



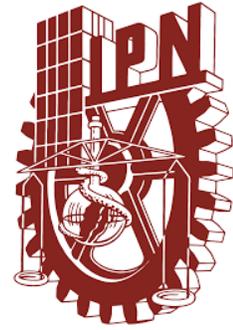
**Sociedad Mexicana de Ciencia y Tecnología  
De Superficies y Materiales A.C.**

***IX International Conference  
on Surface, Materials and Vacuum***



September 26-30, 2016, Mazatlán, Sinaloa, México

**PROCEEDINGS**





**Sociedad Mexicana de Ciencia y Tecnología de Superficies y Materiales A.C.**  
**IX International Conference in Surfaces, Materials and Vacuum**  
**September 26<sup>th</sup>-30<sup>th</sup> , Mazatlan, Sinaloa, México**

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**Dear Colleagues,**

From the very beginning the Annual Conference of the Sociedad Mexicana de Ciencia y Tecnología de Superficies y Materiales (SMCTSM, Mexican Society of Science and Technology of Surfaces and Materials) has been an important forum used by the Mexican scientific community for the discussion of scientific and technological topics related to research in the areas of surface and materials science.

In these ocaion we are pleased to welcome you to participate in the IX International Conference on Surface, Materials and Vacuum (ICSMV) which will held in the city of Mazatlán, Sinaloa from the 26th to the 30th of September 2016.

The scientific program of the Conference is divided into plenary conferences, short courses and the different symposia with oral and poster contributions. For the IX edition the symposium of Photothermal and Plasma and Vacuum was reverted to two symposia the Photothermal Phenomena and the Plasma and Vacuum symposia. We have added the symposium of Advanced Materials Synthesized by Chemical Routes and we have two invited symposia the Atomic Layer Deposition and Luminescence Phenomena: Materials and Applications. Additionally to the scientific program, there is a symposium of Science Divulgation which is a traditional forum for the bringing together of students and the general public with the work undertaken and developed within our Society.

We hope that the efforts of the organizing committee, sponsors and colleagues will result in an interesting friendly meeting, providing the opportunity for closer and new interactions between researchers coming from the diverse institutions.

The IX ICSMV  
Organizing Committee SMCTSM  
September 2016, Mazatlán, Sinaloa, México.



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# **IX INTERNATIONAL CONFERENCE IN SURFACES, MATERIALS AND VACUUM**

## **PLENARY LECTURES**



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# OPENING TALK

## **Foams : new promising materials**

*Dominique Langevin*

*Laboratoire de Physique des Solides, Université d'Orsay*

Foams are dispersions of bubbles in liquids (or solids). Examples of solid foams are insulation materials (glass and polymer foams), and lightweight materials for car industry (metallic foams).

A large amount of work is devoted to the understanding of foaming and foam stability. Improving this knowledge is very important for the control of the different technological processes used to elaborate solid foams. In these processes, the foam is usually liquid and destabilises due to different mechanisms: gravity drainage, coarsening (gas diffusion from small to large bubbles) and coalescence. We will describe the existing knowledge on these mechanisms and show how they can be controlled.

We will present examples of solid foams obtained from various gels (made with surfactants, colloidal particles and polymers) and show how the solidification can be controlled. This will include foams made with microfluidic devices where the bubbles are monodisperse in size.



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# PLENARY LECTURE I

**Tailoring properties of two dimensional transition metal dichalcogenides:  
looking beyond grapheme**

*Talat Rahman*

*University of Central Florida, USA*

To be announced



# PLENARY LECTURE II

## Localized magnetometry of metallic nanowires using off-axis electron holography

Arturo Ponce, Eduardo Ortega and Alfredo Benitez

Department of Physics and Astronomy, University of Texas at San Antonio. One UTSA Circle, San Antonio, TX 78249, USA.

The comprehensive understanding of nanoscale materials and their physical properties are of great interest to the scientific and technological community. In particular, magnetic nanostructures of different size, shape and composition possess a great potential to improve current technologies in areas such as: magnetic data storage, electromagnetic sensing<sup>1,2</sup>. Lately, soft magnetic nanowires, (Co, Fe & Ni) have been studied for a while experimentally and by simulations, but there still some questions to be address. Soft magnetic nanowires can switch magnetization in two different modes depending on their thickness, these modes are known as the transverse wall mode and the vortex wall mode. In thin ferromagnetic nanowires (diameter less than 40nm) a simple domain wall nucleates and propagates along the nanowire axis, while the reversal of thick nanowires (diameter more than 40 nm) is achieved via localized curling or vortex mode. The magnetization direction of each magnetic domain will be influenced by the magnetocrystalline anisotropy; typically following the easy magnetization axis, which minimize the magnetocrystalline energy. The magnetization behavior in this nanostructures is dominated by the competition between magnetocrystalline anisotropy and shape anisotropy. In many cases this competition between can frustrates the magnetization direction. It is expected that the magnetostatic coupling between nanostructures have a strong influence on their response to an external field<sup>3</sup>.

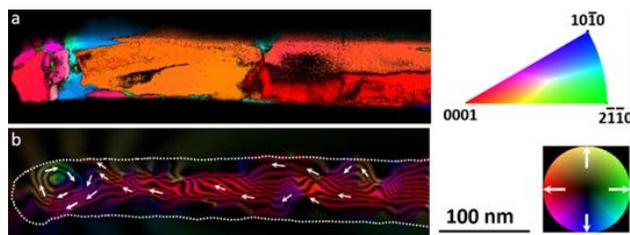


Figure 1. (a) Crystal orientation and (b) magnetic phase contour maps of the Co nanowire. The crystal orientation map is displayed with respect to the direction of observation  $z$  (color key code displayed on the right) and is over-layered with the reliability map to reveal zones where crystallites overlap. The outline of the nanowire is marked by the thin white line. Arrows represent the magnetic flux direction<sup>1</sup>

The talk will cover two folds: 1) crystalline orientation phase mapping assisted by a precession electron diffraction unit for analysis in nanostructures such as metallic nanoparticles and nanowires and 2) the analysis of the magnetic fields within and surrounding metallic nanowires. The combination of electron holography and crystalline orientation phase mapping can provide of important information not only



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about the magnetic behavior but the different orientation of the magnetization as function of the orientations of nano-grains in a polycrystalline structure. The analysis of the magnetic behavior and quantitative measurements has been obtained using off-axis electron holography. The retrieved phase from holography contains information related to the thickness of the sample, electric potential, lattice distortion for crystalline and finally magnetic fields. The magnetic phase utilizes the interference of two electron waves (reference and object) to detect and quantify the electromagnetic field at nanometer scale. In this interference-based approach the magnetic vector potential  $A$  within the ferromagnetic nanowire causes a phase shift in the quantum mechanical wave functions of the electrons passing through this region (Aharonov-Bohm effect)<sup>4</sup>. Once the phase is recovered and separated, the contour of the pure magnetic phase image corresponds to the projected in-plane magnetic induction as well as the crystal orientation map as shown in Figure 1a and 1b. The methods of characterization and image analysis for the interpretation and extraction of quantitative information of the metallic nanowires will be discussed.

1. J. Cantu-Valle, I. Betancourt, J.E. Sanchez, F. Ruiz-Zepeda, M.M. Maqableh, F. Mendoza-Santoyo, B.J.H. Stadler, A. Ponce, *J. Appl. Phys.* 118 (2015) 024302.
2. J. Cantu-Valle, E. D. Barriga-Castro, V. Vega, J. García, R. Mendoza-Reséndez, C. Luna, V. M. Prida, K. Nielsch, F. Mendoza-Santoyo, M. José-Yacaman, A. Ponce, *J. Magn. Magn. Mater.* 379 (2015) 294–299.
3. F. Ruiz-Zepeda, Y.L. Casallas-Moreno, J. Cantu-Valle, D. Alducin, U. Santiago, M. José-Yacaman, M. López-López, A. Ponce, *Microsc. Res. Tech.* 77 (2014) 980-985.
4. Tonomura, N. Osakabe, T. Matsuda, T. Kawasaki and J. Endo, *Phys. Rev. Lett.* 56 (1986) 792.



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# PLENARY LECTURE III

## **In-situ Characterization of Atomic Layer Deposition (ALD)**

*Jiyoung Kim*

*The University of Texas at Dallas, Richardson, TX 75080*

Atomic Layer Deposition (ALD) has been widely utilized to deposit high quality high-k dielectrics with ultra-precise thickness controllability. Particularly, during the initial few cycles of ALD, metal precursors and reactants are exposed to different environments because of a substrate unlike in the middle of ALD process. Anomalous initial growth behaviors, therefore, are frequently observed at the initial ALD process. As devices are being continuously scaled down sub-10 nm node, it is critical to understand impacts of initial ALD process on interface characteristics as well as high-k dielectric deposition. Precursors and reactants for high-k dielectrics frequently exhibit strong interactions with a channel substrate, such as Si and III-V, during the first few cycles of ALD. Particularly, some of ALD precursors show a very high reactivity (or catalytic behavior) with a substrate at a processing temperature. For examples, La(fmd) enhances formation of La-silicate on Si substrate, while TMA (Trimethyl-Al) effectively remove native oxide at GaAs surface. On the other hand, some 2-D materials with hydrophobic nature, such as graphene and Mo<sub>2</sub>S, etc., would prevent appropriate adsorption of reactants on the basal plane, which causes non-uniform nucleation. If a chemical functionalization technique is applied to improve ALD nucleation process, performances of the channel would be frequently degraded. In this presentation, I am going to introduce in-situ XPS system clustered to thermal ALD to investigate surface reactions during the initial few half cycles of ALD on Si and GaAs. I will also mention in-situ electrical characterization on 2D devices for initial few half cycles of ALD process.



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# PLENARY LECTURE IV

## **Manganese nitride magnetic nanopyramids: ab initio calculations**

*Jonathan Guerrero and Noboru Takeuchi\**

*Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México*

Antiferromagnets are very important materials in spintronic devices due to their ability to modify the switching behavior of adjacent ferromagnets. Both  $\text{Mn}_3\text{N}_2$  and  $\text{MnN}$  are antiferromagnetic materials, and their (001) surfaces form nanopyramids. Although structurally similar, these nanopyramids show different electronic and magnetic properties. Since these two materials are potential substrates to form ferromagnetic/antiferromagnetic heterostructures, a good knowledge of their atomic arrangements and magnetic properties is needed. Therefore, we have performed first principles total energy calculations using spin polarized density functional theory calculations of bulk  $\text{Mn}_3\text{N}_2$  and  $\text{MnN}$  and their (001) surfaces. The stability of the different surface terminations is calculated using the surface formation formalism. It has been found that the  $\text{Mn}_3\text{N}_2$  (001) and  $\text{MnN}$ (001) nanopyramids are formed by three and two different terraces, respectively, in agreement with experimental observations. We also compare our Tersoff-Hamman STM and ILDOS simulations with the experimental STM images. A good agreement between them has been found.

We thank DGAPA Project # IN100516 and Conacyt project # 164485. Calculations were performed at the DGCTIC-UNAM Supercomputing Center, with the grant # SC16-1- IG-31.

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# PLENARY LECTURE V

## **Straightforward synthesis of ZnO nanostructures compatible with silicon technology\***

*M. Meléndez-Lira*

*Departamento de Física, Cinvestav -IPN and Departamento de Ciencias Básicas, UAM-A*

Silicon is the base material of the huge technological development in electronic technology. There is no discussion about the importance of this material in the increasing performance of computers and the relatively new Internet of Things (IoT). However because of its electronic characteristics, indirect and low energy band gap, there are some technological applications in which silicon is not an adequate material or its performance is surmounted by other materials. Two examples of the above are photovoltaic and photocatalytic applications; both of them will have a big impact on the future of humanity. By contrast ZnO a transparent semiconductor with a direct bandgap of 3.4 eV is ideal for some applications: detection and emission of UV light, transparent displays, water photolysis, etc. Most of the ZnO electronic properties are enhanced by the formation of nanostructures. The production of ZnO nanoparticles using low cost methods is inadequate for some applications due to chemical residues. We have developed a low cost methodology compatible with silicon technology. ZnO nanoparticles are self-assembled within a silicon oxide matrix by employing RF reactive sputtering. In this talk we will present a general discussion of the recent advances along with some perspectives in the photovoltaic and photocatalytic applications of ZnO.

Our methodology to produce ZnO nanostructures will be presented along with results of the chemical, structural, optical and electrical characterization. Finally, we will comment on the possible applications of the produced material.

\*: Partial financial support by CONACyT is acknowledged.



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# PLENARY LECTURE VI

## **Production of refractive structures and waveguide integrated optical devices by femtosecond laser structuring**

*Javier Solis*

*Laser Processing Group, Instituto de Optica, CSIC*

The use of ultrashort laser pulses enables coupling laser energy inside dielectric materials via non-linear absorption. Already in 1996, the pioneering work of Kazuyuki Hirao and coworkers showed that this approach can be used for writing optical waveguides inside fused silica and other glass materials. Since then, sub-surface, fs-laser structuring has been used to produce a wide variety of active and passive photonics components with a performance comparable to that achievable with more conventional techniques. The presentation will provide an overview on the production of refractive structures and waveguide integrated optical devices by femtosecond laser structuring, with emphasis in our recent work on the use of fs-laser induced ion-migration for the production of high index contrast refractive structures.



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# PLENARY LECTURE VII

## **Design of Metal-organic frameworks: Applications from catalysis to gas adsorption**

*Berenice González Santiago*

*Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa*

Metal-organic frameworks (MOFs) are a class of porous materials which have been shown to exhibit properties that make them strong candidates for post combustion carbon capture and storage (CCS) processes and catalysts. These materials can have a diverse range of framework architectures because of the wide variety of coordination geometries between the metal cations and the organic ligands, which assemble in 2D, and 3D structures. MOFs possess significant potential catalytic advantages over ‘classical’ porous solids, and in this talk I will describe the synthesis and functionalization of known and novel MOFs and their applications in environmental catalysis and carbon dioxide capture.



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# PLENARY LECTURE VIII

## **Second harmonic generation in nanostructured metamaterials**

*W. Luis Mochán*

*ICF-UNAM, Cuernavaca, Morelos, México*

We develop a representation of the linear microscopic response of a nanostructured binary periodic metamaterial that allows the efficient calculation of its macroscopic response and its linear microscopic field for arbitrary geometries, composition and frequencies. The linear field allows us to obtain the dipolar surface contributions and quadrupolar bulk contributions to the nonlinear processes of three wave mixing such as second harmonic generation (SHG). The quadratic response has a multipolar character when the building materials and the geometry is centrosymmetric. However, when the geometry lacks an inversion point the nonlinear response becomes enhanced and acquires a dipolar character even when the building materials are centrosymmetric. This suggests a strategy for obtaining a large SHG from ordinary materials.



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# PLENARY LECTURE IX

**Two-dimensional materials, heterostructures and devices**

*Xiangfeng Duan*

*Department of Chemistry and Biochemistry & California Nanosystems Institute  
University of California, Los Angeles, Los Angeles, California 90095 USA*

Two-dimensional layered materials (2DLMs), such as graphene or molybdenum disulphide, represent an ideal 2D material system for exploring fundamental chemistry and physics at the limit of single atomic thickness. The covalently bonded atomic layers in 2DLMs are bound weakly to each other through van der Waals interactions, which offers considerable flexibility to isolate, mix and match individual atomic layers without the constraints of lattice and processing compatibility. It can therefore open up vast possibilities for nearly arbitrarily combining multiple materials and integrating distinct properties at the atomic scale, and thus enabling entirely new opportunities beyond the reach of existing materials. Here I will focus my discussion on exploring these 2D materials and their heterostructures as new platforms for the creation of a wide of electronic and optoelectronic devices with unique functions or unprecedented performance. Examples discussed include: high-speed transistors; a new design of vertical transistors for ultra-flexible electronics; and several new types of tunable photonic devices.

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# PLENARY LECTURE X

## **Time-of-flight mass spectrometry in laser-matter interaction studies**

*Alexander V. Bulgakov*

*S.S. Kutateladze Institute of Thermophysics, SB RAS, Novosibirsk, Russia*

Mass spectrometry (MS) is one of the most powerful techniques to study processes occurring during/after laser-matter interaction. In this talk, an overview of using MS techniques in laser ablation/desorption/excitation experiments will be given. The main types of mass spectrometers and typical experimental schemes will be considered. The main attention will be paid to time-of-flight (TOF) MS as to the most informative and frequently used technique. The use of TOF MS will be illustrated by examples of author's studies of various aspects of laser-matter interaction including synthesis of nanoclusters, dynamics of laser-ablation plasmas, pulsed laser deposition, laser excitation of gas-phase clusters, and laser-induced forward transfer of nanoparticles.



# PLENARY LECTURE XI

## **Up- and down-conversion in photoluminescent glasses for enhanced photovoltaics: recent advances**

*G.C. Righini*

*Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi, Roma, 00148, Italy*

*Nello Carrara Institute of Applied Physics, CNR-IFAC, Sesto Fiorentino, 50019, Italy*

Efficient light manipulation at sub-wavelength scale is of great interest for the enhancement of the efficiency of solar cells. Performance of any solar cell is determined by the efficiency of the absorption process of light via excitation of electron-hole pairs and extraction of these generated charge carriers (electrons and/or holes). The absorption, in turn, has a number of limiting factors: one is related to the small size and acceptance angle of the active region; another is due to the reduced spectral sensitivity of the active material, which could not make use of a part of the solar spectrum.

Correspondingly, the energy harvesting may be improved in two ways: a) light trapping schemes may be adopted in order to make the cell “thicker” by exploiting scattering and/or reflection effects, which effectively increase the optical path inside the photoconductive material. Plasmonic structures, constituted by patterned metal films or nanoparticles, have demonstrated to be very effective for directing and enhancing the incident light beam. b) up- and down-conversion processes may be exploited to convert the frequencies of the solar spectrum from near-mid-IR and from uv regions, respectively, to the visible region of maximum absorption of the cell. Thin glassy or glass-ceramic films doped with rare earths have proved to be very suitable for this purpose.

Here an overview of recent results achieved, in particular, in the field of up- and down- frequency conversion by different research groups will be reported, and different approaches will be compared.

Acknowledgments: The collaboration and critical discussions with several colleagues (C. Armellini, F. Coccetti, F. Enrichi, M. Ferrari, F. Gonella, A. Łukowiak, S. Pelli, A. Quandt, L. Z. Zur) are gratefully acknowledged



# PLENARY LECTURE XI

**Pulsed Laser Deposition of 2D and Bulk II-VI Materials**  
Manuel A. Quevedo-Lopez  
Department of Materials Science, University of Texas at Dallas

In this talk pulsed laser deposition (PLD) methods are presented to study p-n II-VI homo and heterojunctions fabricated *in-situ*. *In-situ* film deposition allows higher quality p-n interfaces by minimizing spurious contamination from the atmosphere. Morphologic and structural analyses were carried for CdTe films deposited on various substrates and different deposition conditions and the electrical characteristics and performance of the resulting junctions are studied. In addition, a scalable and catalyst-free method to deposit stoichiometric two dimensional molybdenum disulfide (2D MoS<sub>2</sub>) films over large areas is reported with the maximum area limited by the size of the substrate holder. The method allows deposition of MoS<sub>2</sub> layers on a wide range of substrates without any additional surface preparation including single crystals (sapphire and quartz), polycrystalline (HfO<sub>2</sub>), and amorphous (SiO<sub>2</sub>). The films are deposited using carefully designed MoS<sub>2</sub> targets fabricated with excess of sulfur (S) and variable MoS<sub>2</sub> and S particle size. Uniform and layered MoS<sub>2</sub> films as thin as two monolayers, with an electrical resistivity of  $1.54 \times 10^4 \Omega \text{ cm}^{-1}$  were achieved. The MoS<sub>2</sub> stoichiometry was as confirmed by High Resolution Rutherford Backscattering Spectrometry (HRRBS). With the method reported here, *in situ* graded MoS<sub>2</sub> films ranging from  $\sim 1$  to 10 monolayers can also be deposited. thickness control is achieved by controlling the growth kinetics by simply manipulating the repetition rate (frequency) and energy of the laser as well as the deposition pressure. The absorption of the laser energy by this a volume consequently forms a plasma, or plume, at the surface of the target and the species get transferred to the substrate. This process is not dependent on the partial pressures of the constituent cations.<sup>1</sup> However, the deposition pressure can be used to modify the mean free path of the ablated species to either minimize or maximize the energy of the species reaching the surface of the substrate. In PLD processes, only the stoichiometry is transferred from the target to the substrate and the crystalline phase of the resulting film is not necessarily the same as that of the target.<sup>1</sup> Furthermore, MoS<sub>2</sub>



growth on amorphous, polycrystalline and single crystal substrates was also demonstrated. With further work, the method reported here can lead to future large-scale deposition of MoS<sub>2</sub> for various applications.

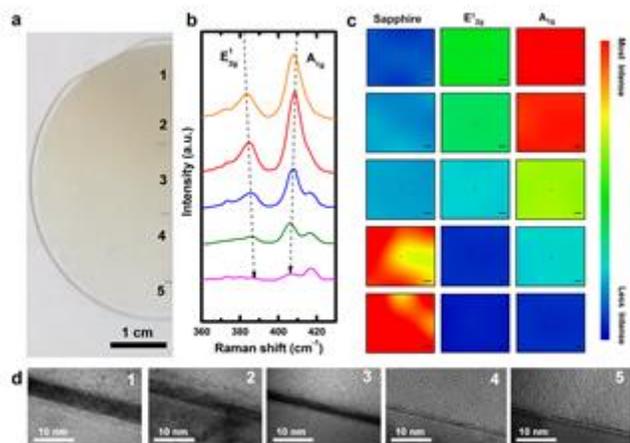


Figure 1. MoS<sub>2</sub> thin film with graded thickness and the corresponding Raman mapping. (a) The optical image shows a MoS<sub>2</sub> thin film thicknesses gradient on half sapphire wafer deposited by PLD thicknesses gradient. Raman spectra and Raman mapping are shown (b-c). Areas of high and low intensity are represented by red and blue colors in the Raman mapping. (d) TEM cross-section results for areas 1 through 5 showing the thickness gradient for the MoS<sub>2</sub> films along the entire substrate.

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# **IX INTERNATIONAL CONFERENCE IN SURFACES, MATERIALS AND VACUUM**

## **SHORT COURSES**



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# SHORT COURSE A

**Physicochemical approach to nanomaterials for nanoscience and nanotechnology**

*Arturo Ponce*

*UTSA, USA*

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# SHORT COURSE B

## **Atomic Layer Deposition (ALD) for Micro- and Nano-Electronics**

*Jiyoung Kim*

*Materials Science and Engineering, University of Texas at Dallas*

Atomic layer deposition (ALD) is highly regarded as one of the most viable ultrathin film formation techniques well-suited for semiconductor devices fabrication with large throughput and relatively low equipment cost. While, ALD is a subclass of chemical vapor deposition (CVD), its self-limited working principle distinguishes it from its siblings. Conventional CVDs inject all gas phase chemicals needed for reaction into the chamber simultaneously and continuously, and thus reactions occur in a relatively uninhibited manner. In contrast, ALD alternates between discrete exposures of separate source chemicals and the purging gas in a sequential manner. Since reactions only occur on the substrate's surface at the reaction sites limited in number per each pulse cycle, saturated dose yields a readily predictable and reproducible amount of film growth, giving ALD a plethora of unique advantages, such as ultra-precise thickness controllability, 3-dimensional conformal deposition and relatively low process temperature. This short course will consist of fundamentals of ALD, ALD applications on semiconductor manufacturing and ALD applications on nanomaterials and nanotechnology. ALD fundamentals will cover principles of ALD, ALD precursors, ALD equipment and characterization techniques. In section of ALD for semiconductor application, conformal high-k dielectric and metal deposition for Si technology will be reviewed. Selective ALD and low temperature ALD will be also discussed. Formation of nanomaterials and hybrid thin films using ALD will be introduced in ALD for nanotechnology section. Dielectric deposition on 2D materials (Graphene and TMD) will be also discussed.



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# SHORT COURSE C

## **Polyelectrolyte aqueous solutions and mixtures with surfactants**

Dominique Langevin

Laboratoire de Physique des Solides, Université d'Orsay

Polyelectrolytes are macromolecular ions that ionize in solution in water. When their concentration is sufficient, they form gels which can adsorb large quantities of water (super-absorbent materials). We will first highlight the differences between polymer and polyelectrolyte solutions, recalling the classical background: radius of gyration, persistence length, dilute and semi-dilute solutions, osmotic pressure of counterions, rheology, behaviour upon confinement. Examples of experiments validating this background will be presented.

Associating polyelectrolytes of opposite charge allow obtaining very interesting materials, such as coatings and capsules. These materials are made of alternating layers of each polymer. Their elaboration will be described, together with examples of applications.

Mixed solutions of polyelectrolytes with surfactants also have a large number of applications. They are the basis of many aqueous formulations: the polymer is used to control the viscosity and the surfactant, to control the surfaces properties. Particularly interesting are the mixtures of species of opposite charges which also lead to interesting materials. The classical background on the mixed solutions will be described: binding isotherms, surface tension, aggregation and precipitation. Examples will be given



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# SHORT COURSE D

## **Raman spectroscopy Workshop for chemical and material identification in materials research**

*Richard W. Bormett  
Renishaw Incorporated*

This workshop will provide a review of the theory and the application of Raman spectroscopy techniques useful to the scientific community. Raman spectroscopy has been proven to be capable of providing material and chemical analyses of samples that may vary in size from the very large to the sub-micron, and that maybe in sealed containers (under glass or plastic). New advances in technology now allow Raman microscopy to be extended from the optical microscopes to AFM and SEM microscopes. Raman imaging supports a number of “fast” chemical and topographical contrast methods that can greatly simplify area composition distribution analysis. There will be emphasis on Raman microscopy, with imaging techniques that reveal layers and material distributions, for example in cells, and advanced materials including composites. A live demonstration of Raman microscopy with 785 nm and 532 nm excitation and the imaging processing and acquisition capabilities of dispersive multi-wavelength Raman system will be available so attendees are encouraged to bring microscope compatible samples.



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# SHORT COURSE E

## **Pulsed laser ablation synthesis of clusters and nanostructured materials**

*Alexander V. Bulgakov*

*S.S. Kutateladze Institute of Thermophysics, SB RAS, Novosibirsk, Russia*

Pulsed laser ablation (PLA) is a promising and fast growing technique to produce individual clusters and cluster-based nanomaterials. Advantages of this method include high purity of the produced nanostructures, universality with respect to material, flexibility and ability to efficiently control the cluster formation process. A number of novel cluster systems such as fullerenes and met-cars have been discovered using PLA. In this course, the main principles of PLA-based synthesis of nanomaterials will be presented and advanced experimental and theoretical methods for investigation of the cluster generation processes will be overviewed. Mechanisms, dynamics and formation conditions of clusters with different types of chemical bonds will be analyzed. Peculiarities of PLA-based synthesis of nanostructures in various ambient environments (vacuum, gas, liquid) as well as upon deposition of PLA products onto substrates will be discussed. Particular attention will be paid to laser generation of novel functionalized nanomaterials promising for application in such fields as catalysis, optoelectronics and medicine.



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# **IX INTERNATIONAL CONFERENCE IN SURFACES, MATERIALS AND VACUUM**

## **TECHNICAL TALKS**



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# TECHNICAL TALK I

## **Determinación de Potencial Zeta como indicador de las características de la superficie**

*Rosario Espinosa Melendez  
Anton Paar México S.A. de C.V*

El potencial zeta es un parámetro que se puede medir entre la interfase de la superficie de un sólido y un líquido. El potencial zeta representa la carga de la superficie y esto se manifiesta en presencia de una solución, una manera de poder conocer este fenómeno es mediante la técnica Streaming Potencial.

El Método Streaming Potencial es una técnica que permite la comprensión de esta propiedad en la superficie de muestras planas y en partículas de tamaño mayor de 25 micras.

Esta evaluación se puede realizar en sólidos de diversas formas y tamaños como son: membranas, películas, filtros, polímeros, composites, materiales semiconductores, biomateriales, fibras sintéticas y fibras naturales, cosméticos, surfactantes, granulados, aditivos, líquidos iónicos, minería, minerales, sistemas de flotación, etc.

Las condiciones experimentales de la técnica nos permite realizar experimentos de manera automática realizando cambios en el equilibrio iónico y curvas de adsorción con líquidos iónicos, surfactantes, polielectrolitos y proteínas permitiéndonos registrar en tiempo real el fenómeno de adsorción en la superficie.



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# TECHNICAL TALK II

**Análisis de nanomateriales en hasta cinco escalas distintas usando una sola plataforma de  
Dispersión de rayos-X**  
*Jorge Pablo Gonzalez Garibay*  
*PANalytical México*

To be announced

TECHNICAL TALKS

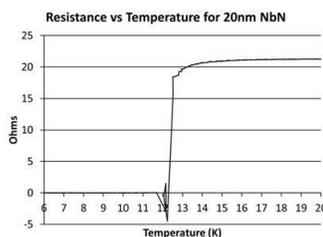


# TECHNICAL TALK II

## Atomic Layer Deposition and Self Assembled Monolayers – From Superconductivity to Selective Area Deposition

Adam Bertuch, Ritwik Bhatia, Laurent Lecordier, Mark Sowa, and Ganesh Sundaram  
Ultratech-CNT, 130 Turner Street, Waltham. MA, 02453, USA

The use of self-limiting deposition techniques such as Atomic Layer Deposition (ALD), and the deposition of self-assembled molecules (SAMs) have made possible a broad range of thin film applications which were previously inaccessible. In this work we describe the function of ALD films in encapsulation, and energy, applications, as well as the development of Nb-based ALD films as superconductors. Additionally, the application of SAMs will be explored for surface functionalization, as well as its use in enabling area selective ALD deposition.



**Figure 1.** Plot of temperature vs resistance for Niobium nitride grown via plasma enhanced ALD. A critical temperature ( $T_c$ ) of 12.4° K has been achieved .



**Figure 2.** The application of SAMs to cotton, to functionalize the material to create a hydrophobic, and oleophobic surface. The untreated cotton (No SAMs) allows the ink and oil to penetrate the material easily, while the deposition of the FOTS allows the surface to repel oil, ink, and water.



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# **IX INTERNATIONAL CONFERENCE IN SURFACES, MATERIALS AND VACUUM**

## **SYMPOSIA**



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# **AB-INITIO CALCULATIONS AND SUPERCOMPUTING SYMPOSIUM (ACS)**

**Chairmen: Naboru Takeuchi (CNYN-UNAM)**  
**María Teresa Romero de la Cruz (FCFM-UadeC)**



[ ACS-134 ] DFT vs. LEED for the determination of the surface structure: The case of the  
Induced Reconstruction by Oxygen of Cu{311}

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DFT method has been widely used to describe the surface structure of complex superlattices, they have shown to be very useful before to embark in a more complex determination by multiple dynamic methods like LEED.

In this work, the structure of (1/3) of monolayer of Oxygen on Cu{311} was determined by LEED, and DFT. It was found that, similar to other Cu surfaces like Cu{100}<sup>1</sup>, Cu{110}<sup>2</sup>, Cu{211}<sup>3</sup>, Oxygen induced a missing row reconstruction of Cu{311} surface along the [01-1] direction, and the Oxygen forms O-Cu-O chains on a (2X2) superstructure on the reconstructed Cu{311}. Some STM results showed that there are a considerable mass transport with the adsorption of Oxygen, The DFT calculations, and the complete I-V LEED analysis show similar results within a 10%.

Keywords: LEED, STM, DFT, Adsorption, Surface Structure

This work was partially supported by DGAPA-UNAM..

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[ ACS-189 ] Ultrafast charge dynamics in bilayer transition-metal dichalcogenides

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<sup>2</sup> University of Central Florida. Department of Physics

We have analyzed the ultrafast response of bilayer semiconductors 2L MoS<sub>2</sub>, 2L WSe<sub>2</sub> and MoS<sub>2</sub>-WS<sub>2</sub> to external laser-pulse perturbations by using a combined Density-Matrix Time-Dependent Density-Functional Theory and Many-Body Theory approach. In particular, we have calculated the binding energies of the excitons, trions and biexcitons in these systems and found that the electrons and holes can form both intra- and inter-layer strongly-bound states. Our time-resolved study of the ultrafast dynamics of electrons and holes, including formation and dissociation of the bound states, shows that one can explain experimentally observed ultrafast inter-layer migration of holes in some of the bilayers [1] by an unusually large delocalization of the hole state. We also discuss the role of the hole-phonon interaction in the inter-layer hole transfer and show that the hole migration time can be further shortened by the interaction of the holes with the transfer phonon modes. Finally, we discuss some general properties of the excitons, trions and biexcitons in two-layer transition-metal dichalcogenides formed by “habitual” electrons and strongly delocalized holes.

[1] X. Hong et al., Nature Nano 9, 682 (2014)

Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354 and by Mexican CONACYT Postdoctoral Fellowship Program Scholarship # 23210 (J.M.G.H.).



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[ ACS-338 ] Surface reactivity of Ge[111] for organic functionalization by means of a radical-initiated reaction: A DFT study

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The current study of interfacial chemistry at semiconductor surfaces is an important area of research due to its future technological impact. Functionalities such as molecular recognition, biocompatibility of surfaces, and molecular computing, could be achieved by the combinations of organic chemistry with the semiconductor technology. One way to accomplish this goal is by means of organic functionalization of semiconductor surfaces such as the bulk-terminated germanium surfaces, more specifically the Ge[111]. Therefore, in this work we theoretically study, by applying density functional theory, the surface reactivity of the bulk-terminated Ge[111] surface for organic functionalization by means of a chain reaction activated by hydrogen vacancies on a previously hydrogen-terminated Ge[111] surface.

The attachment of unsaturated molecules such as acetylene, ethylene and styrene, may lead to the incorporation of some functionalities such as surfaces with a hydrophobic character, the possibility for the construction of multi-component organic layers and finally the design of molecular conductors at the semiconductor surface, respectively. Results derived from this work are compared with those obtained in our previous calculations on the germanene surface by following the same chemical route.

The calculations of this work show an accumulation of electronic charge at the hydrogen vacancy site having as a result electron pairing due to strong lattice-electron coupling and therefore a diminished surface reactivity. Furthermore, the energetic calculations of the transition states of the reaction show that the surface reactivity of the hydrogen-terminated Ge[111] surface is less promising than its two-dimensional analogue, the hydrogen-terminated germanene.

We acknowledge partial financial support from Conacyt project 164485 and DGAPA project IN100516. Calculations were performed in the DGCTIC-UNAM supercomputing center, project SC16-1-IG-31.



[ ACS-419 ] Organic functionalization of hydrogenated silicene with aldehydes

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<sup>2</sup> CnyN-UNAM

We have studied the radical initiated addition reaction of aldehydes on hydrogenated silicene by means of periodic density functional theory. Before the reaction starts, a dangling bond is formed by removing a hydrogen atom from the surface. An incoming unsaturated molecule may be able to react with the dangling bond and attach to the surface. Thermodynamics and kinetics suggest that adsorption is highly probable to occur. Even more, comparison of results with the addition reaction of aldehydes on H-Si(111) and the adsorption of hydrocarbons on hydrogenated silicene, suggest that reaction of aldehydes on hydrogenated silicene is even more favorable. This might be explained in terms of the enhanced polar ambient in H-Silicene with respect to the H-Si(111) surface in the first case, and by the higher stability of Si-O bonds with respect to Si-C bonds in the later. Also, calculations suggest that the reactions proposed here can self-propagate, so we encourage the use of aldehydes in future experimental works to functionalize silicene.

We thank financial support from Conacyt Project 164485 and DGAPA project IN100516. Calculations were performed in the DGCTIC-UNAM supercomputing center, project SC16-1-IG-31.



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**[ ACS-444 ] Two-dimensional boron nitride structures functionalization: First principles studies**

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Density functional theory calculations have been performed to investigate the acetylene (C<sub>2</sub>H<sub>2</sub>) adsorption on two-dimensional hexagonal boron nitride (2D hBN) layers considering the 2x2, 4x4 and 6x6 periodicities. The electron-ion interactions are treated with the pseudopotential method. Calculations have used the van der Waals density non-local correlation functional (vdW-DF) with the PBE correction. Results show two different possible adsorption sites; the first site is on top of boron atom where an interaction boron-carbon is observed and the second site is on top of nitrogen atom where the interaction is nitrogen-carbon. In all cases chemisorption is obtained, adsorption on top boron is the most stable structure with bonding energy of -0.826, -0.838 and -0.915 eV for the 6x6, 4x4 and 2x2 periodicities, respectively. Diffusion energy barriers have been encountered; in the case of boron-carbon interaction an energy barrier of 0.08 eV and in the nitrogen-carbon interaction an energy barrier of 0.80 eV. The total density of states (DOS) displays an energy gap in both cases. The projected DOS indicate that the B-p and N-p orbitals are those that make the most important contribution to the valence band and the H-s and C-p orbitals provide an important contribution to the conduction band. Provided that the interactions of the acetylene with the 2D layer modify the structural and electronic properties of the hBN it may be concluded the possibility of structural functionalization using organic molecules.



**[ ACS-22 ] Many electrons interacting by a Yukawa potential in a AlGaAs/GaAs Quantum Wire under an external electric field.**

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The development of growth techniques such as Molecular Beam Epitaxy or Metal-organic Chemical Vapor Deposition has allowed the synthesis of high-quality semiconductor quantum wires (QWr). The QWrs are one-dimensional (1D) systems in which the discrete states of energy and the strong confinement of charge carriers, photons and phonons lead to unique properties. The use of these properties have plenty potential applications in a wide range of devices such as lasers, solar cells, biological sensors, photodetectors or transistors. On the other hand, an important number of complex theoretical models has been developed to explain and predict many properties of these QWr. Specially complicate has been to study the problem of many electrons interacting into the QWr. In different branches of physics, a simple way to resolve the many-particles problem is by means of the use of a Yukawa potential (YP). However, the YP has been not sistematically studied in the problem of many-electrons interacting into a crystalline QWr.

In this work, we present a study of the problem of many electrons into a square and circular Al<sub>x</sub>Ga<sub>1-x</sub>As/GaAs QWr interacting under a YP, which are affected by an external electric field. The proposed model contains material parameters such as the Al concentration (by using the Varshni model), the substrate orientation (implicit in the effective mass), the dopant level (associate to the screening parameter  $\kappa$  in the YP), the cross section geometry of the QWr (circular or square) and the magnitud of the external electric field. To adjust the model to experimental values, we consider concentrations of  $10^6$ - $10^{22}$  cm<sup>-3</sup>, the (631) Miller orientation of the GaAs substrate, an Al concentration of  $x=0.23$ , a conduction band of  $V=206$  meV and the external electric field in the range of  $10^4$  to  $1 \times 10^5$  V/cm. By using th Yukawa model and these parameters, we calculate the electronic density distribution into the square and circular QWrs for different electronic concentration and values of the external electric field.



[ ACS-27 ] DFT Study of surface F and Cl bonds effects on the electronic states of Si terminated porous SiC

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Porous Silicon carbide (SiC) is a binary compound nanostructure, which has been identified as an alternative semiconductor material for power electronics, because the SiC exhibits some excellent chemical and physical properties. In this work, Porous Silicon Carbide was modeled by removing columns of atoms of an otherwise perfect SiC crystal in the [001] direction using the supercell scheme [1], so that the porous structure exhibits a surface exclusively composed of Si atoms (Si-rich) using different surface passivation agents, such as hydrogen (H), fluoride (F) and chloride (Cl). The results demonstrate that all of the passivation schemes exhibit an irregular band gap energy evolution due to a hybridization change of the surface. The structural analysis shows a great dependence of the bond characteristics on the electronegativity of the bonded atoms, and all of the structural and electronic changes could be explained due to steric effects.

#### Acknowledgments

This work was partially supported by multidisciplinary projects IPN 2016-1770 and 2016-1771 by IPN.

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**[ ACS-28 ] Effect of doping on the electronic properties of diamond nanowires: a first-principles study**

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In recent years large amounts of resources have been devoted to experimental and theoretical research of low dimensional systems in order to reduce the size of technological devices. In particular, great interest has been shown in the diamond nanowires (DNW) from the standpoint of basic science, as one of the multiple innovating solutions in the field of communications, electronics and quantum computing. Therefore, this research uses first principles calculations based on the Density functional theory and the supercell scheme [1, 2], to study the effects of dopants such as Nitrogen and Boron combined with a vacancy on the electronic properties of diamond structures. The studied defects were modeled on bulk diamond and [001] oriented DNWs. The results show that DNW behave like semiconductor, or a conductive material depending upon the dopant or defect; for instance the nitrogen-vacancy defects create trap states around the band gap energy, which would make it suitable as a single photon source, while carbon boron vacancy (CBV) could be useful for sensor applications, and for the NW with just a vacancy behaves like a conductor depending of the spin applied, particularly attractive for application on Field Effect Transistors, because of the nature of the direct energy band gap.

**Acknowledgments**

This work was partially supported by multidisciplinary projects IPN 2016-1770 and 2016-1771 by IPN.

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[ ACS-227 ] First principles calculations on strained BiFeO<sub>3</sub> using Quantum Espresso

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During the last years, the multiferroic material BiFeO<sub>3</sub> (BFO) has received a great deal of attention due to its potential applications for magnetoelectric devices. At room temperature, this material is a single-phase magnetoelectric multiferroic with antiferromagnetic and ferroelectric ordering that exhibits a large spontaneous electric polarization [1].

The aim of this computational work is to calculate the spontaneous electric polarization of BFO thin films deposited on a SrTiO<sub>3</sub> (STO) substrate and to evaluate how the polarization depends on the strain applied to the film.

To this end, we have first investigated the electronic and structural properties of bulk BFO. These calculations have been carried out within the Density Functional Theory + Hubbard U (DFT+U) formalism using the Quantum Espresso package [2]. The spontaneous polarization of BFO in its bulk rhombohedral *R3c* phase has been computed by means of the modern theory of polarization developed by Vanderbilt [3], taking the *Pm-3m* centrosymmetric phase as a reference.

To evaluate the influence of the strain that the STO substrate (belonging to space group *Pm-3m*) provokes on the BFO films, we have built a structural model in which three layers of the BFO in tetragonal phase (*P4mm*) are connected with three layers of STO.

#### Acknowledgements

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[ ACS-324 ] First-principles study of aluminum-phosphorus co-doped monolayer graphene

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### Abstract

In this work we studied the phosphorus-aluminum co-doping effect on the electronic and structural graphene properties using ab-initio calculations in the basis of density functional theory (DFT). The doping of graphene with substituent heteroatoms can transform the band structures as well as the electron transfer, improving their electronic performance that could enhance their sensing ability like gas sensor. The incorporation of heteroatoms on monolayer graphene modifies the structural parameters. Furthermore, the electronic properties were improved through opening a gap up to 0.61 eV produced by the synergistic effect of phosphorus-aluminum co-doping. The semiconductor behavior of co-doped graphene can be tuned by regulating the dopant concentration.

**Keywords:** density functional theory, graphene, co-doping



[ ACS-326 ] Study of structural and electronic properties of a PbS quantum dot supported to  
TiO<sub>2</sub> nano-particle

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The geometric and electronic structure were determined for a junction of two semiconductor nanoparticles: (TiO<sub>2</sub>)<sub>38</sub>[1] and (PbS)<sub>(4-32-364)</sub>, with different geometries reports experimentally for both nanoparticles. In the case of TiO<sub>2</sub> was used Anatase, and Rutile atomic structures with planes [1 0 1]. For PbS: Cubic and centering on plane [1 1 1][2,3], with sizes of (PbS)<sub>4</sub>, (PbS)<sub>32</sub>, and (PbS)<sub>364</sub>. Also was verified different PbS stoichiometries into the TiO<sub>2</sub>-PbS interaction to find the ideal gap sizes. These predictions will be implemented in the laboratory, the structure of the ground electronic state of both nanoparticles were determined using Density Functional Theory (DFT) calculations using FHI-AIMS[4] package and VASP package [5], and Molecular Dynamic using DL-POLY package[6]. The densities of states (DOS) of these particles were calculated in vacuum. Next the atomic and electronic structure of their junction was determined. The calculations were performed at the level of DFT, using a plane-wave basis set, and the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof for the exchange-correlation energy [5]. The core electrons were described with Projector Augmented Wave (PWA) method, also were included relativistic scalars effects (ZORA)[6] and Van Der Waals interactions using Tkatchenko-Scheffler methodology[7]. Since the photocatalytic activity of a system is determined by its atomic and electronic structures the results derived here provide fundamental data to develop and design photocatalytic systems for hydrogen production.

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[ ACS-380 ] First principles study of oxygen adsorption on graphene sheets.

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First principles total energy calculations have been performed to study the structural properties of oxygen adsorption on graphene sheets. Calculations have been performed within the periodic density functional theory as implemented in the PWscf code of the QUANTUM ESPRESSO package. The exchange-correlation energies are treated with the generalized gradient approximation (GGA). Electron-ion interactions are modeled with pseudopotentials. The electron states are expanded in plane waves with an energy cutoff of 30 Ry. 551 hexagonal supercell periodicity has been considered. Oxygen atom was placed at different adsorption sites. The results indicate that the most stable configuration corresponds to oxygen atom placed over the C-C bond with adsorption energy of -3.156 eV, which indicates a chemisorption interaction. The C-C length bond results to be 1.49 Å, while C-O bond is 1.50 Å. Accordingly to electronic structure calculations a direct band gap of 1.318 eV is opened after the adsorption process. Therefore, we conclude that oxygen adsorption significantly modify the electronic properties of graphene.



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**[ ACS-511 ] theoretical study of the novel nitride cluster quasi-fullerenes**

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A theoretical study of new compounds based some new allotropic forms of carbons in the form cage denominated Quasi-Fullerenes ( $C_{48-q}$  and  $C_{60-q}$ ) that due to their size have capacity to encapsulate metal nitride clusters to form some new molecules denominate Nitride Cluster Quasi-Fullerenes (NCQF). They have very interesting chemical reactivity properties, which have not been seen in small carbon molecules. Full geometry optimizations of the systems were performed at the B3LYP level of theory. All formation energies are negative indicating that they are thermodynamically stable. The NBO calculations are done to understand the charge transferred from metal nitride cluster to the quasi-fullerenes. All calculations were performed using the software package Gaussian 09.



[ ACS-572 ] **Ab initio investigation of CsCl, B27(FeB) and B33(CrB/TII) phases of PbS**

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The lead sulphide, PbS, is a direct narrow gap semiconductor, at room temperature, its energy band gap approximately 0.37-0.4 eV and fcc crystal structure with a NaCl type. PbS is suitable for applications in infrared detection, photoresistance materials, laser diode, humidity and temperature sensors, decorative coating and solar control coatings. Recent investigations show that intermediate phases of PbS may occur as pressure-induced, resulting in stable or meta-stable crystalline structures with quantum confinement, which modifies the band structure and the behavior of electrons. In this work, we theoretically investigate the structural phases of PbS: NaCl, CsCl, TII (Cmcm) and FeB (Pnma) through first principles studies within the Density functional theory. The equilibrium lattice constants and atomic positions were calculated as well as the electronic band structures. We have found that the electronic structures of the TII and FeB structures remain semi-conducting in their calculated optimized structures.



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**[ ACS-573 ] Sulfur dioxide adsorption on silicane: First principles studies**

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The sulfur dioxide (SO<sub>2</sub>) adsorption on clean and aluminum-doped silicane is investigated by first principles total energy calculations. Studies are done within the periodic density functional theory taking into account Van der Waals effects. Two molecule configurations are considered to investigate different SO<sub>2</sub> concentrations by dealing with 2x2, 3x3 and 4x4 supercells. The electron-ion interactions are modeled with the pseudopotential method and the exchange-correlation energies are treated with the generalized gradient approximation. The ground state geometries correspond to the interaction of the oxygen atom with a silicon atom (configurations A1-A3) and the oxygen atom with the aluminum atom (configurations A1-Al - A3-Al), for the clean and aluminum doped silicane, respectively. Binding energies indicate that the molecule shows in most cases strong chemisorption in both clean and Al-doped silicane. To explore the electronic properties, calculations are done of the total and projected density of states. Results in both clean and Al- doped silicane indicate the absence of any energy gap. Charge density plots also show strong interactions between the molecule and silicane.



**[ ACS-574 ] First principles study of structural and electronic properties of Zn<sub>1-x</sub>MnxS**

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Diluted magnetic semiconductors (DMS) have attracted interest of the academic and industrial communities, because of their applications in spintronics, integrated optoelectronic devices, and nano-structured quantum devices. The interaction between Mn3d electron and the electronic states of the host crystal is of special interest. In this work, we investigate the structural and electronic properties of cubic Zn<sub>1-x</sub>MnxS using first principles calculations. We have investigated the lattice parameters and band gap energies. Our results suggest that lattice constants and bandgap energies change linearly when the Mn concentration is increased.



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# **ADVANCED MATERIALS SYNTHESIZED BY CHEMICAL ROUTES (AMSCR)**

**Chairman: Veronica de la Luz Tlapaya (UAM-Iztapalapa)**



**AMSCR-24 | Development of Si/PbTe photodiode by combination of Photo Chemical Bath  
Deposition and Chemical Vapor Deposition techniques**

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Semiconductor two-component structures formed by narrow band chalcogenide film like PbS, PbSe or PbTe deposited over Si substrate are of substantial interest due to their possible use as photo diode sensors or elements of multi-junction solar cells [1, 2]. In this work, the diode of p-PbTe/n-Si was made by two-stage techniques involving ecologically friendly and inexpensive chemical routes. At the first stage, the plumbonacrite film  $Pb_{10}(CO_3)_6O(OH)_6O$  was deposited over Si plate by Photo Chemical Bath Deposition (PCBD) that is cheap, simple and easily scalable; ammonia free process at room temperature was used. We have found that addition of UV illumination to traditional CBD process increases the deposition rate and improves the film quality. At the second stage, the plumbonacrite film was converted into PbTe in Chemical Vapor Deposition reactor using Te hot gas transported from the evaporation source to the substrate by neutral transporting gas (Ar in our case). Investigation of the structure obtained with X-ray diffraction, SEM and optical methods have shown that the PbTe film produced has good structural and morphological parameters that are similar to those of the bulk material, and the photo diode thus obtained has a sensitivity of 0.1 A/W that is of the order of the sensitivity of commercial photo diodes.

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[ AMSCR-200 ] ZnAlCe layered double hydroxides for photodegradation of phenol

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ZnAlCe layered double hydroxides (LDH) with different content of Ce (3.5, 5.0 and 10.0% mol) were successfully synthesized in one step by the co-precipitation technique. The partial incorporation of cerium into the layers of the material can be appreciated in the XRD diffraction patterns, showing some deformation in the crystallographic direction (1 1 0) of the ZnAlCe LDHs. In the samples calcined at 400°C, the UV-vis-DRS study showed a shift of the absorption edge toward the blue region of the spectra as a result of the cerium incorporation to the ZnAl LDH; the analysis of XPS confirms the co-existence of Ce<sup>4+</sup> and Ce<sup>3+</sup> in the ZnAlCe LDHs. The photodegradation and mineralization of phenol under UV irradiation was remarkably improved in the sample containing 5% mol of Ce. A mechanism where cerium in the layered material promotes the separation of the photogenerated electron-hole pairs is proposed. In this mechanism, Ce<sup>4+</sup> acts as electron scavenger, facilitating the electron transfer toward adsorbed O<sub>2</sub> and an accumulation of holes, increasing the generation of radicals OH•.



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**[ AMSCR-210 ] Photoelectrocatalytic reactor for degradation of Methyl Red dye in aqueous solution using Au doped TiO<sub>2</sub>**

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Water pollution is a problem that affect us all, leaving no choice but to seek ways to make contaminated water again be fit for human consumption. Photocatalytic processes received great attention in wastewater treatment due to its cheapness, environmental compatibility and optimal performances. Because of this reason, the present contribution aims to deepen the knowledge in Au doped TiO<sub>2</sub>-based systems and their employment in methyl red removal from aqueous solutions. Au-TiO<sub>2</sub> photocatalysts have been synthesized by a microwave assisted sol-gel method and characterized by means of X-ray diffraction techniques (XRD) and transmission electron microscopy (TEM). The synthesis of the TiO<sub>2</sub> catalyst was carried out by a sol-gel synthesis method using titanium isopropoxide (97% Aldrich, TTIP) as a titanium precursor in an organic solvent (isopropanol, 99.9%, J. T. Baker), the hydrolysis process was then performed by adding water into the precursor/solvent solution. The obtained sol was transferred into Teflon vessels and placed on a microwave reaction system. The resultant solution was then filtered and dried at room temperature and a calcination process was carried out at 450 °C for 3 h. The diffraction peaks detected after the calcination process indicates the presence of the crystalline anatase phase ( $2\theta = 25.33^\circ, 37.82^\circ, 48.08^\circ, 53.93^\circ, 62.75^\circ$ ) and no presence of rutile phase ( $2\theta = 27.46^\circ, 36.11^\circ, 41.27^\circ, 54.37^\circ, 69.07^\circ$ ) was observed. According to the TEM analysis, the mean particle size was 10.6 nm with a semi spherical shape. The catalytic activity was evaluated with respect to methyl red photodegradation in different conditions as a function of irradiated light (UV, solar) and the application of an electric current. The photocatalytic test demonstrates the positive influence of the application of an electric current to photocatalytic processes. The degradation profiles of methyl red for the continuous recirculation reaction system, after 4 h of reaction show that the percentage removal of methyl red using one photoanode-cathode pair were 33 %, it is interesting to note that removal of methyl red increase on photoanode-cathode pairs utilized for the process. For the degradation using two pairs of electrodes, the methyl red removal was 53% while using three pairs were 80%. It is possible to calculate a pseudo first order kinetic constant for the degradation reaction of methyl red using the data obtained in the degradation profiles by means of Langmuir-Hinshelwood method. The kinetic constant value using one photoanode-cathode pair was  $0.0017 \text{ s}^{-1}$ , while the largest value obtained was  $0.0068 \text{ s}^{-1}$ , for the process with 3 photoanode-cathode pairs, meaning it is the faster degradation, it is interesting to notice that the value of the constant increase on the number of electrodes. TOC removal profiles were recorded using a TOC Fusion equipment. For the continuous recirculation reaction system, after 4 h of reaction and using three photoanode-cathode pairs, the TOC removal was 45 %.



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[ AMSCR-236 ] Cytotoxicity studies of poly- $\epsilon$ -caprolactone/silver nanoparticles.

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In this study nanofibers of poly-epsilon caprolactone containing silver nanoparticles (AgNPs) were produced through electrospinning technique, in order to be used as cover for wounds and tissue regeneration. Silver nanoparticles were synthesized with concentrations of 12.5 mM, 25 mM, 75 mM and 100 mM of silver nitrate and the *in situ* reduction of the Ag<sup>+</sup> ions by N, N-dimethylformamide (DMF) in tetrahydrofuran (THF), followed by the formation of polycaprolactone-silver fibers (PCL-AgNPs) with the simple addition of the polymer and processing through the electrospinning technique. The results of dynamic light scattering and UV-visible spectroscopy showed the presence of silver nanoparticles with diameters around 15 to 30 nm. The microstructure and chemical composition of the PCL-Ag nanofibers were characterized by optical microscopy, scanning electron microscopy and infrared spectroscopy. The composite presented a fibrillar structure around 900 nm in diameter. Also, it was found that the characteristic bands of the PCL were unaffected by the addition of AgNPs. The determination of toxicity *in vivo* of the PCL-AgNPs nanofibers showed no dermal toxicity for any of the AgNPs concentrations used. The *in vitro* cytotoxicity of the PCL/AgNPs nanofibers showed a decrease in the percentage of cell viability with increasing concentration of AgNPs, in addition to the formation of micronucleus in cells.



[ AMSCR-243 ] Dyes removal by photo and photo-electrocatalysis using TiO<sub>2</sub> doped with Ag and Au

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Photocatalytic process has been used for a variety of applications such as decomposition of organic pollutants present in water and air. This technology is based in the use of a semiconductor that can absorbing light to carry out the hydroxyl radical formation, in this case the catalyst most used is titanium dioxide due to its high superficial area and low toxicity. The application of TiO<sub>2</sub> is limited due to its low photoactivity under visible light. Therefore, attempts to extend its photoactivity to the visible region have been made by substitution of Ti<sup>4+</sup> on the crystalline structure for metallic ions such as Fe, Ni, Co, Ag, Au, Pt.

1%w Ag-TiO<sub>2</sub> and 1%w Au-TiO<sub>2</sub> photocatalysts have been synthesized by a microwave assisted sol-gel method and characterized by Raman spectroscopy, X-ray diffraction (XRD) and UV-Vis diffuse reflectance spectroscopy. Crystal grain sizes has been determined by the Scherrer equation. X-ray diffractions patterns were recorded to study the formation of TiO<sub>2</sub> crystalline species. The diffraction peaks detected after the calcination process indicates the presence of the crystalline anatase phase and no presence of rutile phase was observed. These observations were confirmed with the Raman spectroscopy and the band gap values were 2.9 eV for each doped material.

The photo and photo-electrocatalysis tests shows a color removal up to 80% and 90% respectively, in the demineralization of the total organic carbon the results reached were up to 85% in both cases.



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[ AMSCR-246 ] An infrared and  $^{27}\text{Al}$  NMR study of porous  $\alpha$ -alumina support from aluminum formate

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Alumina is considered an advanced ceramic, and its properties, such as strength, hardness, superficial area, chemical stability, and applications, are derived from its crystal phases. Supported alumina membranes were prepared by sol-gel technique using aluminum formate. Coordination and site distortion of polyhedral Al were estimated by  $^1\text{H}$  and  $^{27}\text{Al}$  NMR spectroscopy.  $^{27}\text{Al}$  NMR data on formed gels showed that aluminum has 6, 5 and 4 coordination numbers. NMR spectroscopy is an easy technique for understand the transition of sol-gel to alumina phase. Thermal decomposition of aluminum formate was characterized by X-ray diffraction and IR spectroscopy. The influence of the aging conditions was determined by NMR. Morphology was characterized by SEM microscopy. XRD and IR spectroscopy showed the presence of amorphous  $\text{Al}_2\text{O}_3$  at 400 °C,  $\eta$ - $\text{Al}_2\text{O}_3$  at 800 °C and the transformation to  $\alpha$ - $\text{Al}_2\text{O}_3$  at 1050°C, while the precursors were present at 25 and 200 °C for Aluminum formate and Aluminum formate hydroxide, respectively. SEM images of sintered catalytic support revealed a porous ceramic microstructure with intertwined microwires. Superficial area of alumina support was 5.48  $\text{m}^2/\text{g}$ , with pore diameter around 3.37 nm.



**[ AMSCR-247 ] Phase transformation from aluminum formate to alpha-alumina by Raman and infrared spectroscopy.**

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Aluminum oxide or alumina is a ceramic material presented in different phases according to the processing temperature and the precursor used. Each phase presents characteristic properties, the alpha phase ( $\alpha$ -Al<sub>2</sub>O<sub>3</sub>) is used as an advanced ceramic given its high chemical stability, hardness, thermal conductivity and electrical insulation. The synthesis methods currently used to obtain  $\alpha$ -alumina involve complicated and long lasting processes. In the present work, phase transformation of aluminum formate (Al(O<sub>2</sub>CH)<sub>3</sub>) to  $\alpha$ -alumina obtained at low temperature by spray drying was studied. Phase transformation was analyzed by infrared spectroscopy (FTIR), Raman spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM). Spectroscopic and diffractive techniques allowed the observation of the decomposition of aluminum formate and the formation of  $\eta$  and  $\alpha$  phases of alumina at 1000 °C and 1100 °C. SEM allowed the observation of alumina particles of 200 – 300 nm forming agglomerates of 1 – 2  $\mu$ m. The  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> obtained has high purity and small particle size, it can be used as an advanced ceramic in different applications such as preparation of heat and corrosion resistant materials or contamination adsorbents.



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[ AMSCR-393 ] Preparation of composites based on polymethylmethacrylate (PMMA) / 3-trimethoxysilyl propyl methacrylate (TMSPM) / aluminum trioxide (Al<sub>2</sub>O<sub>3</sub>) sol gel route.  
Influence of the concentration of Al<sub>2</sub>O<sub>3</sub>

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Were synthesized composites based polymethylmethacrylate (PMMA) / 3-trimethoxysilylpropylmethacrylate (TMSPM) with different concentrations of Al<sub>2</sub>O<sub>3</sub>, the goal of this study is to prove the influence of Al<sub>2</sub>O<sub>3</sub> in the polymerization conversion and properties of the composites. The composites were synthesized by the sol gel process, firstly it has been made radical copolymerization of methyl methacrylate (MMA) was performed with 3-trimethoxysilylpropylmethacrylate followed by hydrolysis of tetraethoxysilane (TEOS), then were added concentration by weight of Al<sub>2</sub>O<sub>3</sub> , 0.1%, 1%, 3% and 5%. The composites were dried at 70 ° C for 24 h. The best yield was when add 0.1% Al<sub>2</sub>O<sub>3</sub> with 83%, concentration of 1% with a yield of 75%, the concentration of 3% with a yield of 78% and when added 5% Al<sub>2</sub>O<sub>3</sub> was used 65% yield, finding that has higher concentration decreases polymerization conversion. The composites obtained were characterized by FT-IR spectroscopy (ATR), scanning electron microscopy SEM, showing the interactions and dispersions between Al<sub>2</sub>O<sub>3</sub> and PMMA / TMSPM. Thermal properties (TGA) where two stages of degradation are observed and evidence that higher concentration of Al<sub>2</sub>O<sub>3</sub> exists an increased degradation temperature. The TGA curves show that with higher concentration of Al<sub>2</sub>O<sub>3</sub> the weight loss is smaller compared with the polymer without Al<sub>2</sub>O<sub>3</sub>.



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**[ AMSCR-406 ] The Sol-Gel Method as a Chemical Alternative for Design New Hybrid Materials**

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The relative soft chemical conditions in which occurs the sol-gel process allows the combination of organic and inorganic species in novel materials with optimized physicochemical properties. The research for the correct trapping of tetrapyrrole macrocycles inside inorganic network has permitted us to improve the methodologies for tune its interesting physicochemical properties. In this form new alternatives have postulated and proved for design the adequate containers in which porphyrins and phthalocyanines, and similar species, used as probes, preserve its stability and those physicochemical properties that display in solution. These studies demonstrate the possibility of use the sol-gel method and functionalized and organo-substituted alkoxides for the attaching and modification of inorganic matrixes with active species from simple ions to proteins, antibodies and cells, for the creation hybrid porous materials with physicochemical environments inside its pores for the effective display properties of those species. Furthermore, the presence and interactions of the active molecules with other reactants, solvents or additives during the sol-gel process has important effect over the textural characteristic of the final hybrid systems. The developed of methodologies here described can help in the synthesis of new kind of materials with properties tuned according with the needed application.



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[ AMSCR-468 ] Thermal and Mechanical Properties of  $Zr_{57.19}Al_{10.7}Ni_{10.7}Cu_{21.41}$  -  
 $Zr_{52.23}Ni_{11.94}Al_{11.94}Cu_{23.88}$  Bulk Metallic Glasses

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### ABSTRACT

The thermal and mechanical properties, as well as fracture morphologies of two bulk metallic glasses ( $Zr_{57.19}Al_{10.7}Ni_{10.7}Cu_{21.41}$  and  $Zr_{52.23}Ni_{11.94}Al_{11.94}Cu_{23.88}$ ) are presented in this paper. Cylindrical and conical ingots were obtained using the suction casting technique. It was found that the obtained glasses have critical glassy diameter,  $D_c$ , 3 mm. The  $\Delta T_x$ ,  $T_{rg}$  and  $\gamma$  parameters of the obtained glasses were similar to other glasses of similar chemical composition. On the other hand, the Blackman diagram and the Poison ratio indicated the same mechanical behaviour of the obtained glasses, such behaviour was corroborated experimentally. The  $Zr_{57.19}Al_{10.7}Ni_{10.7}Cu_{21.41}$  and  $Zr_{52.23}Al_{11.94}Ni_{11.94}Cu_{23.88}$  glasses are high strength materials with Young's modulus,  $E \sim 83$  and yield strength,  $s_y = 1.7$  GPa. Finally, SEM images showed that the fracture morphology on specimens tested by compression was ductile, observing the veined fracture surface for metallic glasses.



[ AMSCR-487 ] Polycaprolactam and Multi Wall Carbon Nanotubes composites

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Carbon nanotubes are materials with extraordinary properties; those outstanding characteristics could be used through polymeric matrices. Electric conductivity, hardness and transparency are potential properties that researchers look after using carbon nanotubes with polymeric matrices. Polycaprolactam (PA 6) is a transparent polymer with industrial applications. The aim of this work was the obtaining of composites from polycaprolactam and Multiwalled Carbon Nanotubes (MWCNTs).

Multiwalled Carbon Nanotubes were synthesized through chemical vapor deposition using benzene as carbon source and ferrocene as catalyst, synthesis conditions for CNTs synthesis were 850 °C, 70 ml/min gas flow rate and 30 minutes as reaction time. PA 6 pellets were purchased from SIGMA-ALDRICH. Composites from polycaprolactam and MWCNTs were obtained using a solution mixing technique.

The first step to produce the composites involved the dissolution of 0.1 grams of PA 6 (10 pellets) with 4 mL of sulfuric acid (H<sub>2</sub>SO<sub>4</sub>), the solution was placed onto a stirring hot plate with a temperature of 200 °C for 3 hours. In the second step different concentrations of MWCNTs (0.2, 0.4 and 0.8 %) were added to the solution. Afterward H<sub>2</sub>SO<sub>4</sub> was evaporated at 200°C during 2 hours. Once the composite was dried out a gauzy thin film was extracted and characterized by Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS) and Fourier Transform Infrared Spectroscopy (FTIR).

Micrographs analyzed by SEM showed a uniform dispersion of MWCNTs with some bundles in the polycaprolactam matrix. FTIR spectra presented a peak appearing around 3400 cm<sup>-1</sup> attributed to the stretching of the hydroxyl groups. Moreover, the characteristic PA 6 absorption bands were observed: NH stretching (3297 cm<sup>-1</sup>), amide I (1637 cm<sup>-1</sup>) and amide II (1540 cm<sup>-1</sup>).

Polycaprolactam and Multi Wall Carbon Nanotubes composites synthesis with sulfuric acid solution technique and their characterization were presented. The composites obtained have potential electronic applications.

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**[ AMSCR-555 ] Nano and microstructural development of strontium aluminate obtained by the Sol-Gel Technique**

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Undoped strontium aluminates powders were synthesized from precursor solutions prepared with aluminum and strontium nitrate salts, and using the Sol-Gel Technique following a basic/anhydrous route. The temperature of drying was of 120° C and annealing interval from 450 until 1,200° C in atmosphere of air. Micro structural and morphological characterization were carried out. The analysis of the X-ray diffraction patterns and images of SEM shows the existence of two phases, a crystalline and other to way amorphous, both associated with the growth of strontium aluminates. The morphology different associate to powders has been related with the development of the crystalline habits and suggests the preferential growth of the hexagonal phase for low temperatures, coexisting with a monoclinic phase that gradually increases as increase the annealing temperature. Due to the structural bi-dimensional forms, the crystallite size was determined from the scale of SEM images. An important result is that growth units preserve their nanometric dimensions even after of the heat treatment at 1,200 ° C so it can be inferred that the materials are identified as nanostructured.



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[ AMSCR-561 ] Synthesis, characterization and testing of bulk catalysts NiMo for HDS of 4,6-DMDBT

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Bulk catalysts of nickel-molybdenum were prepared by solvothermal methods and their catalytic activity was tested in hydrodesulfurization of 4,6-dimethyldibenzothiophene. The precursors and catalysts were characterized by scanning electron microscopy with X-ray microanalysis, XRD and nitrogen adsorption at 77K, Raman spectroscopy and high-resolution transmission electron microscopy. The results indicated that the  $\beta$ -NiMoO<sub>4</sub> phase presented the best activity in the reaction of the HDS of 4,6-DMDBT.



[ AMSCR-41 ] **In situ growth of ZnO using a biopolymeric matrix of galactomannan**

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One of the promising nontoxic and biocompatible semiconductor material is Zinc Oxide (ZnO), which has received extensive application due to its exceptional electrical and optical characteristics. Recently, there are several physical or chemical synthetic methods of preparing ZnO, such as thermal evaporation, pulsed laser deposition (PLD), ion implantation, reactive electron beam evaporation, thermal decomposition and sol-gel technique (Sreetama & Bichitra, 2012).

Synthesis of inorganic crystals or hybrid inorganic-organic materials with specific size, shape, orientation, organization, complex form, and hierarchy has been a focus of recent interest because of the importance and the potential to design new materials and devices in various fields such as catalysis, medicine, electronics, ceramics, pigments, and cosmetics (Shu-Hong & Helmut, 2014).

Of the inorganic antimicrobial materials, ZnO have antimicrobial activity, however, the detailed mechanism for the activity of ZnO is still under debate. ZnO antibacterial action mechanism involves various routes: (a) release of Zn<sup>2+</sup>, (b) release of H<sub>2</sub>O<sub>2</sub>, (c) cellular internalization in case of ZnO nanoparticles, and (d) surface chemistry of sample (Rajeev et al., 2016)

We use an eco-friendly method *in situ* method for the formation of ZnO where properties such as morphology and size can be controlled by adjusting the source species, reaction temperature and time, etc. using galactomannan that is a natural biopolymer extracted from mesquite seeds. The nanocomposites were characterized with XRD and SEM also their microbial properties against *E. coli* and *S. aureus* were tested, finally a reaction mechanism it's proposed.



[ AMSCR-55 ] Synthesis and characterization of zeolites from fly ash obtained from the  
combustion of coal.

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**Abstract.** In this work the synthesis and characterization of zeolites, obtained by hydrothermal route using as crystallization precursor sodium hydroxide, and fly ash (from coal combustion) as raw material, is reported. The synthesis was performed at constant temperature of 100°C, with sodium hydroxide molar concentrations ranging 1.5 to 4.5 M, during 24 hours. The morphological and structural characterization of raw material and synthesized samples were performed by means of scanning electron microscopy (SEM) and X-ray diffraction (XRD); while the specific surface area, and the average pore size and pore volume were determined by nitrogen physisorption. The chemical characterization was carried out using energy dispersive spectroscopy (EDS), and X-ray fluorescence spectroscopy (XRF). The obtained results will allow to evaluate the applicability of the synthesized material for cations removal applications, present in industrial wastewater containing heavy metals.

**Keywords:** Adsorption Surface, Fly-Ash, Hydrothermal Process, Morphology, Zeolites.



[ AMSCR-101 ] SBA-15 with varying magnesium content in Oxidative Dehydrogenation of n-octane

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In recent years there have been works that studied the catalytic properties of silica mesoporous SBA-15 in a 2-D hexagonal array, with different heteroatoms, such as gallium, titanium, lanthanum and vanadium. These catalysts have been tested in different reactions<sup>1,2,3</sup>. One of these reactions is the oxidative dehydrogenation of light alkanes performed using catalysts with acid-base properties. There are been used different metal oxides as catalysts such as vanadium, molybdenum, tungsten and niobium oxides<sup>4,5,6</sup>.

In this work magnesium was introduced into mesoporous silica SBA-15 with the aim of improving the acid-base characteristics of SBA-15 and evaluate its performance as a catalyst in the ODH of n-octane.

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[ AMSCR-197 ] BaTiO<sub>3</sub>-Co<sub>1-x</sub>Gd<sub>x</sub>Fe<sub>2</sub>O<sub>4+d</sub>: Synthesis, characterization and properties

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A modified route of the Pechini method was used to the obtaining of nanometric BaTiO<sub>3</sub>-Co<sub>1-x</sub>Gd<sub>x</sub>Fe<sub>2</sub>O<sub>4+d</sub> (with x= 0, 0.04 and 0.08) powders. As chemical reagents were used BaTiO<sub>3</sub>; metallic nitrates, as source of Co<sup>2+</sup>, Gd<sup>3+</sup> and Fe<sup>3+</sup> cations; citric acid and ethylene glycol as chelating agents and as monomers. The precursor gels were dried for 72 hours and treated at 600 °C for 2 hours. XRD studies show the presence of both crystalline phases; the tetragonal polymorph of the perovskite-type structure of BaTiO<sub>3</sub> (PDF 5-0626) and the spinel-type structure of CoFe<sub>2</sub>O<sub>4</sub> (PDF 22-1086). TEM micrographs show particles of BaTiO<sub>3</sub> covered by Co<sub>1-x</sub>Gd<sub>x</sub>Fe<sub>2</sub>O<sub>4+d</sub> nanoparticles; particle sizes are near to 60 and 20 nm, respectively. Magnetic and electric loops show the typical hysteresis associated to ferromagnetic and ferroelectric behavior and saturation values near to those previously reported.



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[ AMSCR-198 ] Synthesis and characterization of Tb-substituted hydroxyapatite powders for 2,4-dichlorophenoxyacetic acid photodegradation applications

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Tb<sup>3+</sup> doped hydroxyapatite (Tb:HAp) luminescent powders were synthesized by Sol-gel technique, with dopant concentration ranging 2 to 12 wt.%. From the X-ray diffraction patterns and BET measurements, the average crystallite size, the unitary cell parameters, and porous size of the samples were determined for all dopant concentrations. The chemical characterization, performed by XEDS and FTIR, shows that the host matrix corresponds to HAp with calcium deficiency, evidencing that the 10% doping content sample have a stoichiometry of 1.63, having also the best ion substitution efficiency. The photoluminescence emission spectrum agrees with the allowed Tb ion transitions, and shows that the 10% doping content sample exhibit the largest luminescent emission. Finally, the UV light driven photocatalytic activity, in presence of 2,4- dichlorophenoxyacetic acid (2,4D) in aqueous phase was studied as function of the irradiation time and dopant concentration, obtaining the best result in the evaluation of the photodecomposition of 2,4D, for samples with 10% content of terbium.



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[ AMSCR-204 ] Study on grow process and optical properties of ZnO microrods synthesized by hydrothermal method

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ZnO rods were synthesized by hydrothermal method. Physical dimensions of the ZnO rods were changed systematically as a function of: precursor salt, deposition time, molarity, and temperature parameters. Nanorods using zinc nitrate and microrods using zinc acetate were obtained. The nano/microrods morphology was obtained by Scanning Electron Microscope. Zinc acetate resulted as the optimum precursor salt to study the growth process of the rods. Transmittance, diffuse reflectance, cathodoluminescence, and x-ray diffraction techniques were employed to characterize the microrods as a function of methenamine molarity/zinc acetate molarity ratio (MHTT/MZn). Optical results made possible to propose an energy diagram that presents different optical absorption and radiative desexcitation mechanisms. All microrods resulted with an average energy gap of 3.25 eV and several energy levels into it associated to structural defects. The increase of neutral interstitial zinc and/or neutral oxygen vacancy shallow donors with the incorporation of HTT into precursor solution contributed to have ZnO microrods with bigger near band edge. The use of HTT permitted the change of interstitial oxygen defect into oxygen anti-site defect and promoted the migration of zinc ions from intrinsic sites to interstitial sites during synthesis process.



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**[ AMSCR-221 ] “Comparative study of the synthesis of NiFe<sub>2</sub>O<sub>4</sub> by coprecipitation and electrospinning”**

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Two routes of synthesis, coprecipitation and electrospinning, were used to compare the obtaining of NiFe<sub>2</sub>O<sub>4</sub>. The chemical reagents used during a lightly modified coprecipitation route were metallic chlorides, as source of Ni<sup>2+</sup> and Fe<sup>3+</sup> ions, and sodium hydroxide (NaOH), as precipitating agent. The chemical reagents used during the electrospun were metallic nitrates, as source of Ni<sup>2+</sup> and Fe<sup>3+</sup> ions; polyvinylpyrrolidone, as polymeric vehicle; and N,N-dimethylformamide and ethanol as solvents. The products were dried and treated at different temperatures: 300, 600 and 900 °C for 2 hours. XRD results show the obtaining of the characteristic cubic spinel associated to NiFe<sub>2</sub>O<sub>4</sub> in both cases (PDF 74-2081) and a subtle different effect of the temperature on their crystallinity in each technique. Magnetic loops of all products show the typical ferrimagnetic behavior and values of saturation, remanence and coercivity similar to those previously reported for nanometric materials. SEM micrographs of the obtained products show that coprecipitation and electrospinning lead to materials with two different morphologies: nanospheres and nanofibers, respectively.



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[ AMSCR-244 ] Synthesis and characterization of core-shell structures based on Fe<sub>3</sub>O<sub>4</sub>@TiO<sub>2</sub>

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Core-shell structures are versatile materials constituted in its simple form by a single nucleus and an exterior layer of a different material. This led to uncountable properties and applications due to the possible combinations of core and shell materials. Magnetite nucleus is desirable because the structure can be recovered by a magnetic field without affecting the exterior material properties. Combining a magnetite nucleus with photocatalysts like TiO<sub>2</sub> based materials are a great option since these can be recovered and reusable. Titanium dioxide with anatase phase is one of the best semiconductor used on environmental applications due to its easy production and oxidation properties. Another advantage of this material is that works under room temperature and atmospheric pressure. The band-gap of TiO<sub>2</sub> is 3.2 eV which implies an activity range of >387 nm. This activity range can be extended to the visible region by adding metals to the TiO<sub>2</sub> lattice. In this work the complete structure was synthesized by sonochemical via. The formation of the structure was observed by TEM, SEM and EDS. The photocatalytic activity was evaluated by the malachite green color removal under solar radiation on a batch reactor with bubbling agitation. Aliquots were collected every 10 minutes for a total reaction time of 180 minutes then were analyzed by HPLC-UV-Vis. After 180 minutes no presence of the dye was observed. The core-shell structures were recovered by a simple magnetic field showing that is possible to obtain via sonochemical synthesis a material with catalytic activity and easy to reuse without any other expensive recovery method.



[ AMSCR-245 ] Synthesis of Pt-TiO<sub>2</sub> by microwave assisted sol-gel method for hydrogen photo-electrogeneration.

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TiO<sub>2</sub> photocatalysis has been studied as a promising technology for the hydrogen generation. Earlier studies reported that adding a noble metal in the TiO<sub>2</sub> lattice, such as Pt, Pd, Au, Ag, improves significantly the photocatalytic activity of TiO<sub>2</sub>. This behavior could be explained by the action of novel metal as photogenerated electron acceptor. The electron can be quickly transferred from the TiO<sub>2</sub> surface to the metal particle, leading to the electron-hole separation (h<sup>+</sup>/e<sup>-</sup>) and resulting in the improvement of photocatalytic efficiency.

Pt-TiO<sub>2</sub> photocatalysts have been synthesized by a sol-gel process microwave-assisted and characterized by means of several techniques (Scanning electron microscopy (SEM), powder X-ray diffraction (XRD), and Raman spectroscopic techniques) and used in the hydrogen generation under UV irradiation at room temperature. Pt-TiO<sub>2</sub> material was used to make electrodes (working and counter), for its use in a photocatalytic electrolyzer for the hydrogen production. Using platinum to modify the TiO<sub>2</sub> and employing the MW reaction method it is possible to observe changes in surface area, crystalline phase, crystal size and band gap values of the material. These changes could be related to an increase in the photocatalytic activity efficiency. The best material obtained in this study was 10 % Pt-TiO<sub>2</sub> synthesized by 60 min at 215 °C and calcined at 450° C for three hours, with which it is possible to obtain 15ml of hydrogen by volume in an estimated time of 4 min.

Keywords: Microwave radiation; TiO<sub>2</sub>-Pt ; X-ray diffraction; photocatalytic activity; Hydrogen generation; Electrolyzer.



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**[ AMSCR-260 ] Structural and luminescence analysis of ZnS:Mn nanoparticles obtained by the hydrothermal method**

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Zinc sulfide (ZnS) has a band gap of 3.6 eV (in bulk) and presents thermoluminescent properties. These properties are present at micro-scale sizes and can be improved in by changing to an a nano-scale sizes. In addition, property such as luminescence can be increased by adding and impurities such as manganese, which has been chosen for this purpose. Spherical ZnS:Mn nanoparticles with diameters of 30 -50 nm were synthesized at by hydrothermal process, using Zinc Acetate, Thiourea, Sodium Sulfide and Chloride Manganese as precursors. The samples were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), and UV/Vis and thermoluminescent (TL) spectroscopies techniques. The XRD pattern showed that the ZnS:Mn nanoparticles have a zinc blende structure. The results of UV/Vis absorbance indicate a band gap close to 4 eV, which appears to be related to the nanometric size of the obtained powders. Finally, TL glow curves were obtained for the samples showed high sensitivity to rays-x.



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[ AMSCR-262 ] Microwave assisted sol-gel synthesis and characterization of Cu/Fe TiO<sub>2</sub>

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Titanium dioxide has been widely used and investigated due to the stability of its chemical structure, biocompatibility and its physic, optic and electric properties. Its photocatalytic properties have been utilized in many environmental applications to remove pollutants in water and air. In order to improve these properties, attempts to extend its photoactivity to the visible region have been made by modification with noble metals. The aim of this work is to deepen the knowledge in M-TiO<sub>2</sub> systems. TiO<sub>2</sub> nano powders have been synthesized by means of a sol-gel method. The TiO<sub>2</sub> nano powders have been doped with iron and copper; with concentrations of 0.1 wt% and 1.0 wt%, and concentrations of 0.5 wt% and 1.0 wt% respectively. The nano powders were synthesized by a microwave assisted sol-gel method using a precursor of titanium (titanium isopropoxide (IV), Aldrich 97%) and a solvent (isopropyl alcohol, 99.9%), adding water to perform the hydrolysis process. The obtained sol was then placed on a microwave reaction system. A process of chemical reduction was then carried out by adding sodium borohydride in order to obtain a metallic particle. UV-Vis-DRS analysis was carried out to determine band gap energy by means of Kubelka Munk method, crystal structure, particle size, grain size and morphology was characterized by means of XRD, SEM, TEM and Raman spectroscopy. Morphology analysis showed the structure of the nano powders to be agglomerated spherical balls with an average particle size of 11-12 nm. According to the band gap energies, a decrease in the band gap of 6.3 %, a decrease in grain size of 48 % and a decrease in particle size of 54 % with respect to the Degussa P25 TiO<sub>2</sub> was achieved. Raman analysis show a spectrum with well defined vibrational modes characteristic of the crystalline anatase phase (143, 197, 395, 515 and 638 cm<sup>-1</sup>). The diffraction peaks detected in the diffraction patterns indicates the presence of the crystalline anatase phase ( $2\theta = 25.33^\circ, 38.60^\circ, 48.08^\circ, 53.93^\circ, 55.1^\circ, 62.75^\circ, 68.82^\circ, \text{ and } 75.12^\circ$ ), and no presence of rutile phase was observed.



[ AMSCR-266 ] Synthesis of mesoporous TiO<sub>2</sub> using a biological template

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Titanium dioxide (TiO<sub>2</sub>) is a cheap, not toxic, and thermally stable multifunctional material. This material is used for a broad applications such as sensors, pigments, cosmetics, solar cells, photocatalysis, and even cancer therapy.[1] All these applications make TiO<sub>2</sub> one of most important materials for development of different technologies. Nevertheless, remains challenges for synthesis of TiO<sub>2</sub> in order to obtain a best control of shape, size and crystallinity for guarantee the desired properties.[2]

In the last years, biomolecular structures such as virus, proteins, peptides, DNA among others have been used for the synthesis of nanomaterials. Sol-gel method offers versatility in the synthesis of metal oxides, allowing the use of these biotemplates, for example, has been demonstrated that peptides can be used to produce nanoparticles of anatase at room temperature by sol-gel method.[3]

Thus, in this work we present experiments in which the filamentous bacteriophage M13 –virus that infect bacteria, with a capsid constituted of peptides- is used as template in order to synthesize crystalline structures of TiO<sub>2</sub>. On the other hand, M13 phage is able to self-assembly[4] as a liquid crystal depending on concentration, pH among others parameters. Thus, our aim is to obtain crystalline mesoporous structures of TiO<sub>2</sub> using M13 phage as template. The combination of knowledge from biology and chemistry can be a powerful tool for the synthesis of novel materials and the development of new technologies through ambient friendly techniques and biocompatible materials.

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[ AMSCR-269 ] Synthesis of ZnO:Eu<sup>+3</sup> nanoparticles by hydrothermal method

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El principal objetivo de este trabajo fue implementar el método hidrotermal en la obtención de ZnO: Eu<sup>+3</sup>. El óxido de zinc dopado con europio (ZnO: Eu<sup>3+</sup>) nanopartículas se obtuvieron por síntesis hidrotermal con diferente concentración y precursores reactivos, la temperatura óptima de la síntesis y tiempo de residencia para la síntesis se established también. La formación de ZnO: Eu<sup>+3</sup> nanopartículas se confirmó por difracción de rayos x (XRD). Microscopía Electrónica de imágenes de barrido (SEM) mostró que el ZnO: nanopartículas de la UE tienen un cristal con una morfología hexagonal. El acetato de zinc y nitrato de zinc se utilizaron como fuente de zinc y cloruro de europio como fuente de europio, agua desionizada usada como hidróxido de disolvente y de potasio como el cambiador de solución de pH en la síntesis hidrotermal. La composición química se obtuvo por espectroscopia de dispersión de energía (EDS) y las propiedades ópticas y eléctricas se obtuvo por UV-vis. Los tamaños medios de los cristales hexagonales se obtuvieron de 30 de - 40 nm y 480 nm de ancho de largo y fue posible establecer la fase hexagonal wurtzite.



**[ AMSCR-316 ] Use of UV-VIS and partial least square method to determine the Al concentration in ZnO:Al thin films**

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ZnO materials are of great interest for their superior optical and structural properties and also by their chemical stability which are essential aspects for many possible applications. Zinc oxide thin films have been investigated due to their important applications, e.g. as transparent electrodes and windows in solar cells, in gas sensors, and as photocatalytic agents. In this work we use absorption uv-vis measurements together with partial least square in order to determine the Al concentration in ZnO thin films doped with Al prepared by the sol-gel technique on silica glass substrates. The starting solutions were prepared using zinc acetate as precursor, diethylene glycol as organic template, methanol as solvents, diethylamine as chelating agent and aluminium nitrate as dopant. The zinc acetate used was calculated to obtain Zn concentration  $M=2.0$  mol/l. After, we added aluminium nitrate dissolved in methanol as dopant. The resultant solution was kept in magnetic stirring by 5 hours. The content of aluminium in the precursor solution is referred as the atomic percentage with respect to Zinc. Here, we used  $[Al]/[Zn]= 1,3,5,7,9\%$  at. Thin films were grown using the sol-gel dip coating technique on silica glass substrate. The films were sinterized at  $100^\circ\text{C}$  after each immersion during 10 minutes. After that, the films were thermally treated at  $300^\circ$  and  $500^\circ\text{C}$  by 15 min.

The samples were characterized by XRD, UV-Vis, Raman spectroscopies and SEM. Applying partial least square method, we obtain a Calibration/prediction model that correlates the aluminium concentration in the sample and the uv-vis absorption spectra. Results show that spectral variations are highly correlated with the Al concentration present in the ZnO samples analyzed. The model showed a high correlation value of 0.94 and a low RMSEP value of 1.16.



[ AMSCR-353 ] High crystallinity copper sulfide thin films deposited at room temperature by SILAR

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Copper sulfide thin films have been studied due to their wide range of applications, such as solar control and absorbent films in photovoltaic devices.  $\text{Cu}_x\text{S}$  is a *p*-type semiconductor with electrical resistivity ranging from 1.43 to 4.17  $\Omega\text{cm}$ , depending on the composition, and has a high absorption coefficient for wavelengths larger than 1127 nm ( $\sim 10^4 \text{ cm}^{-1}$ ).  $\text{Cu}_x\text{S}$  forms five stable phases at room temperature, however, the  $\text{Cu}_2\text{S}$  phases have received great attention as promising solar cell absorbents due to their structural, optical and electrical properties. The  $\text{Cu}_2\text{S}$  bandgap energy (1.1 eV) is favorable for light absorption under sunlight illumination.

Deposition of  $\text{Cu}_x\text{S}$  has been previously reported using SILAR, however, amorphous or very low crystalline structures have been reported for the as-deposited films. In this work, high crystallinity copper sulfide thin films were successfully grown by SILAR at room temperature. The films were deposited over CdS grown by chemical bath deposition on Corning® glass. The SILAR process was carried out in a Holmarc's SILAR Coating System Model No: HO-TH30C. In this process,  $\text{CuSO}_4$  and  $\text{NH}_4\text{OH}$  formed the cationic solution,  $\text{Na}_2\text{S}$  the anionic solution, and deionized water was employed for rinsing. The properties were evaluated as a function of the number of cycles (25, 50, 75 and 100) of the SILAR process. The films resulted with good appearance, well adhered to the substrate, homogeneous, uniform, and with a deep green color. The chemical composition and morphological characteristics are discussed in this work, as well as the structural, optical and electrical properties, focused in the applicability in photovoltaics.



**[ AMSCR-449 ] Preparation and characterization of TiO<sub>2</sub> nanoparticles in rutile phase.**

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TiO<sub>2</sub> nanoparticles find usage in paint (as pigments) [1], cosmetics [2], dielectrics [3], electrochromics [4], organic pollutant on windows [5], water/air purifier and deodorizer [6], lithium-ion batteries [7], dye-sensitized solar cells [8], gas sensors [9], catalyst supports [10], photocatalysis [11], photo voltaic cells [12], luminescent [13], biomaterials [14].

TiO<sub>2</sub> has four naturally occurring polymorphs: anatase, brookite, TiO<sub>2</sub>(B) and the most stable form, rutile. Anatase is the most widely studied photocatalyst since it exhibits high photoactivity, whereas generally lower photocatalytic activity is noticed for rutile [15].

Several methods of synthesis of TiO<sub>2</sub> nanoparticles have been reported in the literature, e.g., sol-gel [16], hydrothermal [17], citrate-gel [18], hydrolysis [16], or gas-phase pyrolysis of titanium tetrachloride [19], direct oxidation of titanium platelets [20], metal organic chemical vapor deposition (MOCVD) [21].

An alternative route is the sol-gel process that has attracted much attention since it was introduced in the 1980s. The method allows the facile synthesis of stable metal oxides with better purity and homogeneity at ambient conditions [22].

TiO<sub>2</sub> nanoparticles with rutile phase is obtained by sol-gel method. Titanium isopropoxide in solution is used as precursor. Then a precipitating agent is added, which consist in a solution of nitric acid in water. After, it is constantly agitated and allowed for 24 hours aging step. Subsequently it is drying at 80 ° C for 6 hours and finally annealed at 500 ° C for one hour.

In order to perform structural studies, X-ray diffraction (XRD) measurements were performed. As a result, TiO<sub>2</sub> with rutile phase is observed and as a correspondence with the file JCPDS 00-021-1276. Furthermore, particle size from 15 to 45 nm is determined through applying the Scherrer equation.

Moreover, EDS was performed on samples where the presence of the elements of the TiO<sub>2</sub> was observed by RAMAN positions bands corresponding to 235, 447 and 612 cm<sup>-1</sup> belonging to TiO<sub>2</sub> phase rutile was determined and SEM morphology of the nanoparticles was observed.

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[ AMSCR-461 ] Synthesis and NLO properties of L- Histidine HCl-[ErNO<sub>3</sub>]5H<sub>2</sub>O crystals

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Organic crystals have nonlinear optical effects (NLO) that make them attractive for applications in frequency conversion and optical processing. Among these we find the amino acids like l-histidine, and L-histiden HC. These compounds have nonlinear optical properties in some of their polymorphs. However their thermal stability is poor. It has been demonstrated that some mixed crystals of aminoacids with some nitrates improve properties like thermal stability and second harmonic emission. In this work, we synthesize L- histidine- HCl crystals doped with penta hydrated erbium nitrate by slow evaporation at room temperature. The optical absorption spectrum recorded in the wavelength range of UV-vis revealed that the crystal has good optical transparency in the range of 350 to 1100 nm. The crystalline phase was determined by X-ray diffraction and the second harmonic generation efficiency of the crystal measured by using the Kurtz Perry modified method taken as reference the Urea SHG emission. Results obtained in this research shown that of L- Histidine HCl-[ErNO<sub>3</sub>]5H<sub>2</sub>O with a 0.3% of Er (III) has an 0.65% SHG emission respect the Urea.



**[ AMSCR-533 ] Preparation and study of optical properties of ZnO:Eu<sup>3+</sup> nanoparticles by the polyol method**

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In this work, we performed a detailed study for determinate the optimal synthesis conditions for obtaining of ZnO:Eu powders with nanometric particle size by the polyol method. This method allows to produce nanoparticles with a restricted size, controlled morphology and high crystalline quality. The synthesis parameters studied were the molar ratio of chemical compounds used during the synthesis procedure, times and temperaturas reaction. Furthermore, we analyzed the influence of the physical and chemical characteristics of the reagents used such as acetates and metal nitrates, as well as the sources of polyol: ethylene glycol, diethylene glycol and polyethylene glicol. Chemical composition, structural and morphological characteristics of the powders obtained were analyzed by X-ray diffraction, scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS), respectively. The resulting ZnO powders exhibit a crystalline structure as the wurtzite, with particles size of the order of 20 nm. The absorption spectrum shows a peak around 350 nm. The powder doped with the Eu<sup>3+</sup> ion showed an orange-red light emission which corresponds to the transition  $^5D_0 \rightarrow F_2$  with a maximum at 610 nm using an excitation wavelength of 320 nm.



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**[ AMSCR-575 ] Cu-Ag/Mordenite catalysts for NO reduction: effect of silver on catalytic activity and hydrothermal stability**

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Mordenite-supported bimetallic (Cu-Ag) catalysts were prepared for NO reduction. The effect of silver concentration on catalytic activity and hydrothermal stability was analyzed. The synthesis of monometallic catalyst was achieved by Cu<sup>+2</sup> ion exchange. Bimetallic catalysts were obtained adding Ag<sup>+</sup> by ion exchange. Two different ion exchanges were prepared under microwave-radiation. Hydrothermal stability was proved via hydrotreatment by exposing catalysts to a water vapor stream at high temperature during several hours. No significant crystalline change in the mordenite was observed by XRD, suggesting that the use of microwave radiation does not affect the structure of this zeolite. The bimetallic catalysts exhibit higher catalytic activity than monometallic Cu catalyst, and Cu/Ag ratio plays a significant role. FTIR and UV-Vis studies show catalysts to contain Cu<sup>+</sup> and Cu<sup>+2</sup> species, which absorb NO at room temperature. Copper cationic species can be in a configuration similar to bis(μ-oxo)dicopper cores linked to catalytic activity by completing copper cationic red-ox cycle, which is promoted by the presence of silver. XPS studies show copper to migrate from bulk to surface and for hydrotreated monometallic Cu catalyst a dealumination process takes place producing CuO that leads to its catalytic deactivation. In hydrotreated bimetallic catalysts copper cationic species remain and the lower catalytic activity is associated with weakening of the copper-silver interaction. This copper-silver interaction is linked with both copper migration and Ag<sup>+</sup> limited reduction with formation of aggregated silver species, as it was evidenced by NH<sub>3</sub> surface adsorption and XPS studies.

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# **ADVANCED AND MULTIFUNCTIONAL CERAMICS (AMC)**

**Chairmans: Jesus Heiras Aguirre (CNYN-UNAM)**



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[ AMC-237 ] Contact resonance frequencies determination and their use in the scanning probe microscopy technique

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Local characterizations of electric, magnetic, mechanic, electrochemical and structural properties of materials by scanning probe microscopy are usually carried out by sensing variations of the cantilever's resonance frequencies. In this work an automatic method to obtain these frequencies through the control of a lock-in amplifier by a computer with software developed in LabView, is presented. The lock-in possesses an internal ac source. The procedure is helpful and easy to implement for users that are interested in extending the capabilities of their atomic force microscope to carry out techniques like piezoresponse force microscopy, atomic force acoustic microscopy and piezomagnetic force microscopy, to name a few. In order to illustrate the utility of the methodology proposed, resonance piezoresponse force microscopy, linear and non-linear electromechanical studies, discrimination of ferroelectric from non-ferroelectric responses and piezomagnetic force microscopy measurements were conducted.

Thanks are due to PAPIIT-UNAM projects IN109016 and IN106414 and CONACYT No. 174391 and 166286.



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[ AMC-240 ] Fabrication of polymer-clay membranes for heavy metal removal in aqueous systems

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Four different polymer-clay composites were obtained by electrospinning method, in order to be used for adsorption of heavy metals present in aqueous solutions. Both clays employed (Kaolin and Metakaolin) were added in 5% ratio to polymer solutions of poly-ε-caprolactone and Polyvinyl alcohol (10%). Kinetic and adsorption studies were conducted using different solutions of Cadmium (Cd<sup>+2</sup>), Chromium (Cr<sup>+3</sup>), Copper (Cu<sup>+2</sup>) and Lead (Pb<sup>+2</sup>) with 200 mg/L concentration. Composite membrane samples were added to the heavy metal solution at a 0.5 g/L ratio and were magnetically stirred for 72 h. Results obtained by ICP spectroscopy demonstrated that adsorption processes followed a pseudo first order model. Heavy metal amounts adsorbed per gram of material (mg/g) was higher in membranes based on PCL-clay composite. Fibers composed of Kaolin and PCL showed the highest adsorption capacity for Cd<sup>+2</sup>, Cr<sup>+3</sup> and Pb<sup>+2</sup> with 26.6, 24.57 and 29.66 mg/g, respectively. On the other hand, Metakaolin-PCL fibers adsorbed the biggest amount of copper per gram (22.80 mg/g). According to results obtained, it was demonstrated that the polymer-clay fibers prepared by electrospinning showed an important potential for heavy metal removal.



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[ AMC-252 ] Synthesis of Lithium Niobate-Silica ceramic fibers

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Lithium niobate can be synthesized by various methodologies, in this project it was done by the sol-gel method coupled with the electrospinning technique. Using lithium niobium ethoxide as precursor for the synthesis it was possible to obtain coaxial fibers. The inner section of the fiber was composed by Lithium Niobium ethoxide and poly(vinilpirrolidone) (PVP), and the outer section by an solution of tetraethylorthosilicate (TEOS) and PVP. The metalorganic fibers obtained by electrospinning were analyzed and measured using optic microscopy, the process generated fibers with elongated and stable morphology, with a predominant diameter of 1.49  $\mu\text{m}$ . The precursors fibers were dried at 100°C and treated at 800°C, 2 hrs. After thermal treatment ceramic fibers were characterized by Raman and Infrared spectroscopy. In the analysis of infrared spectroscopy the spectrum show the vibrations of  $\text{SiO}_2$  bonds, and the vibration of Nb-O bond, while in the Raman spectroscopy the spectrum show lithium Niobate signals and  $\text{SiO}_2$  bonds, and with vibrations corresponding to Lithium Niobate polarized. The analysis and characterization of the obtained coaxial ceramic fibers demonstrate that the fibers were composed by Lithium Niobate and silica.



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**[ AMC-334 ] Obtaining spheres of alumina-NpsAg with bactericidal properties**

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In this methodology alumina spheres with silver nanoparticles were obtained. The  $\alpha$ -alumina was used for its properties as high hardness and thermal stability, besides being a biocompatible ceramic. The alumina spheres serve as a support for silver nanoparticles, which were added because of its antibacterial properties. Because of its size nanoparticles have a larger surface to volume ratio, and is more effective because there is more surface contact with the environment around them. The spheres obtained have a diameter of 2  $\mu$ m, with irregular surface and then sintering process intertwined particles. Silver nanoparticles were added by the electrodeposition technique, after electrodeposition spheres turned to a dark gray color, where by the deposition of silver nanoparticles on the surface of the alumina particles was displayed. For characterization of the spheres SEM analysis, IR and XRD spectroscopy were conducted. The antimicrobial activity of the alumina-NpsAg spheres, was analyzed by the turbidimetry technique using bacteria strains of *E. coli*, *S. aureus*, *Klebsiella spp.* and *S. mutans*.



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**[ AMC-401 ] Synthesis of LaNiO<sub>3</sub> perovskite by the autocombustion method**

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The lanthanum nickelite (LaNiO<sub>3</sub>) with structure type ABO<sub>3</sub> has been widely studied due its excellent electric, ionic conduction and catalytic properties. There are several factors that affect the purity of the obtained materials, mainly the heat treatment temperature. In this work the synthesis of LaNiO<sub>3</sub> by autocombustion method as a function of heat treatment temperature was performed using urea as fuel. The heat treatment was studied evaluating the purity of the obtained perovskite at different temperature values: 800°C, 850°C, 875°C and 900°C, at 5 hours. The samples were characterized by thermogravimetric analysis (TGA), differential thermal analysis (DTA) and by X-Ray diffraction (XRD). By thermal analysis and X-Ray diffraction was found that LaNiO<sub>3</sub> perovskite take place at 875°C.



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[ AMC-456 ] Reactive Magnetron Sputtering: how it works and some important complications

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Magnetron sputtering is a well-established and much-used technique to deposit thin films of many materials but it is particularly useful for producing ceramic coatings. In general, the processes involved in sputtering are that positive inert gas ions are generated in a plasma, they bombard the negatively target causing the expulsion of atoms, and these condense on the substrate to form the deposit. The particularity of magnetron sputtering, MS, is that the application of a magnetic field traps electrons and increases the production of ions, thus increasing the number of ions that bombard the target and, this increases the expulsion of target atoms. In this talk I will describe in detail what happens during MS and the effect of the various magnetic field configurations available. I will then describe the differences between using DC, RF and pulsed-DC, particularly in relation to reactive MS, and I will try to answer the question “Can you have a RF magnetron? Substrate biasing and heating are often used to vary and control the composition and microstructure of the deposits, however, the understanding of the fine points involved are often insufficient. The idea that the composition of the target and deposit are always the same, and the values sputtering yield, are often used to design a target for a given application. We will demonstrate that this approach is sometimes not correct.

Hopefully this presentation will help students and researchers, who use MS, to be able to help them increase their understanding and maximize the utility of this quite complicated technique.



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[ AMC-539 ] Influence of oxidation state in magnetic behavior of Fe doped LiNbO<sub>3</sub> particles

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We reported ferromagnetic response in reduced and oxidized LiNbO<sub>3</sub> particles doped with Fe. The samples were synthesized using mechano-synthesis of LiNbO<sub>3</sub> powders and Fe<sub>2</sub>O<sub>3</sub> at concentrations of 0.44 to 2.20 % mass, diffusion and mechanic stabilization were performed by thermal annealing in air for 60 h, after that reduction and oxidation state was induced by thermal treatment in hydrogen and oxygen atmosphere respectively. X ray diffraction, scanning transmission electronic microscopy and Raman spectroscopy were used for structural characterization of all samples, vibrating sample magnetometry at temperatures between 50 and 300 K was performed. Results showed ferromagnetic response with very strong dependence of magnetization on Fe concentration for reduced samples, the maximum saturation magnetization was of 0.95 emu/gr at room temperature; in other hand, oxidized samples presented a saturation magnetization 2 orders of magnitude lower. We also found that magnetic response of both oxidation states have a small dependence with temperatures between 50-300 K. Ferromagnetism in reduced samples is attributed to oxygen vacancies and Fe<sup>2+</sup> ions in the structure; meanwhile low saturation magnetization is due to the lack of oxygen vacancies and the Fe<sup>3+</sup> ions in the structure.



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[ AMC-125 ] Effect of Sb addition in a Bi/Pb-based superconductor prepared by solid state reaction

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Bismuth based superconductors have been proposed as an alternative in devices for generation, storage and transportation of energy because of its chemical stability, flexibility in manufacture and processing and its high transition temperature.

The present work focuses on the addition of Pb and Sb in order to stabilize the Bi-2223 phase. Pellets were prepared by solid state reaction. Precursor powders were prepared with different additions of antimony ( $x=0, 0.06$  and  $0.1$ ) and heat treated using two different routes. The addition of Sb in the material stabilized the formation of Bi-2223 in the materials in small quantities, but it was found that the heat treatment is also affected by the dopant; samples doped with antimony required a longer sintering time. Samples with an addition of Sb  $x=0.06$   $\text{Bi}_{1.6}\text{Pb}_{0.4}\text{Sb}_{0.06}\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_y$  sintered for 130 hours and 140 hours at  $860^\circ\text{C}$  presented superconductivity when cooled using liquid nitrogen. A higher composition Bi-2223 will be able to enhance the transition temperature of the material, this can be translated into more compact, simpler cryogenic systems for the use of the material in energy applications.

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[ AMC-191 ] Synthesis and characterization of glasses and glass-ceramics in the  $K_2O$ - $BaO$ - $PbO$ - $B_2O_3$ - $Al_2O_3$ - $TiO_2$  system

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Glasses with high  $TiO_2$  content (titanate glasses) have great interest for their technological applications due to their optical properties and good chemical durability. However, it is well known that a high content of this oxide increases the spontaneous crystallization tendency, which hinders the possibility for obtaining phases and microstructures well regulated after treating them thermally. On the other hand, glass ceramics based on titanate glasses, containing crystalline phases like potassium and/or barium and lead titanates, are very promising in structural and electronic applications. In this work, five glasses in the system of  $K_2O$ - $BaO$ - $PbO$ - $Al_2O_3$ - $B_2O_3$ - $TiO_2$  were synthesized and thermally treated to obtain glass-ceramics. Glasses were characterized by DTA, FTIR, DRX and MEB, while glass-ceramics were characterized by DRX and MEB. The results revealed that homogeneous glasses were obtained and their structure is formed by boroxol rings ( $B_3O_6$ )<sup>3-</sup>, octahedral units of  $(TiO_6/2)$  and  $(AlO_6/2)$ , linked together by divalent cations of  $Ba^{2+}$  and  $Pb^{2+}$ . Glasses were crystallized in the temperature range from 700 to 723° C. Crystalline phases present in glass-ceramics were  $Ti_7O_{13}$  and  $Ba_4Ti_{12}O_{27}$ , which could be promising in the electronic field as n-type semiconductors.



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[ AMC-238 ] **Alternative method to study the local strain in ferroelectric materials by contact atomic force microscopy**

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In this work we develop an alternative simple and low cost method to study the local strain in ferroelectric systems by means of atomic force microscopy (AFM) in the contact mode. This method does not require a lock-in amplifier. The procedure is based in the detection of topography changes at a point, originated by the application of dc voltage pulses with triangular modulated amplitude. The remnant strain after each pulse of voltage is applied, as a function of such voltage, gives rise to a hysteretic curve from which the local piezoelectric coefficient is then calculated. The procedure allows a reduction of the electrostatic effect. To illustrate the appropriate use of this method the above-mentioned hysteresis curve of a PZT film was acquired, and then used to calculate the corresponding local piezoelectric coefficient and coercive voltage. In order to validate the method, the same measurements were carried out by piezoresponse force microscopy in the traditional way, i.e. by using a lock-in amplifier.

Thanks are due to PAPIIT-UNAM projects IN109016 and IN106414 and CONACYT 174391 and 166286.



[ AMC-265 ] Study of the structural stability on polycrystalline superconducting phases of  
RE<sub>3</sub>Ba<sub>5</sub>Cu<sub>8</sub>O<sub>18</sub> (RE = Y<sup>+3</sup>, Sm<sup>+3</sup>) systems

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Superconductors of systems REO-BaO-CuO with general formula RE<sub>3</sub>Ba<sub>5</sub>Cu<sub>8</sub>O<sub>18</sub> (RE=Y<sup>+3</sup>, Sm<sup>+3</sup>, Nd<sup>+3</sup>) are phases with orthorhombic crystal structure with similar values of unit cell. Within this family of superconductors, those based on yttrium (RE= Y<sup>+3</sup>), Y<sub>3</sub>Ba<sub>5</sub>Cu<sub>8</sub>O<sub>18</sub>, have been the most investigated. In this work we replaces the Y<sup>+3</sup> for Sm<sup>+3</sup> in different proportions given the similarity of radius among cations. The Y<sub>3</sub>Ba<sub>5</sub>Cu<sub>8</sub>O<sub>18</sub>, (Y<sub>2</sub>Sm)Ba<sub>5</sub>Cu<sub>8</sub>O<sub>18</sub>, (YSm<sub>2</sub>) and Sm<sub>3</sub>Ba<sub>5</sub>Cu<sub>8</sub>O<sub>18</sub> superconducting phases were prepared by the solid-state reaction method. The optimal conditions of Sm<sup>+3</sup> doping and oxygen content were established using the equilibrium curves for the Y<sub>3</sub>Ba<sub>5</sub>Cu<sub>8</sub>O<sub>18</sub> phase. The atomic composition of the samples was measured by the energy dispersive spectroscopy technique (EDS) and changes in the structural parameters were studied by X-ray diffraction. By means Resistance vs Temperature measurements in the samples obtained were established the synthesis parameters that influence the variation of the critical temperature (T<sub>c</sub>).



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[ AMC-349 ] Molecular oxygen generation in the glass system ZnO-CdO-TeO<sub>2</sub> doped with  
Eu<sup>3+</sup>

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TeO<sub>2</sub> (tellurium dioxide) is not stable above 700°C and tends to decompose into TeO (tellurium monoxide) and O<sub>2</sub> (molecular oxygen). Whenever TeO<sub>2</sub> based glasses are heated, some molecular oxygen escape producing changes in the intrinsic defects (related to oxygen deficiency). These defects include Te-Te. A vacancy, in general is an efficient trap of electrons, and the change in intrinsic defects contributes with the structural disorder to the glasses creating attractive sites for rare earth dopants. Tellurium oxide glasses have a structural network consisting of Te-O bonds, and can be obtained easily when a modifier oxide is incorporated. The glass matrix is mainly constructed of trigonal bipyramids and trigonal pyramids of TeO<sub>4</sub> and TeO<sub>3</sub> structural units, respectively. If the glass network is dominated by TeO<sub>4</sub> groups, the Eu<sup>3+</sup> ions are not incorporated into the vitreous network. When the modifier oxide is added, the concentration of TeO<sub>3</sub> increases owing to the gradual change from TeO<sub>4</sub> units to TeO<sub>3+1</sub> intermediate groups until reaching TeO<sub>3</sub> units. This is, Te ions can change its oxidation state and produce hollow structures around.

In this research, the generation of O<sub>2</sub> in ZnO-CdO-TeO<sub>2</sub> glasses doped with different concentrations of Eu<sup>3+</sup> ions and thermal treatments in the range of 300°C and 400°C is studied. Raman spectra characterization showed the variation in intensity of the band at 1556-1565 cm<sup>-1</sup> which is related to molecular oxygen as a function of the thermal treatment. The increase in temperature causes structural changes in the as-cast glasses, leading to the development of crystalline phases as observed by XRD. At 420°C, crystalline phases related to Zn ions are predominant and this can be associated to the enrichment in Zn derived of the volatilization of TeO<sub>2</sub> and CdO during fusion.



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[ AMC-359 ] Synthesis of Aluminum Alloys 2024-Cerium Oxide Composite by Mechanical Alloying

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Aluminum alloys are excellent candidates for the metal matrix composite synthesis. The aluminum alloys reinforced with hard particles combine the ductility and low density of the metallic matrix with the high hardness and stiffness of reinforcement particles, resulting in a metal matrix composite which shows excellent mechanical properties.

The oxides are adequate for use as reinforcement material in aluminum matrix. Moreover, the incorporation of nanometric oxides significantly improves mechanical properties of the metal matrix composite by reducing the inter-particle spacing.

Aluminum-based composites can be synthesized in the solid state by powder metallurgy (PM) process, which presents versatility and cheap production costs. PM process involves the mixing of reinforcement particles with the aluminum powder, followed by consolidation and sintering processes. PM can include mechanical alloying (MA) and mechanical milling (MM), which favor homogeneous particles dispersion.

CeO<sub>2</sub> nanoparticles and A2024 burr aluminum alloy were used as reinforcement to synthesize the composites by mechanical alloying. The mixture of starting materials comprises 5 wt. % of CeO<sub>2</sub> nanoparticles. Mechanical alloying of the powder mixtures was carried out at room temperature in a high energy ball mill SPEX 8000M. Milling time was set to 3 h. Methanol was used as process control agent. Consolidated bulks of composites were fabricated by cold pressing the milled powders at ~ 900 MPa. Compacted products were sintered for different times at 550 °C under argon atmosphere.



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The dispersion by ball milling of CeO<sub>2</sub> nanoparticles into aluminum alloys 2024, produce dramatic variation of the microstructure and hardness. The remarkable microstructural variation of both metal matrixes is the reactivity of Ce with the Cu in the aluminum alloys 2024.

**[ AMC-361 ] Chromia and alumina oxide scales formation in high entropy alloys**

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For structural and high temperature applications, the development of structural alloys with enhanced mechanical properties and good oxidation and corrosion resistance against aggressive environments is required. The thermal barrier coatings (TBC), are highly advanced materials systems that provide thermal insulation for metallic components at high temperature applications. The operating temperatures of the gas turbine were significantly increased thanks to the developments of TBC, the gas turbines reach temperatures from 1400 to 1500 °C, above the superalloys melting point (1300 °C). The TBC are typically composed of metal substrate, metallic bond coat, thermally grown oxide (TGO) and ceramic top coat (yttria-stabilized zirconia). The bond coat serves to improve the adherence of the metallic substrate to the top coat and to protect the substrate from environmental attack by the formation of the TGO. The chromia (Cr<sub>2</sub>O<sub>3</sub>), alumina (Al<sub>2</sub>O<sub>3</sub>) and silica (SiO<sub>2</sub>) are the preferred oxide scales to protect the high-temperature alloys substrates against oxidation due to their inherent slow growth rates at elevated temperatures. The scale is a weak link that must be almost ideally adherent to retain the top coat. Therefore, characterizing the formation and growth of this oxide scale is an initial method for assessing the potential of new alloys as bond coats.



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The high entropy alloys, composed of at least five principal elements in equiatomic or near-equiatomic compositions, are potential replacements to high-temperature superalloys due to their attractive properties like high strength, high thermal stability, excellent resistance to softening at relative high temperatures and good oxidation resistance. In this investigation was studied the effect of short oxidation treatment at high temperature on the mechanical and microstructural evolution of equiatomic high entropy alloys with Al and Cr content, to understanding their potential as high-temperature alloys in TBC systems.

The high entropy alloys were synthesized by mechanical alloying followed by cold-pressing and conventional sintering at 1200 °C in vacuum. The solid products were subjected to oxidation treatments at 1000 and 1100 °C in air. The structural and microstructural evolution of these alloys were studied by X-ray diffraction and electron microscopy. Sintered and thermal treated samples were also tested by Vickers microhardness. At the sintering condition, the formation of FCC and BCC phases as well as Tetragonal-type phases in the high entropy alloys was observed. The hardest alloy is NiCoAlFeMoCr. The formation of alumina and chromia oxide scales is evident since 1000 °C.



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[ AMC-409 ] Fabrication and structural characterization of lead-free ferroelectric ceramics of  
BCTZ-BFN system by alternative route

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In this work we present results on the fabrication and structural characterization of lead-free ferroelectrics perovskite-type  $ABO_3$  ceramics of BCTZ-BFN system. Ceramics were fabricated by an alternative to the solid state reaction route using precursor powders:  $BaCO_3$ ,  $CaCO_3$ ,  $TiO_2$ ,  $Fe_2O_3$ ,  $ZrO_2$  and  $Nb_2O_5$ , which they were subsequently milled and sintered. Dry milling was carried out in a SPEX 8000 mill for 2 hours, and a single thermal cycle consisting of two stage of temperature (calcination-sintering). The process involves a first step of high energy milling of the powders in the stoichiometric proportions. Zirconia balls as grinding media (10 mm diameter) in a vial along with nylamid powders were used. The weight ratio of balls: powder was 10:1. Dry milling was carried out in a SPEX 8000 mill for 2 hours, and a thermal subsequent process (sintering) of 1050 and 1250 °C for calcining and sintering, respectively. The obtained ceramics were characterized by X-ray with radiation of Co and  $\lambda = 1.7889 \text{ \AA}$  into the range  $2\theta$  of 24 to 94° and analyzed by Rietveld refinement. Theoretical density was calculated using the lattice parameters of the unit cell obtained by Rietveld refinement, in addition to the ceramic density by the Archimedes method. X-ray diffraction patterns show us that the high-energy milling process fails to complete reaction between precursors for the synthesis but creates a metastable phase by further thermal process allows the reaction of the milled powders obtained high density (> 90%) ceramics with perovskite  $ABO_3$  structure.



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[ AMC-457 ] Synthesis of TiO<sub>2</sub>-ZnO system by the combustion method

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In this work TiO<sub>2</sub>-ZnO system was studied by combustion method modified for its application in the degradation of dyes from textile industry. The TiO<sub>2</sub>-ZnO system using oxides and nitrates as precursors and urea as fuel was studied. Samples were prepared with different molar ratios of ZnO (0.25, 0.50, 1.00, 1.50 and 2.00). The powders obtained were characterized by X-ray diffraction (XRD). Comparing the pattern JCPDS (Joint Committee on Powder Diffraction Standards) with the obtained XRD diffractograms, was obtained a TiO<sub>2</sub> - ZnO system with presence of mixtures of Zn<sub>2</sub>TiO<sub>4</sub>, ZnO, anatase and rutile (TiO<sub>2</sub>). To determine the efficiency of the samples in the degradation of dyes, studies with methylene blue were performed at 10 ppm, finding that the samples prepared with nitrates and oxides with a molar ratio of 0,5 and 2,0, respectively, showed the best results; for samples synthesized with oxides, efficiency degradation was 3.84% at 2h and the sample synthesized with nitrate, degradation efficiency reached 57.9% at 1h. For longer times, the sample saturates and the degradation process is stopped.



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[ AMC-521 ] Effect of MoO<sub>3</sub> on cordierite ceramics sintering and crystallization

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Cordierite (2MgO-2Al<sub>2</sub>O<sub>3</sub>-5SiO<sub>2</sub>) is a technically important ceramic which is applied in a great variety of areas. Cordierite and cordierite based glass ceramics, well known because of their low dielectric constant, high resistivity, elevated thermal and chemical stability and very low thermal expansion coefficient, are promising materials for electronic applications. Due to its lower processing costs and its better electrical properties, cordierite is an alternative material to be used as substrate in replacement of alumina, conventionally employed in the electronic industry. Cordierite is difficult to sinter because of the very narrow sintering temperature range functional ads which can allow easier process of sintering at lower temperature. The melting temperature of these ads should be lower than that of the precursors. In addition, the cationic radius should be larger than the radius of the metals in MAS to avoid the substitution into cordierite sites. Different components have been used as sintering aids: Cr<sub>2</sub>O<sub>3</sub>, ZrO<sub>2</sub>, K<sub>2</sub>O, B<sub>2</sub>O, TiO<sub>2</sub>, and BiO<sub>2</sub>. MoO<sub>3</sub> has necessary criteria to form a liquid phase and support cordierite sintering, such as large atomic radius of 145 pm and low melting temperature (795°C). Molybdenum trioxide forms eutectics with magnesium and aluminum. In the present work are reported the results obtained from the study of the effect of MoO<sub>3</sub> in the crystallization of cordierite, which shows that the temperature of formation of cordierite is less than reported in the literature. The composition, thermal analysis and microstructural evolution were followed by X-ray diffraction, differential thermal analysis and SEM characterization.



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[ AMC-537 ] **Second Harmonic Generation from Lithium Niobate powders Synthetized by a New Approach**

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Second-harmonic generation (SHG) is reported for a set of lithium niobate powder samples obtained by a new-hybrid approach. The approach involves mechanic activation of Lithium Carbonate and Niobium Oxide, followed by a chemical dissolution in H<sub>2</sub>O at 90°C. Mechanic activation was carried out at different milling times 180, 270 and 360 min, using air and water as different environments. The resulting solutions were evaporated obtaining dry and amorphous powders that were identically annealed at a fixed temperature 850 °C for 2 h in room atmosphere. The powders samples were characterized by X-ray diffraction (XRD) and Raman spectroscopy. XRD and Raman characterization confirmed the formation of pure LiNbO<sub>3</sub> powders; a totally stoichiometric sample was obtained for the case of dry-milling for 270 min, for which an average crystallite size of 100 nm has been determined by means of fitting of the broadening (012) peak to Scherrer equation. Second harmonic generation was performed using a fundamental wavelength of 1064 nm. The obtained results reveal that, at the nanoscale, a stoichiometric composition of LiNbO<sub>3</sub> is not the main driven mechanism for high-conversion efficiency, as could be expected. Instead a direction toward narrow distributions in particle size and lowering of surface energy, both accomplished by higher milling times of the precursors, seems to take place in the attempt of obtaining stronger harmonic signals; in the case of wet-milling it can be seen that this is not necessarily correct, probably due to the fact that water presence obstructs the lowering of surface energy mainly because it acts as a lubricant instead of oxygenation coming from breaking the O-H bonds.



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**[ AMC-538 ] Temperature dependence of Raman scattering in LiNbO<sub>3</sub> powders**

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We reported the temperature dependence of Raman scattering in reduced and oxidized pure near stoichiometric LiNbO<sub>3</sub> powders. The samples were prepared using mechanosynthesis of a stoichiometric mix in molar weight of Li<sub>2</sub>CO<sub>3</sub> and Nb<sub>2</sub>O<sub>5</sub> as precursors, after that, annealing in reduced or oxidized atmosphere using hydrogen and oxygen were performed. X ray diffraction, scanning transmission electronic microscopy were used for structural characterization of samples. Raman spectroscopy at temperatures between 300 and 500 K was performed. Results showed a reversible blue shift for Li-O vibrating modes in reduced sample. On the other hand oxidized sample presented no changes with temperature variations.



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[ AMC-547 ] Size effects in ferroelectric BaTiO<sub>3</sub> nanometric powders

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The ferroelectric materials present behaviors on the permittivity and cycles of hysteresis which are relevant for various applications in industry and technology. Increasingly smaller and more compact components are required, by what is done to determine what the effect of the low dimensionality on the properties of these materials. This work sought to obtain and characterization of fine powders of barium titanate (**BTO**) through the process of solvothermal synthesis and co-precipitation. From these results, found that control of the fundamental parameters as the concentration, temperature of reaction, Ba/Ti ratio and the use of a mineralizing agent for accelerating the nucleation, were sufficient and adequate for obtaining the **BTO** compound. *XRD* studies revealed that the observed diffraction patterns are associated with cubic **BTO**, in both that studies performed after the process of sintering of powders, shown diffraction peaks associated with tetragonal **BTO**. The estimation of the size of crystal revealed that powders with longer reaction time showed a higher growth of crystal. These results were confirmed by images of transmission electron microscopy. Finally, the measurement of dielectric properties and ferroelectric in the obtained powders, were obtained for the permittivity values near 3,500 units and cycles of hysteresis with characteristic forms of materials presenting diffuse phase transition.



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[ AMC-562 ] Synthesis of silicon carbide using the IER-UNAM solar furnace

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Silicon carbide (SiC) has been prepared successfully using concentrated solar energy provided by the IER-UNAM solar furnace. This has led to the development of a low CO<sub>2</sub> emissions process for the production of this material via carbothermic reduction of a silica/carbon (SiO<sub>2</sub>/C) nanocomposite, which has shown a more reactive carbon for formation of composite, being more thermally stable. Silica (obtained by a sol-gel process) and sucrose were used as precursors of silicon and carbon, respectively, at a temperature of 700°C in controlled atmosphere (nitrogen) for the formation of the SiO<sub>2</sub>/C composite. This composite was used in a second step to obtain SiC at a temperature of 1500°C, in argon atmosphere. The experimental setup used a Pyrex® glass spherical vessel designed to work with concentrated solar power and controlled atmospheres. The experiments were carried out with solar Direct Normal Irradiance (DNI) values close to the 900 W/m<sup>2</sup>. The structure and morphology of the solar obtained SiC were analyzed with Fourier Transform Infrared Spectrometer (FTIR), X-Ray Diffractometer (XRD) thermal analysis TGA/DSC, Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) techniques. Results show that it is feasible to use concentrated solar energy for the synthesis of SiC. The solar SiC obtained is nanostructured and is mainly β-SiC.

Keywords: concentrated solar energy, solar furnace, silicon carbide, SiO<sub>2</sub>/C composite, solar SiC.



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**September 26<sup>th</sup>-30<sup>th</sup> , Mazatlan, Sinaloa, México**

# **ATOMIC LAYER DEPOSITION (ALD)**

**Chairmen: Pierre Giovanni Mani González: (UACJ)**  
**Eduardo Martínez Guerra: (CIMAV-Monterrey)**



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[ ALD-141 ] Synthesis of Dielectric and Semiconductor Nanotubes, through Atomic Layer Deposition, using MWCNT as Template

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Recently, one-dimensional (1D) nanostructures such as wires, rods, belts, and tubes have also become the focus of intensive research owing to their unique physics and chemical properties. Based on their unique geometric characteristics, 1D nanostructures are believed to play an important role as next-generation building blocks for electronic or photoelectronic devices, for chemical or biological sensors, and for energy harvesting, storage, and conversion. One of the most popular 1D nanomaterial is the carbon nanotubes (CNTs) due their promising applications in materials science and medicinal chemistry. Nanotubes have the simplest chemical composition and atomic bonding configuration but exhibit perhaps the most extreme diversity and richness among nanomaterials in structures and structure-property relations.

Preparation of hollow nanotubes of ceramic oxides has recently attracted wide attention, due their wide spectra of applications expected. The use of CNTs as removable template has been a reliable method to obtain this 1D nanoscale materials. A well-controlled synthetic approach is required in order to deposit either particles or thin films onto carbon-based materials in accurate manner, and due to the atomic control on layer growth, atomic layer deposition (ALD) is actually most applied technique. ALD allows the coating of flat surfaces as well as complex and high surface area nano-structures in a conformal and homogeneous manner, with a precise control of the thickness of the deposited film at the angstrom-scale. In this work, we report the synthesis dielectric and semiconductor nanotubes, through Atomic Layer Deposition, using MWCNTs as removable templates. The templates were subsequently removed by controlled heating in oxygen atmosphere. Transmission Electron Microscopy reveals the presence of tubular structures after template removal. EDS, XPS and FTIR spectroscopies were used to analyze the nanotubes composition.



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**[ ALD-233 ] SPECTROSCOPIC ELLIPSOMETRY AS A RESEARCH TOOL IN THE STUDY  
OF ULTRATHIN FILMS DEPOSITED LAYER BY LAYER**

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The interest in materials prepared by atomic layer deposition (ALD), for applications different from the typical electronic research, is considerably increasing worldwide. Currently, this technique has expanded to areas like corrosion protection, polymer impermeabilization and water splitting, among others. The main features of the ALD materials demand advanced and sophisticated characterization tools, which often are very slow, of restricted access and expensive. Spectroscopic Ellipsometry is an optical technique that allows the research of several aspects of the materials deposited by ALD. Almost all the applications of the ALD films fall into the ultrathin regime and in this work the fundamentals, potentialities and some interesting results related to the ellipsometric characterization of different systems deposited by ALD will be discussed. Two different examples were selected to accomplish such goal. By one hand, HfO<sub>2</sub> films deposited with different ALD modes were analyzed to determine thickness and density variations. The ALD modes compared here are the typical continuous mode (CM) and a modified continuous mode known as the discrete feeding mode (DFM). The results show better surface saturation and higher growth rate when the discrete mode is used. Moreover, through the analysis of the ellipsometric angles, a trend of the films density can be discussed. On the other side, the system TiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub>/c-Si were deposited with the DFM and the ellipsometric characterization of this bilayered system allows to elaborate on the thickness of individual layers, the optical properties, as well as the presence of interfaces. In this case, the results complement those obtained in the HfO<sub>2</sub> films, in the sense that the DFM promotes films with better quality than the typical CM. These results can have a significant impact on the development of recipes depending on the films properties required for specific applications. In addition, the ellipsometric analysis shown here serves as an evidence of the potentialities of the applicability of SE as a research tool in the study of ALD materials.



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**[ ALD-235 ] Growth of Hf-Ti-O by Atomic Layer Deposition and Atomic Submono-Layer Deposition**

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In order to expand the range of research and applications in Atomic Layer Deposition (ALD) a growth technique based on its principles has been proposed, Atomic Sub-monoLayer Deposition (ASLD) to study the possibility of creating well controlled alloys. To demonstrate the capabilities of this technique, samples of HfO<sub>2</sub>/TiO<sub>2</sub> were prepared as conventional nanolaminates through the repeated exposure of separated metal-precursor and reactant, and HfO<sub>2</sub>-TiO<sub>2</sub> ASLD growth mode samples, varying precursor doses. Thickness and structure of samples were studied by X-Ray Reflectivity (XRR). Surface topography were studied with Atomic Force Microscopy (AFM) along with Kelvin Probe Force Microscopy (KPFM) for surface potential mapping where clear differences on surface contrast from conventional HfO<sub>2</sub>/TiO<sub>2</sub> nanolaminates and ASLD growth. The films were analyzed with depth profile X-Ray Photoelectron Spectroscopy (XPS) where well-defined HfO<sub>2</sub> and TiO<sub>2</sub> contribution were acquired for both nanolaminates and ASLD plus an additional contribution to ASLD growth that is assigned to a Hf-Ti-O.

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[ ALD-261 ] Electrical behavior of IGZO transistors and MIM structures using HfO<sub>2</sub> as dielectric layer by ALD

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We investigate the effect of oxygen Pressure on the electrical, optical and structural properties of amorphous InGaZnO (a-IGZO) deposited by RF-Sputtering and Pulsed Laser Deposition and at room temperature. Films were prepared onto highly doped p-type silicon <100>, glass and collagen as substrates. The electrical resistivity and the carrier density showed large variation with changes in the oxygen pressure. It was found a minimum resistivity for those films deposited at 10 mTorr and a huge increment in those films deposited at 80 mTorr.

It was found by XRD that all films deposited at room temperature exhibit an amorphous structure. On the other hand, the physical properties of the films like transparency, electron mobility, and free-electron concentration were found to be correlated to the oxygen pressure during the deposition and in turn to the possible oxygen vacancies or metallic interstitial in the film. The energy gap estimated from the optical transmittance showed an increasing tendency with increasing oxygen pressure. When carrier concentration was less than  $10^{19} \text{ cm}^{-3}$ , the temperature dependence of hall mobility showed thermally-activated behavior while carrier concentration was independent of temperature, showed almost degenerated conduction at  $N_e > 10^{18} \text{ cm}^{-3}$ .

Films with better performance were used as active channel in TFT fabricated by shadow mask and photolithography. For films deposited at low pressure, less than 20 mTorr, transistors showed low  $I_{ON}/I_{OFF}$  ratio with high saturation current ( $I_{Sat}$ ) which suggest low resistivity. For those films deposited



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at pressures higher than 30mTorr, the  $I_{ON}/I_{Off}$  increase up to  $10^7$  with  $I_{Sat}$  in range  $10^{-3}$  to  $10^{-5}$ . Field Effect mobility is higher than  $10 \text{ cm}^2/(\text{V}\cdot\text{s})$  for those films with oxygen treatment. Our results suggest that oxygen pressure can be exploited as key parameter to control the electrical and the optical properties of a-IGZO films deposited by RF-Sputtering and PLD. A strong dependence with voltage and frequency is found as a consequence of intrinsic defects from dielectric layer.



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[ ALD-348 ] Determination of the characteristic times of surface coverage of HfO<sub>2</sub> on Si substrates by ALD

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Actually Atomic Layer deposition has been used for electronic devices ensemble. The high quality at the interface permit uses this technique as a deposition method. But when is growing any material is important to think in three important points: Aperture-times of each precursors, number of ALD cycles and times of surface saturation. The present work shows the process of surface saturation in function of pressure and physical models. This way of obtaining films is innovative because it has not been considering in all of ALD equipment. As well as increasing the superficial area, stoichiometric control and thickness. Those features can be controlled using variables such temperature. In previous researches were found that is formed an interface and some defects in film when it is grown for ALD. Those works do not considered this propose model.



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[ ALD-363 ] Temperature effect of the substrate on the growth of Gallium Nitrogen by Atomic Layer Deposition

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In this work we present the results of growth of GaN by atomic layer deposition, ALD. As precursors of trimethyl Ga Gallium was used as a precursor of N hydroxide ammonio was used. The temperature range used was from 150 to 400 C for the substrate temperature and the temperature of the precursor was from room temperature to 40 C. To characterize the effect of temperature during growth atomic force microscopy was used. The results show a trend towards more homogenous growth at high temperatures even encouraging a crystalline phase.



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[ ALD-371 ] Customizing properties of nanostructures by ALD

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The significance of technology based on nanostructured materials has becoming greater as the years go by. The properties of nanostructures govern its applications, thus, a comprehensive approach for understanding the matter behavior is of key importance. All at the same time while controlling its size, shape, topology, etc. This means that having control of the physical placement of matter is the first step towards that approach. It is well known that the fundamental properties of nanostructures are extraordinarily transformed as the size of their constituent materials decreases to the nanometer scale and below Atomic layer deposition is a chemical tool that allows the control of matter at that kind of dimensions for a great variety of materials: from oxides to metals to semiconductors. Thus, this tool offers the possibility to build unique structures with entirely different properties than its micro-sized counterpart. This way, the resulting novel properties (electrical, optical, mechanical, magnetic, etc.) and materials become the building blocks to create the upcoming nano-technological stages.

In this work, it will be shown the use of ALD to build nanosized structures and to control some properties of technological importance.

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[ ALD-377 ] Comparative studies on electrical properties in nanolaminates films base on  
 $\text{Al}_2\text{O}_3/\text{ZrO}_2$  AND  $\text{ZrO}_2/\text{Al}_2\text{O}_3/\text{ZrO}_2$  bilayers

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With the density increase and the minimum feature size of dynamic random access memory (DRAM), high-k dielectric materials in metal-insulator-metal (MIM) capacitor have been investigated to obtain sufficient capacitance for refresh requirements. Metal-Insulator-Metal capacitors, with  $\text{ZrO}_2/\text{Al}_2\text{O}_3/\text{ZrO}_2$  (ZAZ) - nanolaminate thin-films as a dielectric layer, exhibit reduced leakage currents compared to capacitors based on pure  $\text{ZrO}_2$  respectively. These systems providing a high dielectric constant suitable for DRAM applications. ZAZ dielectric laminate grown by atomic layer deposition (ALD) has a mixture of both crystalline and amorphous phases caused by the presence of  $\text{ZrO}_2$  and  $\text{Al}_2\text{O}_3$  oxides in order to coordinate the balance between capacitance and leakage current in the capacitor performance. Although the crystallization of  $\text{ZrO}_2$  may induce the presence the leakage current in the thin films, the dielectric constant of  $\text{ZrO}_2$  can be significantly enhanced, when  $\text{ZrO}_2$  film it is remains in tetragonal phase ( $k=47$ ), but the combination with another dielectric that has higher bandgap as amorphous  $\text{Al}_2\text{O}_3$  could avoid the leakage current in the material. in addition,  $\text{Al}_2\text{O}_3$  layer will produce capacitance loss due to its relatively lower dielectric constant ( $\sim 9$ ).

In this work, we studied the electrical properties in ultrathin nanolaminate films based on bilayers of  $\text{Al}_2\text{O}_3/\text{ZrO}_2$  deposited on Si (100) by thermal atomic layer deposition (ALD) technique, changing the thickness between bilayers (0.1, 0.5, 1, 2, 5 y 10 nm). Deposited films were electrically characterized through measurements of the capacitance as a voltage function. Also we made studies of current vs. voltage in order to obtain the electrical properties of the material. Finally, the dielectric constant, equivalent oxide thickness (EOT) and charge density were calculated by these measurements.

**Keywords:** High-K oxide, ALD, electrical properties, thin films.



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[ ALD-439 ] Optical properties in Al<sub>2</sub>O<sub>3</sub>-Y<sub>2</sub>O<sub>3</sub> dielectric ultrathin multilayer films grown by atomic layer deposition

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The purpose of this study it is provide a valuable knowledge about the behavior of the refractive index and optical bandgap energy in ultrathin multilayer films based on Al<sub>2</sub>O<sub>3</sub>-Y<sub>2</sub>O<sub>3</sub> bilayers grown via thermal atomic layer deposition (ALD) technique on Si(100) substrates. The multilayer configuration stack consists in alternate layers of constant thickness (2 nm) Al<sub>2</sub>O<sub>3</sub> and varying thickness Y<sub>2</sub>O<sub>3</sub> layers for a total thickness of ~100 nm. A set of 6 samples based on bilayers with different thickness ratio, 2:X, were prepared. X refers to the Y<sub>2</sub>O<sub>3</sub> layer thickness (in nm), which is proportional to the number (*N*) of cycles, from 10 to 100 of the Y<sub>2</sub>O<sub>3</sub> precursor. Refractive index *n(l)* and optical bandgap, *E<sub>g</sub>*, of each multilayer were studied via spectroscopic ellipsometry (SE). Cross-sectional mode scanning electron microscope (SEM) images verified the multilayer total thickness and corroborated the accuracy of the optical model used for fitting the SE measurements. Ellipsometry data treated through a General Oscillator optical model was utilized to obtain the total thickness and optical constants. Single effective oscillator model (MSEO) proposed by Wemple and DiDomenico (W-D) allowed establishing a relationship between the refractive index *n(l)* and the optical bandgap energy. Results reveal that the refractive index and optical bandgap in this material can be modulated systematically as a function of bilayer thickness and showing that this material can be exploited for optical multilayered coatings development, suitable for optoelectronic devices in potential applications in nanotechnology.

**Keywords:** Nanostructured materials; Atomic layer deposition; Optical properties; Refractive index modulation.

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**[ ALD-567 ] State of the art in new approaches in ALD: Large Area Spatial ALD, Rotary ALD and Particle Coating by ALD.**

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<sup>1</sup> *BENEQ OY*

We present the results of the latest developments in ALD technology, mainly with focus on unorthodox approaches, such as Large Area Spatial ALD, Rotary ALD and Particle Coating by ALD. The presentation focuses solely on motivation to design such equipment, potential applications, equipment design and updated results of the process development based on such platforms. Each approach has its unique drivers and motivators, in the case of Large Area Spatial ALD we have, the large area substrates. On this field we see as main potential applications the barrier layers by ALD, which have historically shown outstanding performance. We also comment on the plasma integration breakthrough to this ALD approach. The case of Rotary ALD, takes us to a whole new window of opportunity in the fields of optics, and semiconductors, with a documented unparalleled deposition rate for key materials on these fields. Then we move to showcasing the new generation of particle coating equipment, resolving all challenges identified during the previous generation of tools for research on this field, and opening new windows for researchers interested in this ever interesting field of material science. The presentation is made by Beneq team, however it is technologically oriented and if needed Beneq logos can be limited to the last slide, the presentation has no commercial purpose.



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[ ALD-64 ] Growth and Characterization of TiO<sub>2</sub> Films Grown by Atomic Layer Deposition for photocatalytic applications

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Due to the current global needs of efficient processes for purification of waste waters has recently been a significant increase in research, in particular, heterogeneous photocatalysis by titanium dioxide (TiO<sub>2</sub>), due mainly to its ability to induce chemical reactions of oxidation and reduction of the oxygen molecules adsorbed on the semiconductor/medium interface , producing the proven effect biocide and sterilizing of TiO<sub>2</sub> . Although studies have been conducted with other semiconductor photocatalysis mainly CdS and CdSe , it has been observed that with TiO<sub>2</sub> the higher is obtained. In addition, the TiO<sub>2</sub> material is inexpensive, non-toxic and chemically inert biological. The study of the photocatalytic properties of TiO<sub>2</sub> were performed with films formed from a suspension of titanium powder (in anatase phase) TiO<sub>2</sub> thin films can be grow by other methods as: Sol- gel, sputtering, spray-pyrolysis and Atomic Layer Deposition. In this paper we present the results for establish the parameters for the growth of thin films of titanium dioxide (TiO<sub>2</sub>) in anatase phase by Atomic Layer Deposition (ALD), their optical characterization through photoluminescence (PL) , and surface characteristics by atomic force microscopy (AFM) . It also proposes a study of the efficiency of photocatalytic TiO<sub>2</sub> films grown by ALD, depending on the film thickness, by means of the time-dependent decrease in the degradation of color units using as one model contaminant solution of methylene-blue, for potential applications in sewage purification.



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[ ALD-87 ] Refractive index and bandgap variation in Al<sub>2</sub>O<sub>3</sub>-ZnO Ultrathin Multilayers  
Prepared by Atomic Layer Deposition

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This research focuses on the study of the refractive index and bandgap behavior in ultrathin multilayer films of Al<sub>2</sub>O<sub>3</sub>-ZnO bilayers grown via atomic layer deposition (ALD) technique on Si(100) substrates. The multilayer configuration stack consists in alternate layers of constant thickness Al<sub>2</sub>O<sub>3</sub> (2 nm) and varying thickness ZnO films in order to obtain a total thickness of ~100 nm. A set of 10 samples based on bilayers with various 2:X thickness ratios were prepared, where X refers to the ZnO layer thickness. X is proportional to the number of cycles (N) of the ZnO precursor, varying from 1 to 100. The sample morphology was studied via Atomic Force Microscopy and the results show that the surface roughness of the multilayers varies from 0.2 to 1.2 nm, as the ZnO layer thickness increases. In all cases, the roughness values remain below 2% of the total thickness of the multilayer. The refractive index  $n(l)$  and optical bandgap,  $E_g$ , of each multilayer sample were studied via spectroscopic ellipsometry (SE). A General Oscillator optical model was utilized to fit the experimental data in order to obtain the total thickness, refractive index and absorption coefficient. Cross-sectional mode scanning electron microscope images verified the multilayer total thickness and corroborated the accuracy of the optical model. The refractive index varies significantly from values close to the Al<sub>2</sub>O<sub>3</sub> refractive index when the bilayer thickness is small, up to values corresponding closely to ZnO for thicker bilayers. The refractive index, as a function of bilayer thickness, varies between 1.63 eV and 2.3 eV, for  $l = 370$  nm (UV region), showing high sensitivity. In addition, the optical bandgap energy,  $E_g$ , determined using the *Tauc* model, decreases when the bilayer thickness increases, with a maximum variation of  $\Delta E_g \sim 1.6$  eV.



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These results reveal that the refractive index and optical bandgap of Al<sub>2</sub>O<sub>3</sub>-ZnO material can be modulated systematically as a function of the bilayer thickness. Such behavior is of great importance for optoelectronics applications, in particular for the development of devices with response in the UV spectral range.

**Keywords:** Tunable refractive index; Optical bandgap modulation; Ultrathin multilayers; Atomic layer deposition.

#### ACKNOWLEDGMENTS

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[ ALD-88 ] Influence of the bilayer thickness on the optical properties of Al<sub>2</sub>O<sub>3</sub>-Y<sub>2</sub>O<sub>3</sub> dielectric nanolaminate films grown by thermal atomic layer deposition

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This work focuses on the study of the optical properties of ultrathin nanolaminate films comprised of Al<sub>2</sub>O<sub>3</sub>-Y<sub>2</sub>O<sub>3</sub> bilayers. Nanolaminates of increasing bilayers thickness (1, 2, 4, 10 and 20 nm, 1:1 thickness ratio) were grown on Si(100) by means of thermal atomic layer deposition (ALD). Refractive index ( $n$ ) and optical bandgap ( $E_g$ ) were studied via spectroscopic ellipsometry (SE). Thickness of the multilayers was determined through SE measurements and the accuracy of the model was corroborated by means of scanning electron microscope images obtained in cross-sectional mode. Ellipsometric data treated through the Cauchy dispersion model revealed an increase of the refractive index,  $n(l)$ , (e.g. from 1.9 to 2.2 at 190 nm wavelength) when the bilayer thickness increases from 4 to 10 nm. The increase is observed in the whole spectral range measured (190-1200 nm wavelength). Furthermore, for all bilayer thicknesses,  $n(l)$  decreases monotonically as the wavelength increases within the 300 - 1200 nm range. These results demonstrate that the refractive index can be modulated by varying the nanolaminate thickness. The optical bandgap values of the samples, obtained via Wemple and DiDomenico (W-D) model indicate that the bilayer thickness decrease leads to an increase of the optical bandgap. A change of  $\Delta E_g = 0.8$  eV was found for bilayer thickness variation between 20 and 1 nm. Although the optical bandgap values obtained via Tauc model show a smaller variation of  $\Delta E_g \sim 0.1$  eV, they also confirm that there is a dependence between  $E_g$  and the bilayer thickness. Such dependence allows modulation of the optical bandgap values as a function of the bilayer thickness in the nanolaminates. The Al<sub>2</sub>O<sub>3</sub>-Y<sub>2</sub>O<sub>3</sub> optical properties show that this material can be exploited for designing optical multilayered coatings suitable for nanoscale optoelectronic devices.

**Keywords:** Nanolaminates; atomic layer deposition; Optical properties; Optical spectroscopy.



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**[ ALD-203 ] Analysis of Al<sub>2</sub>O<sub>3</sub> as coating for solar cells by ALD**

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Atomic layer deposition (ALD) has emerged as an important deposited technique in thin films for variety applications. Inorganic coating protection barriers are very important in applications as new OLED technology and solar cells grown in plastic substrates, both needs an efficient encapsulation. The permeability of polymer substrates can be reduced around two orders of magnitude using single-layer inorganic coatings (Al<sub>2</sub>O<sub>3</sub>). High quality Al<sub>2</sub>O<sub>3</sub> films can be deposited by ALD at temperatures as low as 33 °C. These temperatures are compatible with most thermally fragile plastic substrate. With ALD technique is possible to obtain a defect-free, continuous thin-film coating of an inorganic material should ideally be impermeable to environment. A good coating with ALD technique could increase the degradation time in solar cells exposed to environment. In addition, thermal annealing process associated with the ALD deposition is shown to improve the open-circuit voltage and power conversion efficiency of the solar cells.



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[ ALD-214 ] Fabrication of Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> Nanotubes, through Atomic Layer Deposition, using MWCNT as Template

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Bilayer of Aluminum oxide/Titanium oxide (Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub>) nanotubes was synthesized by atomic layer deposition (ALD) method, using multiwalled carbon nanotubes (MWCNTs) as templates. The bilayer of Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> material was deposited on the MWCNT at 100 °C by a hotwalls ALD reactor. First, the MWCNT were coated with a layer Al<sub>2</sub>O<sub>3</sub>, and then coated to a TiO<sub>2</sub> layer. A Trimethyl-Aluminum (TMA) and Tetrakis(dimethylamino)Titanium (TDMAT), were used as precursors. In both cases deionized water were used as oxidant. Transmission Electron Microscopy (TEM) shows that the wall thickness of Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> coatings is precisely controlled by adjusting the number of ALD-cycles of TMA/H<sub>2</sub>O and TDMAT/H<sub>2</sub>O. The Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> coatings on the MWCNTs were confirmed through a XPS and a FTIR analysis. In order to remove the carbon template by oxidation, the Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> -coated MWCNT were heated under air flow from ambient temperature up to 800 °C. The correlation between thicknesses and thermal properties of the Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> -coated MWCNTs were studied in detail by thermogravimetric analysis (TGA). EDXS confirmed the production of amorphous Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> nanotubes that retained the cylindrical shape of the parent MWCNTs template with excellent control of wall thickness.

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[ ALD-374 ] Electrical characterization of ALD Al<sub>2</sub>O<sub>3</sub>/ Y<sub>2</sub>O<sub>3</sub> nanolaminates

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Dielectric materials based on metallic oxides as ZrO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, Y<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, are very interesting properties and exhibiting high - K dielectric constants which improve the electrical properties in the different devices for microelectronic and optoelectronic applications in nanotechnology specially for microchip-embedded that provides energy storage in high-capacitance capacitors. Aluminum oxide (Al<sub>2</sub>O<sub>3</sub>) is one of the most widely used materials in the family of ceramics. It is known as a material with good chemical stability, extremely high hardness and relatively high thermal conductivity. Al<sub>2</sub>O<sub>3</sub> thin films are used as dielectric gate in electronic devices, because it has a high - K dielectric value, being a material with interesting physical properties useful in areas such as micro and optoelectronics. Yttrium oxide (Y<sub>2</sub>O<sub>3</sub>) is a material with several interesting diverse applications due to its thermal stability with a high melting point (2439°C), optical transparency from 300 nm to ~11 μm range, high refractive index, and useful electrical properties. In optical applications, its high refractive index can be used in the manufacturing of optical waveguides and multilayer dielectric coatings that might enhance the optical surfaces for optoelectronic applications in order to modify the transmittance and reflectance properties of the materials to which are applied. Atomic layer deposition (ALD) is an ideal technique for fabricate composite thin films. The thickness and stoichiometry of composite thin films prepared using ALD is dependent on the underlying surface chemistry during ALD film growth. Composite thin films may be fabricated by co-depositing two or more materials that may be combined in alternating, discrete layers to form multilayered laminates. These composite materials can be homogeneously mixed to form alloys. A wide range of physical properties may be achieved by varying the relative proportions of the components. This strategy has been used previously to control numerous thin film properties including refractive index, dielectric constant, lattice constant, hardness, charge storage capacity, and surface roughness.

Deposited films were electrically characterized through measurements of the capacitance as a voltage function. Also we made studies of current vs. voltage in order to obtain the electrical properties of the



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material. Finally, the dielectric constant, equivalent oxide thickness (EOT) and charge density were calculated by these measurements.

**Keywords:** High-K oxide, ALD, electrical properties, thin films

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[ ALD-376 ] Comparative studies on electrical properties in nanolaminates films base on  
 $Y_2O_3/ZrO_2$  and YSZ bilayers

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Silicon dioxide (SiO<sub>2</sub>) has been used as the primary gate dielectric material in field-effect devices since the advent of the first integrated circuit. However, this kind of material has limitations when applied as gate dielectrics due to the exponential increase in tunneling current with decreasing its thickness. Currently, different investigations carried to improve the limitations caused for the silicon oxide thickness, have suggested the use of several materials that can replace the SiO<sub>2</sub>. For example, gate dielectrics, such as Ta<sub>2</sub>O<sub>5</sub>, TiO<sub>2</sub>, Y<sub>2</sub>O<sub>3</sub>, and ZrO<sub>2</sub> can be used. Unfortunately, most of these materials are not thermally stable on silicon. However, often occurs the possible formation of SiO<sub>2</sub> or metal silicides when these materials are deposited on silicon or during subsequent annealing. It is known that SiO<sub>2</sub> has a lower dielectric constant; therefore an underlying SiO<sub>2</sub> layer can reduce the effective capacitance of the film. Yttria-stabilized zirconia oxide (YSZ, with dielectric constant 25–29.7), It is a material with interesting dielectric properties that can be used as alternative gate dielectrics due to it is considered as one of the few materials that can be thermodynamically stable in contact with silicon at 1000 K. In this work, we studied the electrical properties in ultrathin nanolaminate films based on bilayers of Y<sub>2</sub>O<sub>3</sub>/ZrO<sub>2</sub> deposited on Si (100) by thermal atomic layer deposition (ALD) technique, changing the thickness between bilayers (0.1, 0.5, 1, 2, 5 y 10 nm). Deposited films were electrically characterized through measurements of the capacitance as a voltage function. Also we made studies of current vs. voltage in order to obtain the electrical properties of the material. Finally, the dielectric constant, equivalent oxide thickness (EOT) and charge density were calculated by these measurements.

**Keywords:** High-K oxide, ALD, electrical properties, thin films.

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would

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[ ALD-390 ] Enhancing the Oxidation resistance of diamond powder by the application of Al<sub>2</sub>O<sub>3</sub> conformal coat by atomic layer deposition

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Diamond powders have been coated with thin layers of Al<sub>2</sub>O<sub>3</sub> by atomic layer deposition. The modified powders were studied by Fourier Transform Infrared Spectrometry (FTIR), Transmission Electron Microscopy (TEM) and X-ray Photoelectron Spectroscopy (XPS); the results show that the coats were successful and conformal. Thermal properties were studied by ThermoGravimetric Analysis (TGA) and Differential Thermogravimetric analysis (DTG); it was found that the weight loss onset temperatures (T<sub>onset</sub>), that denotes the temperature at which decomposition diamond to CO<sub>2</sub> begins, is shifted towards higher temperatures (an increment of ≈ 50 °K) as result of protective effect of the Al<sub>2</sub>O<sub>3</sub> layer. It is concluded that diffusion mechanism across the protective layers is responsible for the moderately increase of oxidation temperature. The amount of improvement is fairly small to be of use for technological applications; however our results confirm that a protective coat can be used to shield diamond from oxidation. Further work is in progress.

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[ ALD-415 ] Synthesis and characterization of TiO<sub>2</sub> and HfO<sub>2</sub> nanofilm compounds by ALD

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Hafnium Oxide (HfO<sub>2</sub>) and Titanium oxide (TiO<sub>2</sub>) films are being studied for their high-k constant in CMOS applications. Atomic layer deposition (ALD) is a novel technique used to deposit oxides, metals and nitrides with high quality and control thickness. Some applications for HfO<sub>2</sub> and TiO<sub>2</sub> are optical coatings, sensors and MOSFETs. The HfO<sub>2</sub>-TiO<sub>2</sub> nanofilm compounds were synthesized through Tetrakis(dimethylamido)hafnium(IV) and Tetrakis(dimethylamido)titanium(IV) as precursors and H<sub>2</sub>O as oxidant-agent varying substrate temperature (120 °C, 200 °C and 250 °C). X-Ray Reflectivity (XRR) and Spectroscopic Ellipsometry (SE) were used to determine HfO<sub>2</sub> and TiO<sub>2</sub> compound thickness and dielectric function respectively. Stoichiometric films were studied with X-Ray Photoelectron Spectroscopy (XPS). Leakage current and dielectric constant were studied through I-V, C-V measurements respectively.



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**[ ALD-417 ] Design, assembly and control of an Atomic Layer Deposition System (ALD)**

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The atomic layer deposition (ALD) is a technique of layer-by-layer growth at nano-metric level in a controlled and highly accurate form. The purpose of this work is to describe the basic features of the ALD system that is being built. The specific design of key parts of the system allows to obtain certain fundamental properties during the cycle. The reactor is the element that holds the growth process, also is the main stronghold of the structure. Made of stainless steel, it features a design that allows optimize tasks that facilitate the accumulation of cycles in the process. This has an input duct for the precursors and another for the output. The growth zone of the films is at the center with a gap depth to prevent movement of the product during the process. Just below the growth zone is found a hole which will hold a flat circular resistance responsible to provide the required heat to the system. An important feature to consider is the system protection against leakage during the cycle. This ALD system has an Oring in the reactor that provides a pressure seal that isolates the system of large leaks. The skeletal of the system consists of pipe and stainless steel connectors with standardized measures. To provide the low vacuum and purge required to the reactor during the process is used a vacuum pump of medium power capable of providing a maximum vacuum of  $1 \times 10^{-4}$  tor. The use of electro-pneumatic valves 2/2 to control the flow of precursors during the cycle. To control the system is used an embedded system Arduino UNO. With a low cost and flexibility this controller uses a high-level language for creating routines and subroutines with a specific purpose in the process. Capable of handling digital inputs and outputs, also has a section aimed to analog inputs which allows to introduce important variables for optimal control of the system such as temperature, pressure, flow, etc. The ability to communicate with a platform of design and graphic control, such as Labview, allows us to optimize and extend the control/monitoring of the ALD system.



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**[ ALD-438 ] Thickness effect on the optical and morphological properties in Al<sub>2</sub>O<sub>3</sub>/ZnO nanolaminate thin films prepared by atomic layer deposition**

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In this work, we studied the optical and morphological properties of ultrathin nanolaminates films based on Al<sub>2</sub>O<sub>3</sub>/ZnO (AZ) bilayers stack. The films were deposited on Si (100) by means of thermal atomic layer deposition (ALD) technique. The bilayer thicknesses (ratio = 1:1) were 0.2, 1, 2, 4, 10 and 20 nm. Refractive index (n) and band gap (E<sub>g</sub>) of each nanolaminate were studied via spectroscopic ellipsometry (SE), and spectral reflectance ultraviolet-visible spectroscopy (UV-vis). Surface morphology and roughness parameters of the nanolaminates were measured by Atomic Force Microscopy (AFM). The optical and morphological properties were shown highly dependent on the bilayer thickness. Ellipsometric data treated through the Cody - Lorentz optical model revealed that the refractive index decreases for thinner bilayers. A sharp intensity decay of refractive index and peaks at the UV region (200-400 nm) indicated increased transparency for thinner bilayers. It is also shown that the band gap is tunable. The maximum band gap value was 4.8 eV. These results reveal that ZnO combined with Al<sub>2</sub>O<sub>3</sub> as bilayers stack can be converted into a dielectric material with enhanced band gap, opening the possibility for new optical and dielectric applications.

**Keywords:** Nanolaminates films; Atomic layer deposition; Optical properties; Band gap modulation

**ACKNOWLEDGMENTS**

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[ ALD-508 ] Flexible dye sensitized solar cells using Atomic Layer Deposition

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Flexible and rigid dye sensitized solar cells (*flex*-DSSCs) were built using hexagonal-shaped small ZnO nanorods synthesized on PET (Polyethylene terephthalate)/ITO and Glass/FTO substrates. In the synthesis, Atomic Layer Deposition (ALD) was used to deposit a textured ZnO film which acts as seed layer. ZnO nanorods growth was carried out by a chemical method assisted by ultrasound using  $Zn(NO_3)_2$  and hexamethylenetetramine (HMT) as precursors. The reaction was carried out in two steps: i) ZnO textured film deposition and ii) ultrasound-assisted growth. After, synthesis, aligned ZnO nanorods (ZnO-NRs) with lengths and thicknesses between (240-350 nm) and (25-80 nm) on substrates were obtained and characterized by HRTEM, SAED, EF-SEM, UV-Vis and Raman spectroscopy. Structural analysis revealed that the ZnO nanorods are well crystalline, possessing a perfect hexagonal structure characteristic of Wurtzite zinc oxide with preferential growth in [0001] direction. ZnO-NRs/(PET/ITO) and ZnO-NRs(Glass/FTO) transmittance ranged between 50% and 80%, this variation depended on the synthesis conditions. Optical band-gap of the synthesized materials was approximately 3.3 eV and this value was independent of the nanorods dimensions. Through EF-SEM, it is evidenced that the nanorods grew on ZnO seed layer of 200 nm, which allowed good contact with the conducting surface of the substrate. Analyses on the effect of synthesis parameters on NRs growth, fabrication of solar cell prototype using working electrode and collector electrode were formed by (Glass/FTO/ZnO-film/ZnO-NRs/ruthenium-dye) and (Glass/FTO/Pt-layer) respectively. Experimental details, structural, electrical and optical characterization details are discussed.



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[ ALD-509 ] Doped ZnO Nanorods grown by Solvothermal-ALD method

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The synthesis of one-dimensional single crystalline ZnO nanostructures has been of increasing interest due to their promising applications in nanoscale devices. Doped and vertically aligned ZnO nanorod arrays with different aspect ratios were synthesized by hybrid wet chemical route. In this study, it was possible to obtain vertically aligned ZnO nanorods using a method that consists in two steps: i) the growing of a textured ALD film to grow a ZnO seeded surface on glass and silicon single crystals (111). ii) and the nanorod array growth by solvothermal synthesis. ZnO thin films are firstly produced by means of ALD deposited on glass substrates and silicon single crystal (111). Subsequently a solvothermal method is employed to grow vertical-aligned doped-ZnO nanorod arrays on ZnO films. A textured ZnO layer with preferential direction in the normal *c*-axes is formed on substrates by the decomposition at 190°C and  $\sim 2.51\text{E}-1$  torr of diethylzinc (DEZn) to provide nucleation sites for vertical nanorod growth. ALD parameters such as exposure time (0.05 and 0.03 s) and number of cycles 400 were varied to modulate the crystallographic nature of seed layer. Doped ZnO nanorods (ZnO-NRs) growth over the substrates was performed by wet chemical procedure in which  $\text{Zn}(\text{NO}_3)_2$  and hexamethylenetetramine were used as the main precursors.  $\text{C}_6\text{H}_9\text{O}_6\text{In}$ ,  $\text{Ru}_3(\text{CO})_{12}$  and  $\text{Ce}(\text{C}_2\text{H}_3\text{O}_2)_3 \cdot 1.5\text{H}_2\text{O}$  compounds were used for doping. Crystallographic orientation of doped ZnO nanorods and ZnO-ALD films was determined by X-ray diffraction analysis. The XRD measurements indicate that the prepared nanoparticles have a hexagonal wurtzite structure and are high-quality single crystals growing along [0001] direction with a high consistent orientation perpendicular to the substrate which is quantified through the texture coefficient. Composition, morphologies, length, size and diameter of the nanorods were studied using a scanning electron microscope, energy dispersive x-ray spectroscopy (EDS) and atomic force microscopy (AFM) analyses. Length and thickness of the ZnO-NRs ranged between 40 and 90 nm and 300 and 600 nm, respectively. It is demonstrated that crystallinity of the ZnO-ALD films plays an important role on the vertical-aligned doped ZnO nanorod growth. SEM images in plane and tilted view show that nanorods have smaller average diameters when compared with conventional hydrothermal synthesis.



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# **BIOMATERIALS AND POLYMERS (BIO)**

**Chairman: César Márquez Beltrán: (BUAP)**



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**[ BIO-90 ] Polycarbonate Material to Detect Gas Radon in the Ancient Cuexcomate Geyser in Puebla City, Mexico.**

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The polycarbonate CR-39 (Columbus Resin Number 39) and the polymeric compound of CD-DVD were used as radiation sensitive materials in order to detect alpha particles emitted in the disintegration of Radon gas. The Radon measurements were collected over a period of nine months in the area of the ancient Cuexcomate geyser, in Puebla City. It was found that Radon concentrations varied in strong anti-correlation with the rainfall intensity. And are lower compared to other locations, in concordance with the stratigraphic composition, as travertine and deposits of volcanic origin, corresponding to the geyser chemical composition and the active environment in the north part of the Trans-Mexican Volcanic Belt with an andesitic and basalt composition.



[ BIO-201 ] Polymer nanocomposites for heat exchangers. properties evaluation

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Heat exchangers play a major role in thermal management into several processes and their design is subjected to the appropriate materials selection[1]. Polymer nanocomposites with carbon nanoparticles exhibit an extraordinary increase in their physicochemical properties, positioning them as the best candidates to replace metals and specialty alloys in the fabrication of heat exchangers or fuel cells [2,3]. Several studies have put emphasis in the aspect ratio and geometry of carbon fillers, and in the combination of nanoparticles to increase the thermal conductivity [4]. The aim of this study is to test several carbon nanoparticles as individual fillers to increase the thermophysical properties of polymer nanocomposites of polyethylene obtained by melt extrusion. Four types of carbon nanoparticles like graphene nanoplatelets (GNP), carbon black (CB), carbon nanotubes (CNT) and carbon nanotubes modified (CNTM) were added in high loadings to a high density polyethylene (HDPE) by means of ultrasound assisted melt extrusion [5] and their thermophysical properties were evaluated. The thermal stability exhibits an average increase of 34 °C at 50% of weight loss, which suggest that thermal stability is enhanced by carbon nanoparticles. On the other hand, heat capacity exhibit an increase of 23% with the adding of CB, suggesting that this nanoparticle would have more ability to heat transfer. CNT can raise up to 0.43 W/mK the thermal conductivity of PE, this means an increase about 87%. The evaluation of mechanical properties had shown a reinforcement effect for all carbon nanoparticles with an outstanding increase for GNP and CNT. Dielectric constant, shown an increase up to 3 orders of magnitude with the addition of CNT, CNTM and CB; and only 1 order of magnitude of increase with GNP. Electrical conductivity as a function of frequency shown a behavior as a conductive material for nanocomposites with CNT and CNTM, being this effect more pronounced with the use of CB, meanwhile the behavior of PE-GNP corresponds to an insulator material. From all carbon nanoparticles tested in this study, CNT showed a better balance in thermophysical and mechanical properties, which suggest that this nanoparticle could be employed to compound a polymer nanocomposite able to the fabricate a heat exchanger prototype.



[ BIO-215 ] Synthesis and characterization of alumina/hydroxyapatite spheres

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Alumina is a ceramic material with excellent properties including hardness and chemical stability. Hydroxyapatite is a bioceramic whose chemical composition is similar to the inorganic part of bone. The objective of this project was obtain porous alumina ceramic spheres coated hydroxyapatite by a route of encapsulation using sodium alginate. In this study, an alumina slurry was prepared adding polyvinyl alcohol and sodium alginate as binder and gelling agents respectively. The alumina slurry was dropped drip in a solution of barium chloride to carry out the gelation process, while the hydroxyapatite was synthesized by the method of chemical precipitation. For the sintering process, the alumina spheres were heated to 600 °C at 1 for 2 h, then they were coated with hydroxyapatite and again sintered at 800 °C for 2 h. Characterization by infrared spectroscopy, X-ray diffraction and scanning electron microscopy, confirmed the stability of the chemical composition of alpha-alumina and hydroxyapatite after heat treatment. The final composite has a porosity about 50% and crystallinity. In conclusion, the method of encapsulation using sodium alginate allowed obtaining porous ceramic spheres, which can be used as a material for biomedical applications.



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**[ BIO-234 ] Development of hydroxyapatite and bio-glass composite through the electrospinning.**

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The materials which designed to induce a specific biological activity are called biomaterials. There are three important aspects to account in a biomaterial must be in contact, biochemically and mechanically compatible with adjacent tissue. Calcium phosphate ceramics are used widely for dental and orthopedic reasons, because they can join tightly through chemical bonds and also promote bone regeneration. Synthetic Hydroxyapatite (HA) has been researched to replace hard tissue because it's composition is similar to that of human bone. However, there are three characteristics that restrict HA use for biomedical applications: brittleness, lack of antimicrobial properties and limited contact with the host tissue. This research proposed the incorporation of glass to counteract the brittleness of HA in a composite formed by coaxial fibers which will be used for bone regeneration. Precursors HA and SiO<sub>2</sub> were synthesized through the sol-gel method and then incorporated into a polymeric PVP matrix; later they were processed by coaxial electrospinning to obtain fibers which were characterized with techniques such as ATR-FTIR, DTA, SEM. The obtained fibers showed a coaxial disposition with a glass core and hydroxyapatite cover. Through ATR-FTIR and SEM analysis was determined the fiber composition and the presence of characteristic chemical groups and microstructure was also observed.



**[ BIO-273 ] Synthesis and characterization of a chitosan-cholesterol composite projected to tissue engineering applications.**

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*Keywords.* Chitosan, Glycidyl methacrylate, Cholesteryl Hemisuccinate, biopolymers, tissue engineering.

The Nanotechnology and Biomedical Engineering have been converted in crucial factors for tissue engineering, especially with the use of biocompatible materials, between them, biometals, bioceramics and biopolymers. This work presents the synthesis and characterization of a Cholesterol/Chitosan-g-GMA composite; the objective is to obtain a composite and to study its behavior as biomaterial. Inside this composite the function of Chitosan and Chitosan-GMA is to promote the tissue regeneration and avoid the bacterial growth, and de main function of cholesterol is providing the necessary conditions to growth quickly and orderly, due to the nature of cholesterol and its relation with epidermal tissue.

The composite synthesis pathway is divided in three stages; the production of Cholesteryl Hemisuccinate, the functionalization of Chitosan to produce Chitosan-GMA and the last step, the conjugation of both products, and a film with raw Chitosan is used as reference. The cholesterol succinate was incorporated to hybrid Chitosan-GMA, or raw chitosan, and dispersed by different methods; after dispersion a film was obtained by casting and was used to subsequent for characterization by melting point, infrared spectroscopy and calorimetry; and its application as a film in wounded tissue under controlled conditions is under evaluation. After the properties shown the film is proposed as a material which could allow accelerated epidermal regeneration.



[ BIO-391 ] Synthesis of a resin recycled polyethylene terephthalate and evaluation of their influence on the mechanical properties of a particular modified

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**Abstract:** The object of study of this research is a new concrete made with the replacement of natural aggregate coarse fraction (AGN) by recycled coarse aggregate (AGR) (25%), moreover with the addition of a polymeric resin (RR) (9, 13 and 17%), which was synthesized from chemical container recycling post-consumer polyethylene terephthalate (PET acronym in english); reuse of materials is one of the pillars on which the current development in terms of sustainability focuses on what is considered of great importance the manufacture of a new concrete that has its genesis in the use of recycled materials. Since the mechanical properties are considered some of the most interesting to assess during the manufacture of a concrete, have been selected the modulus of elasticity and compressive strength of concrete as the characteristics analyzed. It has been found that replacing 25% of AGN by AGR, have been shown averages decrements 5 a 8% in their mechanical properties, however it is noted that this loss is offset by the addition of different percentages of RR, so directly proportional.

**Keywords:**

Polymer modified concrete; polyethylene terephthalate; mechanical properties.



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**[ BIO-515 ] In vitro Comparative Study of Adhesion Force in Dentin of Three Cement Sealers  
BC-Sealer, AH-Plus and MTA Fillapex**

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Sealants based on calcium silicate have the ability to provide excellent sealing and bioactivity. Usually, it is recommended to be used in a single cone technique. The purpose of this study was to evaluate the adhesion forces of EndoSequence BC-Sealer® a bioceramic based premixed calcium silicate-phosphate (BC; Brasseler USA, Savannah, GA), compared with a cement-based MTA (Mineral Trioxide Aggregate) Fillapex® MTA (Angelus), and a cement based on epoxy resin AH-Plus® (DeTrey/Dentsply, Ballaigues, Switzerland). The objective of this project, is to compare adherence to dentin between filled teeth with single cone technique (CU) BC- Sealer®, lateral condensation (CL) MTA Fillapex® and AH-Plus®. For this, 45 uniradicular extracted teeth, palatal roots of upper molars and distal roots of lower molars with large and straight canals were used, they were randomly divided into 3 groups (n = 15), Group 1, BC-Sealer® CU; Group 2, MTA Fillapex® CL; Group 3, AH-Plus® CL. The roots were cut into specimens of 4 mm thick in the middle and apical thirds, leaving 30 specimens per group and the adhesion strength was measured using a standardized test compression. As a result, Group 1, BC- Sealer® CU had the bond strength statistically superior to Group 2, MTA Fillapex® CL; Group 3, AH-Plus® CL. Finally, it was concluded that BC-Sealer® CU material proved to be the best adhesion in both thirds of the root canal being significantly more noticeable in the middle third, compared to MTA Fillapex® CL, and AH-Plus® CL.



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**[ BIO-545 ] Analysis of Mechanical Properties of RBC Membrane Obtained by RT-AFAM**

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The scanning probe microscopy covers several related technologies for imaging and surface measurements to metric micro- and nano- scales to the level of molecules and groups of atoms. The development of this technology is already having profound effects that in many areas of science and engineering as in the case of medicine. The SPM techniques (for its acronym in English, Scanning Probe Microscopy) share the concept of exploration with a probe or tip very sharp (3-50 nm radius of curvature) on the surface of the object. The probe is formed by a flexible cantilever with a tip at its end, allowing to follow the surface profile. When the probe is moved in the vicinity of the sample being investigated, the interaction forces between the tip and the surface influence the movement of the probe. Several interactions may be studied in terms of the mechanics of the probe. Atomic Force Microscopy (AFM) measures the interaction force between the tip and the surface. The cantilever shaped probe can be dragged across the surface and can simultaneously vibrate as you go. Interaction strength depends on the nature of the sample, the probe geometry and the distance between them. In the study of biological systems using techniques (Atomic Force Microscopy, for its acronym in English) AFM, particularly, they have been carried out by conventional contact and tapping modes as allowing you to observe the topography of the sample. In this paper we will focus on conventional modes, as well as resonant methods, such as, acoustic atomic force microscopy (AFAM, atomic force acoustic microscopy) is a technique that is commonly used in conventional materials or hard coatings, in the present work used for the study of mechanical properties of erythrocyte membrane, nanofricción to determine blood cell adhesion through dry smear on glass and get the range of forces to be used, to avoid damaging the cell.



[ BIO-15 ] Glucose sensors based on carbon nanotubes

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New technologies are designing sensors of biologic material detectors with some types of carbon-rich substances. Previously organic materials were limited to a small group of materials but today it has expanded the use of synthetic substances whose composition is not only the carbon. The manufacture of such devices offers a lower cost and an analysis in real-time of a sample obtained from a few ml thanks to that we have an accurate answer on the biological material to be analyzed, GOx. We have made use of Multi Wall Carbon Nanotubes in this design.

The construction was carried out from a previous design based on a FET device architecture metal-insulator-semiconductor (MIS) which substrate is flexible by the use of thin films of polymer MEH-PPV and MWNT, gate and / or source-drain electrodes deposited on a flexible substrate PET film. MWCNTs were synthesized by the technique of microwave irradiation. A mixture of graphite powder and a bimetallic catalyst (CoMo). The devices were electrically characterized, characteristic behaviors of  $I_D$ - $V_{DS}$  are obtained with an interval 0 to 10V between source and drain, with gate voltage of 0, 5, 10, 15, 20, 25 V; finding an  $I_D$  of the order of  $\sim nA$ , for the case in which the device is added GOx, the linear behavior of the current is greater than observed in the device without glucose oxide; in conclusion this devices could be good candidates for their use in medicine as biosensors .



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**[ BIO-63 ] Biological and mechanical properties evaluation of glass ionomer cement added with quaternary ammonium compounds and silver nanoparticles.**

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**Introduction**

The glass ionomer cements are composed by silicate glass and polyacrylic acid. They have clinical applications in dentistry. These materials have undergone different modifications, it is important to evaluate if these modifications altered the other properties.

**Objective**

Determine whether the addition of cetrimide (C), cetylpyridinium chloride (CCP), benzalkonium chloride (CB) and silver nanoparticles (AgNP) at 1 and 2% modifies biocompatibility, compressive strength, surface roughness and micro hardness of glass ionomer cements Gc Fuji PLUS y Gc Fuji ORTHO LC.

**Materials and methods**

An experimental in vitro study was conducted. The biocompatibility of glass ionomer cements Gc Fuji PLUS y Gc Fuji ORTHO LC with C, CCP, CB y AgNP at 1 y 2% was evaluated in MA 104 cells by MTT assay and calcein AM. The compressive strength was evaluated in the universal testing machine. The surface roughness was determined by atomic force microscopy. The surface Vickers hardness was measured. Descriptive statistics were performed.

**Results**

The values for surface roughness ( $\mu\text{m}$ ), hardness (HV), cell viability (%) and compressive strength for GC Fuji ORTHO LC was 23.18, 54.19, 11.16, 23.4; with C 1% 29.82, 50.69, 10.95, 23.41; C 2% 15.43, 45.76, 10.37, 43.05; CB 1% 21.75, 51.41, 11.25, 31.94; CB 2% 22.18, 44.11, 9.41, 26.78; CCP 1% 29.77, 41.02, 9.6, 27.78; CCP 2% 17.35, 36.60, 10.62, 37.77; AgNP 1% 14.68, 50.98, 10.83, 64.02 and Ag NP 2% de 17.06, 33.22, 11.95, 52.01.

The values for surface roughness ( $\mu\text{m}$ ), hardness (HV), cell viability (%) and compressive strength for GC Fuji PLUS was 24.51, 31.17, 9.83, 66.31; with C 1% 14.29, 34.06, 9.75, 93.18; C 2% 20.98, 32.03, 10.83, 85.06; CB 1% 28.39, 28.55, 9.45, 62.46; CB 2% 24.87, 24.52, 10.37, 66.63; CCP 1% 24.19, 24.36, 9.79, 69.9; CCP 2% 22.04, 23.98, 11.25, 78.93; AgNP 1% 20.92, 47.40, 10.16, 106.39 and AgNP 2% 17.30, 36.46, 12.33, 91.27.

Staining with calcein AM exhibit cellular damage in all study groups.

**Conclusions**

The addition of quaternary ammonium compounds and silver nanoparticles modified the properties of glass ionomer cements.



[ BIO-192 ] Determination of loss of Ca<sup>+</sup> in fluorotic dentin and its effect on the microhardness, with pretreatment of NaOCl and self-etching techniques with silver nanoparticles incorporat.

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**Introduction:** The teeth with fluorosis to often need to be restored with composite resin because these have a higher esthetic demand, in addition to having higher recurrence of dental caries. Retention of restorations depends largely micromechanics obtained from the etching effect, however this etching causes demineralization dentinal substrate to achieve adequate retention and adhesion to dentin. Recurrent caries, is the main reason for failure of these restorations. For this reason, self-etching systems with antibacterial can flow in the dentinal tubules and kill residual bacteria in the tooth cavity, which can be beneficial to the inevitable formation of marginal microintervals through time. **Objective:** The aim of this study was to determine the Ca<sup>2+</sup> loss and its effect on microhardness of the fluorotic dentin following pretreatment of NaOCl and self-etching with silver nanoparticles. **Methods:** Thirty-six extracted human molar were selected and divided into four groups: Healthy (control) group, Mild (MI) group, Moderate (MO) group, and Severe (SE) group, according to the severity of dental fluorosis. The occlusal enamel and tooth root were removed to expose the flat dentin surface, which was longitudinally sectioned into three parts with a high-speed diamond bur under water spray. Samples were divided into three groups based on different self-etching techniques to apply. Each group was immersed in the test solutions for different self-etching techniques (1) Self-etching (Control), (2) NaOCl+SE, (3) NaOCl+SE with NAg, unt of Ca<sup>2+</sup> and Mg<sup>+</sup> release intuerdo a la tontacto en 5uml de primer autograbado )control)after which the same samples were subjected for the evaluation of amount of Ca<sup>2+</sup> release into the solution by Atomic Absorption Spectrophotometer. Then the samples were evaluated for the microhardness testing. **Results:** The results showing the effect of self-etching techniques on the healthy and fluorotic dentin desmineralization, also the affects the microhardness. The loss of Ca<sup>2+</sup> in each of the study groups was compared with the control group, having a greater amount of Ca<sup>2+</sup> in affected dentin with fluorosis when it is treated with the technique NaOCl+SE and a lost less of Ca<sup>2+</sup> when is treated with NaOCl+SE with NAg, similarly microhardness values are directly proportional to the loss of Ca<sup>2+</sup>. **Conclusions:** The desmineralization with NaOCl+SE self-etching technique leads to structural changes, as evidenced by reduction of dentin microhardness.



**[ BIO-219 ] Weathering studies of polypropylene carbon nanoparticles nanocomposites for solar water heaters**

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Polymeric materials are proved to be suitable materials for the fabrication of solar water heaters, where they are exposed to direct sunlight where the absorbed heat is transferred to the water,<sup>1,2</sup>. Thus, it is very important to protect the polymeric material against the photodegradation induced by UV light in outdoor conditions. Several UV light stabilizers from the family of benzophenones have been proved successfully in the past, however one of their disadvantages is the tendency to migrate reducing the protection over the time.<sup>3,4</sup> The addition of carbon nanoparticles has been proved successful to reduce dramatically the photodegradation of several polymers besides they are non-migrating additives, with the advantage of increasing thermal stability, mechanical strength, thermal and electrical conductivity.<sup>5</sup> In this study three types of carbon nanoparticles with different morphologies (i.e. carbon nanotubes CNT, graphene nanoplatelets GNP and carbon black CB) were mixed with a polyethylene resin in different concentrations of 1, 2.5 and 5% wt/wt of each nanoparticle. Specimens for tensile test were obtained from compression molding plaques and placed in an artificial weathering chamber QUV and irradiated with a wavelight of 340 nm with cycles of 16 h irradiation and 8 h condensation during 0, 250, 500, 750 and 1000 h exposure. The tensile test were performed in a universal testing machine, with 10 kN load force at a 50 mm/min rate, 5 specimens were tested for each exposure time. With the addition of only 1% wt/wt of nanoparticles the tensile strength and elongation at break of is retained after 1000 h of UV light exposure, this behavior is similar in nanocomposites with 2.5 and 5% wt/wt. Best results were obtained for the nanoparticles in the following order CB, GNP and CNT.



**[ BIO-278 ] Chemical characterization of Agave tequilana leaves as alternative of biomass for second generation biofuels production**

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Second generation biofuels are developing as an attractive alternative to fossil fuels with the aggregate value that does not compete with the food chain production, and therefore is not affecting the food security of a nation. Common source for second generation biofuels are the agricultural waste. The present work is focus on the agave leaf crop considered as a residue in the tequila industry which represents approximately 38 % of the total weight of the plant. The objective of this work is to study the chemical composition of the agave leaf crop residue and its viability as alternative of biomass for biofuel production. Percent chemical analysis, photocolometric, fourier transform infrared spectroscopy (FTIR) and high performance liquid chromatography (HPLC) was employed to study the system. We observed a high concentration of fermentable carbohydrates (~ 70 %); nonstructural (direct reducing sugars and reducing sugar polymers such as fructans) and structural (cellulose and hemicellulose) in the agave leaf. Sugars detected in agave leaf were fructose, glucose, sucrose and arabinose. As a result is found that the high concentration of sugars present in the agave leaf supports is potential as a valuable biomass for second generation biofuels. As an attractive alternative source of renewable energy and generate added value to this material waste.



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**[ BIO-284 ] Synthesis and thermal characterization of hydroxyapatite-collagen composite  
powders obtained by sol-gel technique**

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In this work, the synthesis and characterization of hydroxyapatite/collagen powders synthesized by the sol-gel route, using ultrasonic agitation is presented. The XRD diffractograms shows that the synthesized powders crystallize in the hexagonal phase and that the unitary cell parameters agree with those for synthetic hydroxyapatite. The FTIR and XEDS spectrums demonstrate that the obtained samples have a chemical composition corresponding to calcium-deficient hydroxyapatite. The analysis of nitrogen adsorption isotherms shows the effect of the collagen into the textural properties of the synthesized samples. Finally, by employing the frequency-resolved photoacoustic technique, the values of thermal effusivity of the synthesized powders have been determined and compared to the value corresponding to human mandibular bone tissue.



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**[ BIO-310 ] Development extrusion method for encapsulation of spermatozoa**

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With the encapsulation of sperm the protection of the cells from the environment is wanted by extending their life time out of female reproductive system, therefore enchasing the possibility of artificial insemination and cutting the cost in comparison to conventional insemination techniques. The encapsulation it's made by the extrusion technique, in which an sodium alginate solution mixed with an extensor and the sperm sample. Once mixed, a needle was used to create small drops that were dropped in a bath of barium chloride (BaCl<sub>2</sub>) by the time a cross-linking reaction occurred, trapping the sperm without apparently damaging their morphology, thus forming an spherical polymeric matrix, which gradually degrades due to hydration and mechanic forces of the uterus.



**[ BIO-320 ] Effect of drying temperature on Agave tequilana leaves: A pretreatment for releasing reducing sugars for biofuel production**

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The leaves of *Agave tequilana* Weber variety Blue represents a viable, inexpensive and renewable source of lignocellulosic biomass and fructans for the production of second generation biofuels. The objective was to study the effect of drying temperature on the release of reducing sugars for the agave leaves. It was found that with pretreatment-drying at 100 °C for  $30.5 \pm 1.0$  min had a maximum of the release of reducing sugars with a 66 % increment compared to 60 °C. An aqueous extract obtained from the powder of the leaves after drying did not show the presence of furfural and hydroxymethylfurfural compounds. Phenolic compounds were detected in order of  $120.8 \pm 1.0$  mg L<sup>-1</sup> below 1 g L<sup>-1</sup> reported to causes inhibition of the alcoholic fermentation. In addition the drying of the leaves also can be used as preservation of agave leaf for biomass storing. The results show that pretreatment-drying allow increase the release of reducing sugars, avoids thermal degradation and does not produce significant concentrations of fermentation inhibitors.



[ BIO-332 ] Layer-by-Layer Self-Assembled polyelectrolyte multilayer on maghemite nanoparticles

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In this study, we have studied functionalized magnetic nanoparticles (MNPs) by using the layer-by-layer self-assembly technique (LbL). The  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> nanoparticles were obtained by co-precipitation method. The TEM image of this nanoparticles shown spherical particles with an average particle size about 8.53 nm and standard deviation of 0.21. By X-ray diffraction we have obtained a maghemite phase. The surface charge of nanoparticles was modified with sodium poly(styrene sulfonate) and poly(allylamine hydrochloride) polyelectrolyte by using the layer-by-layer self-assembly technique. The assembly of anionic and cationic polyelectrolytes adsorbed on  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> nanoparticles (PSS/PAH multilayer -NPMs) leads to reversal the surface charge which was measured by the  $\zeta$ -potential. We have observed that the magnetization properties decreased little bit when the polyelectrolyte multilayer is adsorbed on the MNPs, where the saturation magnetization of the bare nanoparticles and PSS/PAH multilayer-nanoparticles found were 63.4 and 46.6 emu g<sup>-1</sup>, respectively.



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**[ BIO-368 ] Modified zinc nanoparticles encapsulated in a polymeric matrix**

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In order to improve the efficiency of encapsulation and compatibility between nanoparticles of zinc and polymers is necessary to make a surface modification with siloxane, after that their incorporation into the polymeric matrix is more easy. This modification increase surface area increasing nanoparticles and microorganisms interaction. Due nanoparticles of zinc oxide have antimicrobial capacities have been using to develop a variety of formulations that contain zinc oxide, the use of zinc oxide as microbial agent and solar protector has been studied and do not have side effects for humans, and its antimicrobial activity of zinc oxide of nanoparticles is better in comparison with zinc particles oxide when it dispersed into the polymer. Nanoparticles of zinc oxide have antimicrobial capacities and have been using to develop a variety of formulations that contain zinc oxide, the use of zinc oxide as microbial agent and solar protector has been studied and do not have side effects for humans. Studies have demonstrate nanoparticle are better than particles. One challenge using nanoparticles is get a good disperse into polymer. In order to improve the efficiency of encapsulation, disperse and compatibility between nanoparticles of zinc and polymers is necessary to make a surface modification with siloxane, after that their incorporation into the polymeric matrix is more easy. This modification increase surface area increasing nanoparticles and microorganisms interaction.



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**[ BIO-431 ] Extracellular matrix, Chitosan and PRP in tissue regeneration**

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Previously obtaining an extracellular matrix of the small intestine of a rat was presented. On this occasion the use of an extracellular matrix obtained starting from a pig's bladder with chitosan and PRP to support the regeneration of skin tissue occurs. IR spectroscopy to discard the presence of trace amounts of the reagents used and the presence of collagen tissue.

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**[ BIO-433 ] Proposed treatment in wound healing in diabetes patient using activating growth factors and chitosan**

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The objective of this study is to propose treatment for healing skin lesions in diabetic patients by the application of PRP in the damage area for activation of growth factors that help healing and chitosan as antibacterial means and protector. Healing results are presented injury in a patient. Chitosan and PRP was obtained by synthesizing in the laboratory

This work has been partially supported by projects VIEP-BUAP 2016, Mexico.



[ BIO-475 ] Synthesis, characterization and cytotoxic activity of europium-doped nanohydroxyapatite

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The main objective of this study was to synthesize europium-doped nanohydroxyapatite using a simple aqueous precipitation method and then characterize and impregnate selected samples with 5-fluorouracil in order to explore the properties and releasing capacity of this material. For this, calcium nitrate tetrahydrate, ammonium dihydrogen phosphate and europium nitrate, were used in aqueous solutions, respectively, as Ca, P and Eu precursors. The nanohydroxyapatite was doped with 3, 5, 10 and 20 wt.% of europium. The obtained samples were characterized after they were dried at 80 °C and hydrothermal treated at 120 °C by 2 h. The samples were analyzed by transmission electron microscopy, X-ray diffraction analysis, fourier transform infrared spectroscopy and, photoluminescence. Also, impregnation and release of 5-fluorouracil were assessed in PBS. The possible toxicity effects of the Eu concentration in the europium-doped nanohydroxyapatite samples were studied using viability assays on human fibroblasts cells (HGF-1) *in vitro*. After the characterization process we found that the sizes of the crystallites were about 10-70 nm with irregular morphology and present the phase corresponding to the JCPDS card 9-0432 for hydroxyapatite. The Eu-doped samples present photoluminescence lines at 590, 615, and 699 nm. The results of the toxicity experiments indicated that doped and undoped powders are biocompatible with fibroblasts cells. Hydroxyapatite sample doped with 5% of europium release almost 7 mg/L after 60 minutes in PBS and decrease the viability of HeLa cells after 24 h. The main objective of this study was to synthesize europium-doped nanohydroxyapatite using a simple aqueous precipitation method and then characterize and impregnate selected samples with 5-fluorouracil in order to explore the properties and releasing capacity of this material. For this, calcium nitrate tetrahydrate, ammonium dihydrogen phosphate and europium nitrate, were used in aqueous solutions, respectively, as Ca, P and Eu precursors. The nanohydroxyapatite was doped with 3, 5, 10 and 20 wt.% of europium. The obtained



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# **CHARACTERIZATION AND METROLOGY (CHM)**

**Chairman: Roberto Machorro (CNYN-UNAM)**



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[ CHM-223 ] Effects of Ar/CdS annealing on the optical properties of Cd<sub>2</sub>SnO<sub>4</sub> thin films  
deposited by sol-gel

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Roberto Sanginés<sup>1</sup>, Oscar Hernández-Utrera<sup>1</sup>, Rebeca Castanedo-Pérez<sup>2</sup>, Roberto Machorro-  
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The effects of Ar/CdS annealing on optical properties of polycrystalline Cd<sub>2</sub>SnO<sub>4</sub> thin films obtained by the dip-coating sol-gel technique are studied by spectroscopic ellipsometry (SE). The films were grown by sol-gel dip-coating technique using CdO and SnO<sub>2</sub> as precursor solutions. These are constituted of 7 coats and have an average thickness of ~260 nm. Each coating was deposited at a withdrawal speed of 2 cm/min, dried at 100°C for 1 hour and subsequently sintered at 550°C for 1 hour in air. After that the films were annealing in an Ar/CdS atmosphere at different temperatures (450°C, 500°C, 550°C and 600°C). The optical constants of the as-deposited and annealed films have been obtained in the wavelength range of 200–1700 nm by using spectroscopic ellipsometry at 45°, 55°, 65° and 75°. The optical model used for the films without annealing is composed by a dielectric layer for the quartz substrate follow by the CTO layer simulated by a Cauchy oscillator. The CTO film for the films annealed in AR/CdS is composed by two layers; the first is described by a Tauc-Lorentz oscillator, the second layer is an EMA consisting of Tauc-Lorenz Oscillator and void material. The surface roughness of the films was fixed according to the values obtained by AFM topography images for each film. It was found that as the temperature increase the values of *n* decreases. However, the values of *N* are comparable with those reported in the literature.



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[ CHM-241 ] Low thermal emissivity filters (Low-e) with Al deposited by magnetron sputtering technique

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Low-e coatings or low thermal emissivity filters, are used in industry for windows that do not let pass the heat. This type of windows are used in the housing market and self-sustainable buildings. They are characterized by high transmission about 80%, but a low thermal emissivity in the infrared (IR). Although there are different companies that trade, and there is little information scientifically. Currently, the cost of this type of windows is too high, this is due to the use of silver (Ag) in its construction. One of the disadvantages of Ag is that it tends to oxidize more easily, that is why a double glass vacuum assembly is needed to protect it. In this work the use of aluminum (Al), as a replacement of silver in Low-E coatings, is proposed. An advantage of using the Al is its similarity to the behavior of the silver, besides having a low transmittance in the infrared about 20%, and higher transmittance in the visible wavelength region. First theoretical designs and experimental results are shown with Low-e construction with 3 layers, and their optical characterization of aluminum (Al).



[ CHM-352 ] Ellipsometric optical characterization of nanolaminates grown by atomic layer deposition

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Ellipsometry is a powerful technique to characterize optical properties of materials. It is very sensitive, non invasive, non destructive, and relatively fast to do. Of course, it has also its limitations: high price, difficulties in the modeling to fit experimental data, available optical information to make the modeling. In this work we applied spectral ellipsometry to characterize nanolaminates, which are thin films composed of layers of different materials, characterized by having alternated individual layers of nanometer thickness. They are deposited via atomic layer deposition (ALD). This technique is used for depositing thin films with precise control of thickness down to atomic scale and the possibility to deposit several materials, including different oxides. ALD is a powerful tool to fabricate ultra thin, highly uniform and conformal material layers. The main contribution of this work is a discussion about the feasibility to applied ellipsometry to measure nanolayers. Do the optical refractive index has a meaning at this level? Our thickness measurements correlate very well with those of transmission electron microscopy (TEM); although, the sample preparation for TEM is tedious and time consuming. Aluminium and Yttrium oxide multilayer were coated on a silicon wafer by ALD. Effective medium approximation is used to fit ellipsometric parameters, from which the evolution of refractive index relative to Al<sub>2</sub>O<sub>3</sub>/Y<sub>2</sub>O<sub>3</sub> thickness combination is obtained, then the gap of the multilayer is drawn.

### Acknowledgements

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[ CHM-379 ] Determination of thermal conductivity using the scanning thermal microscopy module (S<sub>Th</sub>M) in AFM

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Experimental measurement of thermal conductivity is a complex process, it often requires an isolated system and preferably under vacuum, however to achieve these conditions is typically difficult, and the best measurements are obtained with 90-95% accuracy. The complexity increases when we descend to micrometer scales, given the fact that to generate favorable experimental conditions is even more complicated than macroscopic scale. Appropriate equipment for this task is the atomic force microscope (AFM); this tool allows to obtain images of individual atoms, this includes topography imaging, capacitance, static load, magnetic, etc. Thermal analysis can be performed by AFM module by scanning thermal microscopy (S<sub>Th</sub>M). The S<sub>Th</sub>M module is a tool that has been developed for thermal measurements of microscale and nanoscale materials with micro and sub-micro structures, such as powders, grains, films, etc. In this work, the thermal scanning microscopy module (S<sub>Th</sub>M) was evaluated as a means to estimate quantitative values of thermal conductivity, for this, a heating point was performed by DC current in various representative materials (gold, glass, graphite and epoxy resin), and the signal obtained was adjusted by the numerical solution of the diffusion equation considering thermal heat loss by convection and thermal modeling as a Gaussian pulse source. Similarly, thermal mapping of representative materials were performed. By the results obtained it can be concluded that the use of S<sub>Th</sub>M module is suitable for estimating thermal conductivity by a configuration in which local heating is induced by the DC power supply and is suitable for conductive materials, and not for materials with low thermal conductivity.

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**[ CHM-434 ] Synthesis of TiN hard coatings using magnetron sputtering and their  
characterization by surface analysis techniques.**

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Currently, there is the problem of developing measurement standards for surface metrology and the incipient nanometrology in Mexico, because of the difficulty of synthesizing or manufacturing materials and devices that achieve the necessary homogeneity for good evaluation, as well as the difficulty in equipment for the characterization of these materials for further certification, therefore, this project is part of the global development trends accelerated in thin films and devices for its enormous potential in technological applications in materials and to develop benchmarks for measuring physicochemical properties such as thickness, roughness, chemical composition, optical and electronic properties. Hence, the synthesis of materials by magnetron sputtering for control at the atomic level is a strong candidate for producing surfaces with high homogeneity.

On the other hand, there has been a growing interest in hard TiN coatings due to their physico-chemical properties that have allowed them to be used as functional coatings in cutting tools, as well as in electrical applications or as anti-corrosion coatings, offering extremely high hardness, fracture toughness with excellent resistance to oxidation and high temperature corrosion. In this study, the synthesis of TiN films and characterization of their morphological, chemical and hardness properties by different surface analysis techniques are presented.



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**[ CHM-514 ] The unsolved physics behind X-ray photoelectron spectroscopy**

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X-ray photoelectron spectroscopy (XPS) is a very popular surface characterization technique; it is currently mentioned in excess of 10,000 publications every year. This is not surprising since, through XPS, it is possible to obtain the oxidation state of the elements present in a surface together with its composition. In addition, if angle resolved is employed (ARXPS), it is also possible to assess the structure of multilayered nanofilms.

However, there are important basic— and practical— issues about photoelectron-spectroscopy still unresolved, mostly about its baseline or background. Part of the background signal is well understood as due to electron losses caused by scattering with plasmons (mostly) and other electrons (i.e., electronic transitions). This is known as the Tougaard background (a brief description will be provided in this talk). Conversely, the physical origin of a large fraction of the signal, known as the Shirley background, remains unknown.



[ CHM-516 ] Study of the spectral behavior of a photoelectric converter and evaluation of performance-enhancing parameters

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A photoelectric converter (PEC) is a device that can transform light energy into electrical energy through the photoelectric effect. Recent studies have shown the feasibility of direct energy conversion using these devices [1]. In particular, a MOS structure made of silicon and aluminum electrodes has shown that the light from an incandescent lamp can be transformed into electricity and the electron flow is made of the semiconductor material toward the aluminum electrode; that is, the semiconductor material acts as emitter and the aluminum electrode as collector. The photoelectric effect in this structure has also been tested with solar radiation. In both cases the experiments were performed with white light and full spectral content. The development of such structures requires from the theoretical point of view; study the effect of the work function of the material and the spectral response of the device. The theoretical model presented by Perez and Moreno said that the reduction of the work function in both electrodes substantially improves the performance of the PEC [1, 2]. This article describes the experimental results obtained in the PEC after applying different types of light and its comparison with theoretical studies obtained by the proposed theoretical model are presented.

1.-L. A. Moreno Coria, "Study of the photoelectric effect in a MOS structure and its possible application as an electric generator", PhD Thesis, Graduate Semiconductor Devices, BUAP, 2015, in spanish.

2.-J.G. Perez Luna, "Development of an AC thermionic generator" PhD Thesis, DEPFI, UNAM, 2001, in spanish.



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**[ CHM-531 ] Deposit and characterization of hydrogenated amorphous silicon carbide films for the fabrication to ultraviolet light sensors.**

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The majority of ultraviolet radiation that come to the earth is absorbed in the atmosphere, such radiation is harmful to the human body, but some of this radiation cross the atmosphere and reaches to the Earth's surface. Others sources of uv radiation are employed in measuring instruments, water purification systems and in medical applications. Therefore, it is necessary measuring this radiation through of portable and flexible devices.

The objective of this work is to develop a highly efficient uv sensor that satisfies the requirements of portability and flexibility. The device employed as sensor will be a Schottky diode with sensible layer of a-SiC:H. The feature characteristic of a-SiC:H is its wide optical gap. For this reason a-SiC:H films were studied and their Uv absorption characteristics have been improved with the incorporation of phosphorus as dopant. Such characteristics are conductivity and photocurrent. Also it shows the link between the optical characteristics and the dopant content. All the films were deposited in RF PECVD at 100°C, this will allow us fabricate devices on flexible substrates.



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**[ CHM-559 ] Improvement of resistance to mechanical compression in Portland cement mortars induced by the addition of poly-hydroxy-indole**

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Morphological and microstructural evolution of cementitious phases was analyzed due to the nanometric dispersion of hydroxy-poly-indole (HPI) in mortars of Portland cement and its influence on developing of mechanical properties. The behavior of the addition of 0.8, 1.6, 2.4, 3.2 and 4% of HPI in specimens of ordinary Portland cement with ratios of 0.4, 0.6, 0.8 and 1.0 water/cement for periods of 7, 14, 28, 90 and 360 days was analyzed. The resulting samples were tested in a universal machine and was observed that mixtures with better resistance to the mechanical stress had 1.6 and 3.2 percent of HPI in the initial composition for a ratio of 0.8 water / cement. The results of the microstructural characterization by X-ray Diffraction and images of Scanning electron microscopy allow infer the increase of resistance to the strength with a better development of cementitious phases due to a optimal retention of water in the hydration process and to the inhibition of the formation of secondary ettringite as a responsible of the structural weakening. Analysis by infrared spectroscopy to specimens of mortars confirmed the persistence of hydration water for samples containing higher proportions of HPI compared with specimens of reference elaborated using only water.



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**[ CHM-566 ] Cyclic voltammetric and first principles studies of ferrocene modified carbon paste electrodes.**

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Carbon paste electrodes are usually modified from redox mediators like ferrocene. Understanding role of mediators at the electrode interface is very important and interesting in surface electroanalysis. Usually electron transfer of redox mediators are affected by surrounding environment. In this work, we have used Triton X-100 (TX-100) as surrounding environment. We have used Quantum chemical calculation based on the density functional theory to support experimental observations. Mediated electron transfer process of ferrocene was proved by analytical Fukui functions. We are able to explain the cyclic voltammetric observations based on the Quantum calculations. In the current work both Quantum and cyclic voltammetric results are in well agreement with each other.



[ CHM-25 ] CNTs-TiO<sub>2</sub> nanotubes via ALD: influence of sidewall functionalization and nitrogen doping.

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One of the most suitable techniques for synthesizing TiO<sub>2</sub> nanotubes are via CNT template approach. However, different types of chemical groups attached to the CNT surface or dopants can affect the nucleation and subsequent growth of TiO<sub>2</sub> on the template. In this work chemically functionalized multi-walled carbon nanotube with various chemical groups such as COOH, OH and N<sub>2</sub> doped were used. A detailed characterization of the CNT functionalized is presented. Then, by means of atomic layer deposition (ALD) technique, TiO<sub>2</sub> was grown on MWCNT. The effects of different functionalization groups on the nucleation process of Titania were systematically studied using transmission electron microscopy (TEM). Direct observation revealed grain-like growth of the Titania over the functionalized CNTs. On the other hand, N<sub>2</sub> doped CNTs were coated in a more conformal and controlled manner.

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**[ CHM-180 ] Optical characterization of Titanium Dioxide TiO<sub>2</sub> by Spectral Correlation technique in transmission and Backscattering configuration.**

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We present the optical characterization of thin films of Titanium Dioxide (TiO<sub>2</sub>) in transmission configuration. The technique of spectral correlation in frequency domain is employed to obtain the main optical properties in real time such as the diffusion coefficient and the absorption length via of photons scattered in a random turbid medium. We employed the photon diffusion approximation theory, and using the correlation function fitting. Using simulation algorithm for generating a sequence of correlated speckle patterns we recover the results obtain in the experiment.

We show a theoretical analysis developed in the backscattering configuration. We employed a Teflon slab to corroborate the theoretical and experimental results.



[ CHM-254 ] Mechanical properties of TaN<sub>x</sub>/TaC<sub>y</sub> stack coatings

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In this work, TaN<sub>x</sub>, TaC<sub>y</sub> and TaN<sub>x</sub>/TaC<sub>y</sub> stack coatings were synthesized by sputtering. The coatings were characterized by Auger electron spectroscopy, X-ray diffraction, transmission electron microscopy, and nanoindentation. In the TaN<sub>x</sub> coatings the maximum content of nitrogen was  $x = 1.34$  when the sample was synthesized at room temperature (*RT*), while for the TaN<sub>x</sub> coatings synthesized at 500 °C the maximum content of nitrogen was  $x = 0.53$ . The maximum content of carbon in the TaC<sub>y</sub> coating was  $y = 1.26$  when the samples were synthesized at *RT*. When the substrate temperature was increasing up to 500 °C during the synthesis of the TaC<sub>y</sub> coating, the content of carbon decreased to  $y = 0.56$ . All the samples synthesized at 500 °C of substrate temperature showed cubic structure. The results of nanoindentation showed that the highest values of hardness ( $H$ ) and reduced elastic modulus ( $E_r$ ) for TaN<sub>x</sub> coating were  $H = 38.0$  GPa and  $E_r = 390$  GPa; for TaC<sub>y</sub> coating were  $H = 30$  GPa and  $E_r = 260$  GPa. When those materials (TaN<sub>x</sub> and TaC<sub>y</sub>) were utilized for synthesizing TaN<sub>x</sub>/TaC<sub>y</sub> stack coatings, the highest values were  $H = 45.7$  GPa and  $E_r = 477$  GPa, which were higher than the values obtained for the coatings made of a single layer.

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[ CHM-290 ] Kinetics and mechanical characterization of AISI 4340 steel borided by using a mixture of own formulation

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This study evaluates the growth kinetics of hard coatings FeB/Fe<sub>2</sub>B type, on the surface of a AISI 4340 steel. The coatings were achieved by using an own boriding mixture consisting of 70% w. of SiC, 20 % w. of B<sub>4</sub>C and 10 % w. of KBF<sub>4</sub>. The study evaluates the evolution of the layers as a function of the treatment time which was established at 2, 4 and 6 h. The temperature of treatment was 850 °C, and was constant for the three times. Also, the behavior of the layers was evaluated by means of a profile of micro hardness Vickers from the surface to the substrate, to compare the results with those presented in literature attained with other boriding source. The optical examination showed a compact and homogenous layer consisting mainly of Fe<sub>2</sub>B phase, especially in the samples treated during 2 h. The morphology of the layers was of saw-toothed shape, consistent with those expected for this kind of steel. The total thickness of the layers was in the range of 29.842 ± 4.7µm to 53.09 ± 8.39 µm. The hardness values were in the range of 1291.34 ± 98.28 to 1429.7 ± 66.25 HV, which indicates that the boriding source applied in the process can be an alternative to generate boriding layers.

**Keywords:** boriding process, growth kinetics, own mixture



[ CHM-292 ] Characterization of hard layers FeB/Fe<sub>2</sub>B type obtained on the surface of a AISI H13 steel by using a mixture of own formulation

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This research assesses the growth kinetics of hard layers FeB/Fe<sub>2</sub>B achieved by boron diffusion. The layers were obtained by powder-pack boriding process using an own mixture consisting of 70 % wt. SiC, 20 % wt. B<sub>4</sub>C and 10 % wt. KBF<sub>4</sub>. The process was conducted on AISI H13 steel samples at constant time of 2 h. The treatment temperature was established in 850, 900 and 950 °C. The growth kinetics was established as a function of the treatment temperature. The hardness of the layers was evaluated by Vickers microindentation. Optical examination of the samples revealed the presence of a biphasic layer type FeB/Fe<sub>2</sub>B on the samples treated at 950 °C, while the samples exposed to 850 °C exhibited only small isolated zones of FeB phase. The morphology of the layer was similar to those reported in different studies where commercial boriding sources were used. The results show that the thickness of the layers is highly dependent on the temperature process as the thickness achieved to 850 °C was 8.507 ± 1.19 μm in average while at 950 °C the thicknesses of the layer was 28.66 ± 4.18 μm in average. The hardness values of the layers were estimated in the range of 1238-1576 HV, which are consistent with those reported in literature.

**Keywords:** boriding process, growth kinetics, own mixture



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[ CHM-313 ] Study on patents of surface treatment gasoline injectors

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**Abstract:** This work present a study on boride coatings on fuel injectors AISI 304. This paper will give a tool in the automotive engineering area; focused on increment surface properties of a fuel injector by thermo-chemical treatment whit boron atoms, by process dehydrated boron paste, increases the adhesion of the boron layer on the surface of steel by gradients hardness from on surf; obtaining boron layer whit an appropriate toughness and mechanical properties on base material, and decreasing delamination of the surface layers during different mechanical loads. The process initially forming boride layers on with a steel AISI 304 (fuel injector). The surface treatment on nozzle and formation hard layers type FeB and Fe<sub>2</sub>B; are obtained whit temperature range of 1223 K and 1273 K using exposure times of half hour to one hour. Boride layers formed on the surface characterization and are obtained by the method X-ray diffraction (XRD), the distribution of alloying elements were detected by energy dispersive spectrometry (EDS) on surface, evaluating the adhesion of the layers it is determined by the technique Rockwell-C. The hardness and Young's modulus of the layer was also studied by nanoindentation technique with a load of 200 mN.

**Keywords:** patent, surface hardening, boronizing, fuel injection nozzle.



[ CHM-321 ] Thermal characterization on porous silicon

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Samples of porous silicon (PS) were prepared by electrochemical anodic etching on n-type phosphorus doped, (100)-oriented crystalline silicon (CS) wafer (thickness: 530  $\mu\text{m}$ ) and resistivity of 1-5  $\Omega\text{cm}$ , as well as, on p type boron doped (111)-oriented crystalline silicon (CS) wafer (thickness: 430  $\mu\text{m}$ ) and resistivity of 120-230  $\Omega\text{cm}$ . It was used a constant current density of 40  $\text{mA}/\text{cm}^2$  in all cases and a HF (40%) solution. The porous layers were prepared with etching times of 5, 10, 15, 20, and 30 minutes. Infrared photothermal radiometry (IR-PTR) technique was used to obtain the photothermal response in the PS samples as a function of the etching time and photoacoustic spectroscopy (PAS) was used to obtain the corresponding optical absorption spectra.

Photothermal (PT) techniques have proved to be powerful to study the optical, electronic and thermal properties of various samples in a noncontact and nondestructive way without particular sample treatment. In particular, Photothermal Radiometry (PTR) originally proposed by Nordal and Kanstad (1979) is one of the most important techniques because its detection method involves non-destructive, non-contact remote sensing.

Our results show that the photothermal response depends of the etching time, finding the highest optical absorption capacity in the PS samples elaborated with 20 minutes of etching time in the electrochemical etching process, which is consistent with their corresponding optical absorption spectra.

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**[ CHM-423 ] Piezoresponse Force Microscopy: A simple method to obtain phase switching and amplitude butterfly loops**

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A simple low cost procedure to obtain the electromechanical response of non-conductive materials is presented. The technique makes use of amplitude modulated voltage pulses in an atomic force microscope with standard configuration. Material response obtained as signals of amplitude and phase from a lock-in amplifier as well as the input signal introduced to the conductive tip are stored in the AFM images which act like a data acquisition card. The acquired data are processed with a program that eliminates the necessity of voltage pulses with constant time-widths, enabling the system to study the domain stability in the case of piezo-ferroelectric materials as well as relaxation times in electrochemical phenomena. Additionally, a diagram of an electronic circuit for the construction of a signal adder that produces the excitation signal needed for the execution of this procedure is presented. All the codes for the implementation of the technique are available in free-format via our web page.



[ CHM-425 ] Electrical measurement for Schottky junction of n-ZnO:Al by means of Atomic Force Microscopy

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In this work, by means of the conductive Atomic Force Microscopy (C-AFM), the electrical characterization of n-ZnO:Al is carried out. A Pt-Ir conductive probe was used to form the Schottky nano-contact with the thin film surface. The electrical I-V curve was measured in order to determine the Schottky barrier height ( $\Phi_B$ ). The  $\Phi_B$  value was estimated between 0.35 to 1.1 eV fitting the I-V experimental data to the Schottky model. The measurements of the Schottky barrier height got by means of C-AFM were compared with measurements got by other researchers.



[ CHM-467 ] Synthesis and characterization of three-dimensional opal/Fe<sub>3</sub>O<sub>4</sub> magnetic photonic crystals

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Magnetic and optical of three-dimensional magnetic photonic crystals (MPCs), based on an SiO<sub>2</sub> artificial opals infiltrated with 0(M0), 1.34(M1), 2.03(M2) and 24.4(M3) wt % Fe<sub>3</sub>O<sub>4</sub> nanoparticles were investigated. Synthesis of SiO<sub>2</sub> microspheres was performed by the methods of Stöber, while synthesis of Fe<sub>3</sub>O<sub>4</sub> nanoparticles were prepared by co-precipitation of ferric and ferrous salts under the presence of N<sub>2</sub> gas. Trimethylammonium hydroxide has been used how surfactant to prevent agglomerations. Scanning electron microscopy (SEM), X-ray diffraction (XRD), Surface-enhanced Raman scattering (SERS), and Vibration sample magnetometer (VSM) were used to study the physical of the samples. The magnetization curves (M-H) at 300 and 2 K revealed that the magnetic properties of the Fe<sub>3</sub>O<sub>4</sub> nanoparticles increase with a symmetric hysteresis loop, suggesting the superparamagnetic Fe<sub>3</sub>O<sub>4</sub> nanoparticles switched to ferromagnetic nanoparticles in the samples. The reflectance spectroscopy and Kubelka-Munk theory were applied to determine the energy band gap of the samples. From Tauc plots the energy band gap E<sub>g</sub> is found to be 1.97 eV for bare Fe<sub>3</sub>O<sub>4</sub> nanoparticles, while it is 3.98 eV, 3.44 eV, 3.04 eV, 2.96 eV for samples M0, M1, M2 and M3, respectively.



[ CHM-496 ] Mechanical and Optical Properties of Coatings obtained from Functionalized Nanoparticles for Self Cleaning Applications

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Modification of materials is of great importance, and the modification of the material surface is one of the main strategies. Moreover, when the surface is modified, it brings new characteristics from the initial state and these changes are possible through different mechanisms, and one of them is the functionalization. This process, brings new features and properties to a material by changing the surface chemistry of the material, generating a novel material [1-3]. In this work is described the functionalization of metallic oxides nanoparticles with a coupling agent, after the functionalization, the nanoparticles systems were dispersed in a ethanol-water media, followed by addition of acrylic acid acting as the polymer matrix. Coatings were casted in different concentration on glass substrates by means of spin coating technique. The nanocomposite was characterized by water contact angle, SEM, UV-Vis as well as mechanical properties of the coating.

Keywords: functionalization, nanoparticles, self cleaning, nanocomposite.

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[ CHM-541 ] Microstructural properties of alpha-amylase enzyme immobilized on mesoporous SBA15.

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The successful use of biological catalysts in industrial processes is that enzymes have certain characteristics which give them advantages over the use of chemical catalysts, as is the high catalytic activity of the enzymes, enzyme-substrate specificity and require moderate conditions of temperature and pressure, the latter being of great importance as it involves a decrease in the cost of the process where they are used. Amylases today constitute the most important group of enzymes in biotechnology because of its wide area of application, including most industrial application and greater market volume are alpha-amylase and glucoamylase. Alpha-amylase enzyme catalyzes the hydrolysis of random alpha-1,4 glycosidic bonds in the central region of the amylose and amylopectin chain except near molecules branch, and obtaining as result maltose oligosaccharides of different sizes.

This paper focuses on the study of the immobilization of the alpha-amylase from *Bacillus licheniformis* in a mesoporous support siliceous SBA-15 type, this material was characterized by nitrogen physisorption. It was noted that the textural properties as ASE, VP and DP in SBA-15 enzyme indicating decreased adsorption of the enzyme on the support. The optimum pH for immobilization of  $\alpha$ -amylase in SBA-15 is 5. The kinetic parameters obtained are  $V_{max}$  reaction was for the free enzyme with a value of 0.0093 (g / L) s while  $K_m$  increases significantly for immobilized enzyme in SBA-15.



[ CHM-550 ] Remote-plasma nitridation of hafnium oxide thin films grown by ALD

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Hafnium oxide thin films are nowadays employed in CMOS devices. The nitridation of HfO<sub>2</sub> films is used to prevent crystallization during annealing [1]. The thickness and composition of HfO<sub>x</sub>N<sub>y</sub> films is susceptible to the processing parameters. In this work we present an study of HfO<sub>2</sub> nitridation through remote plasma.

P-type crystalline silicon substrates were cleaned with a RCA I-II process. The oxide films were grown with an ALD Savannah Cambridge 100 using tetrakis (dimethylamino) hafnium (TDMA-Hf) as Hf precursor and water (Type I) as the oxidant precursor. The reactor was set to 250°C with an ultra high purity N<sub>2</sub> flow (20 sccm) as purging gas. The exposure time to TDMA-Hf and water were 0.08s and 0.04s per cycle respectively, resulting a growth rate of 1 Å per cycle [2]. The characterization of the film was done through ARXPS with an instrument assembled by Intercovamex equipped with an XR5 monochromatic X-ray source (TermoFisher-VG). To enhance resolution, we employed 10 eV as the pass energy of the spectrometer.

The analysis was done employing the multilayer model (MLM) [3]. It was possible to identify the formation of an oxygen-rich hafnium silicate ~9 Å interface (Hf<sub>0.81</sub>Si<sub>0.18</sub>O<sub>2.46</sub>N<sub>0.26</sub>) and an hafnium oxide layer with almost no nitrogen. This indicates that nitridation is preferential in regions where silicon is present.

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**[ CHM-576 ] Terahertz transmission spectroscopy of tequila and red wine fingerprints**

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THz technologies is a very attractive research field that make use of frequencies of the electromagnetic spectra in the range from 1 to 0.03mm wavelength. This range is also known as the "gap THz", for which there are very few natural radiation sources, and it has also been undoubtedly the range that presented historically greater technological challenge for both emission and detection. The importance for the development of these technologies lies in the ability of these waves to penetrate almost everything except high density materials, some few metals and water. This region also shares a basic property with infrared and microwave, its radiation is nonionizing, i.e., does not carry enough quantum energy to remove an electron from a molecule. Instead of generating ions, energy is barely enough to promote electrons from a low energy state to a higher state. For biological materials, the exposure to THz radiation, will not cause them any injury, contrary to what happens with X-rays exposure. This study presents the use of THz radiation to characterize the organic fingerprint of Tequila and red wine using a transmission spectrometer in the THz range of 200 GHz to 1600GHz. Organic fingerprint from different Tequila brands and types were acquired by distillation successfully removing all ethylic alcohol (which is a highly absorbent substance in the THz band). Then the organic residual compounds were deposited onto a polystyrene cover slip using spinning techniques. Finally, THz spectra of deposits was extracted for analysis and characterization. Rotational and vibrational modes of many molecules contained in the organic fingerprint are distributed in the THz band. These modes can be observed as absorption peaks in the spectrum of THz and using the location and extent of these absorption peaks we were able to identify the composition molecules.

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# **Luminescence Phenomena: Materials and Applications (LPM)**

**Chairmen: Ciro Falcony: (Cinvestav-IPN)**

**Giancarlo C. Righini: (Centro Fermi)**



[ LPM-56 ] Zinc phosphate glasses doped yttrium-europium oxide, a luminescence study

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Zinc phosphate glasses doped with yttrium-europium oxide, were obtained by melting at 1100 °C; suitable precursors of these glasses quantities was grinded mechanically and dried at 400 °C for 2hrs, then the temperature was raised to 800 °C for 2hrs again, finally the temperature was raised at 1100 °C for 3hrs until a liquid is achieved, this liquid is emptied in a copper block to produce a thermal shock and observe the formation of a glass; a final heat treatment at 300°C for 12hrs is practiced.

Luminescent studies were conducted in these glasses, it is observable, that when excited with  $\lambda_{exc} = 396\text{nm}$  are present the  $^5D_0$  to  $^7F_1$ ,  $^7F_2$ ,  $^7F_3$  y  $^7F_4$  transitions in 590, 616, 650, and 697 nm; the main emission is achieved at 616 nm and a high red light emission is observable at naked eye, due to the presence of europium ions. Absorption spectra, transmission and reflectance are obtained; these glasses are transparent in the region of 400 nm to 1100 nm UV; XRD indicates that samples are amorphous; the emission spectra of these glasses were doped with different amounts of yttrium-europium oxide; they depend on the amount of dopant.

The luminescent properties of  $Y_2O_3:Eu^{3+}$  powders have been studied, luminescent  $Y_2O_3:Eu^{3+}$  polycrystalline powders were synthesized by a simple evaporation method. The photoluminescence and cathodoluminescence emission spectra these samples show, luminescence peaks associated with transitions within the electronic energy levels of  $Eu^{3+}$  ions. The dominant peak is at 612nm corresponding to the  $^5D_0$  to  $^7F_2$  transition and present  $^5D_0$  to  $^7F_1$ ,  $^7F_2$ ,  $^7F_3$  y  $^7F_4$  transitions in 590, 616, 650, and 697 nm, when excited with  $\lambda_{exc} = 260\text{ nm}$  and  $\lambda_{exc} = 396$  at room temperature. The intensity luminescence  $Y_2O_3:Eu^{3+}$  powders with different dopant concentrations,  $Eu^{3+}$  ion dependent percentage, finding the optimal concentration is 17 mol%.

XRD of powders  $Y_2O_3:Eu^{3+}$  show these correspond to space group: Ia-3(206), with Cell: 10.5961 10.5961 10.5961 90.000 90.000 90.000, Volume: 1189.702 and Crystal System Cubic; CSD: 86814(ICSD) (No: 01-089-5592); these powders were evaporated at 200 °C and then calcined for two hours at 1100°C. EDS analysis shows that the corresponding  $Y_2O_3:Eu^{3+}$  powders, showing that the achieved yttrium is stoichiometric according to general  $Y_2O_3$  formula. According to the results of the photoluminescence of these powders  $Y_2O_3:Eu^{3+}$ , to excite  $\lambda_{exc} = 396\text{nm}$  have the energy required for luminescence is less and therefore can obtain low-cost LEDs for red light; so it can be considered that this type of compound is a good candidate to have red light and its preparation is simple and inexpensive.



[ LPM-222 ] Carbon-induced optical quenching on nitride-based high electron mobility transistor

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Intensive efforts have been made to improve electrical performance of GaN-based HEMT transistors but it has not been identified factors that limit the breakdown voltage, electrical mobility and lead to the early device failure[1]. Incorporation of impurities, point defects, dislocations and grain boundaries formed at semiconductor layers of the device are good candidates to explain their electrical limitations. This work was focused to study the effect of non-intentional carbon concentration on optical recombination processes in AlGa<sub>N</sub> buffer layer and GaN channel of HEMT transistors grown by MOCVD technique. Samples were grown by changing growth temperature from 950 to 1040 °C, which reduced carbon concentration from  $8 \times 10^{19}$  to  $5 \times 10^{17}$  atoms/cm<sup>3</sup> (measured by SIMS). Low temperature photoluminescence (PL) spectra of AlGa<sub>N</sub> buffer layers where show yellow band(YL), blue band(BL) and near band emissions (NBE), whose relative intensities are well related with dislocation density and carbon incorporation. Optical quenching phenomena on YL, BL and NBE was observed as temperature increases and NBE peak position suffers a redshift as carbon concentration decreases [2]. In samples with high carbon concentration ( $8 \times 10^{19}$  and  $2 \times 10^{19}$  atoms/cm<sup>3</sup>) only carrier redistribution within localized state was observed, while for samples with lowest carbon concentration ( $5 \times 10^{17}$  to  $3 \times 10^{18}$  atoms/cm<sup>3</sup>) two optical quenching process were identified (carrier redistribution and delocalization). Carrier delocalization was confirmed by yellow-band intensity increase when this process was thermally activated at 150 K. Results are explained in terms of carbon-generated localized states with different depth and aluminum fluctuations within AlGa<sub>N</sub> buffer layers. High-resolution PL spectra of C-doped layers show free A exciton and acceptor bound-exciton whose intensities are correlated with crystal quality and carbon concentration. Complementary analysis will be presented for GaN channel of HEMT transistors.



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[ LPM-253 ] Luminescent properties of bicomponent polyester/perylene fibers

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Luminescent properties are very important in several applications mainly as a labeling or watermark for clothing and apparel, also in high value accessories for recognized brands. Due the growing interest to develop a simple and fast check up system that responds under external stimuli and remains non-visible all the time, fibers made of polyester/perylene were obtained and the photoluminescent properties studied for several fiber configurations. PET and perylene were melt mixed to obtain a composite with 1% wt/wt of perylene, then successive dilutions with 0.1, 0.01 and 0.001% wt/wt of perylene were obtained and their photoluminescent properties were evaluated. The sample with 0.1% wt/wt of perylene was choose to fabricate multi-filaments by a melt spinning process with different configurations i.e., the perylene composite was located in the core and PET in the sheath, in other configuration the core was of PET and the sheath of perylene composite with different proportions 50/50 and 75/25, for comparison purposes a 100% perylene composite fiber was obtained. A draw ratio 5:1 was employed in all cases. Then the multi-filaments were braided to obtain a thread and used to weaving a square of 1 inch over a cotton fabric and their photoluminescent properties were evaluated again. In order to quantify the emission of perylene composite with different contents, fluorescent spectra was evaluated and show a typical emission band for perylene located around 529 nm and a slight displacement to 539 nm as the content increases. And the maxima emission was for the sample with 0.1% wt/wt. When the perylene composites were transformed into fibers, the same behavior was observed and it is enhanced for fibers where the composite was located in the sheath. Photoluminescent quantum yield was evaluated for selected fibers weaving on cotton fabric and the best result was for the sample core/sheath (50/50) with 0.1% wt/wt of perylene located in the sheath.



**[ LPM-259 ] Luminescent and structural properties of microwave synthesized HfO<sub>2</sub> and HfO<sub>2</sub>:Eu<sup>3+</sup> nano-powders**

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HfO<sub>2</sub> and HfO<sub>2</sub>:Eu<sup>3+</sup> nanopowders were synthesized in a microwave reactor at temperatures in the range from 180 to 190 °C. Hafnium chloride (HfCl<sub>4</sub>) and hydrated europium chloride (EuCl<sub>3</sub>·6H<sub>2</sub>O) were employed as precursors and Ethanol and desionized water as solvents. Different ratios of Europium (Eu<sup>3+</sup>) to Hafnium (Hf); (Eu<sup>3+</sup>/Hf) \* 100), were considered. The synthesis of the powders lasted about 25 minutes. The structural and luminescent characteristics of the powders were determined by XRD, SEM, TEM, EDS, and PL measurements. The powders resulted polycrystalline with the HfO<sub>2</sub> monoclinic phase, independently of temperature of synthesis or the amount of europium in solution. The average size of the crystallites resulted in the nanometer range (4 - 7 nm). Photoluminescence spectroscopy of the powders revealed the incorporation of Eu<sup>3+</sup> into the monoclinic crystalline structure of HfO<sub>2</sub>, showing a maximum PL emission in powders synthesized from solution with 10 % of europium. A high PL emission was also shown in intrinsic (undoped) HfO<sub>2</sub>. The excitation and emission PL spectra, as well as the corresponding color of green to red in chromaticity diagram as function of the europium concentration, suggest that the nanopowders might have potential applications as highly efficient red emission materials considered in the White Led's technology.



[ LPM-271 ] High-pressure photoluminescence spectroscopy of LiNbO<sub>3</sub>:Cr<sup>3+</sup>; W<sup>4+</sup>. Pressure dependence of spectroscopic parameters and local structure of Cr<sup>3+</sup>

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Room temperature photoluminescence spectra of congruent LiNbO<sub>3</sub>:Cr<sup>3+</sup>; W<sup>4+</sup> were studied. The crystals have been systematically investigated in the 0 - 280 kbar pressure range. Basically, we focus on the influence that hydrostatic pressure has on the  ${}^2E \rightarrow {}^4A_2$  (R-lines) transitions of Cr<sup>3+</sup>. It has been observed the pressure dependence of the spectral position of the R-lines, two centers are identified as centers  $\beta$  y  $\gamma$  Cr<sub>Li</sub><sup>3+</sup>). These show a bilinear behavior until an abrupt change in its slope occurs around 210 kbar. This change is related to the existence of a pressure-induced structural phase transition in the LiNbO<sub>3</sub> host. The analysis of experimental results provides the Racah parameters  $B$  and  $C$  and the crystal field parameter  $10Dq$  at 200 kbar, through the crystal field theory and equation of state.



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**[ LPM-510 ] Quantum yield enhancement of zno nanoparticles by plasma surface modification**

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Over the last two decades, significant scientific and technological interest has focused on ZnO nanoparticles due to their potential in optoelectronic applications, such as gas sensors, piezoelectric transducers, optical waveguides, UV-laser emitter, and solar cells. Moreover, ZnO nanoparticles are cheap, chemically stable under ambient conditions towards sunlight, water and air, and also have a non-toxic nature. In this work we demonstrated that the use of plasma cold improves the quantum yield of ZnO nanoparticles. ZnO nanoparticles were treated by acrylic acid plasma during 30 min at 40 W. Thermogravimetric, transmission electron microscopy and photophysical properties were used to characterize the untreated and treated ZnO nanoparticles. Both samples present the electronic transition attributed to ZnO at 370 nm with a broad absorption to 1000 nm due to light scattering. The normalized emission spectra, were a first peak appear around 380 nm on modified and unmodified nZnO. However, it can be noticed that the peak is very intense in the case of nZnO while for modified-nZnO is only a small shoulder. This is due to the excitonic emission of the material. In addition, a band at longer wavelength can be identified (194 nm for nZnO and 445 nm mod-nZnO) attributed to the emission of defects (“trapped emission”). Plasma treatment of ZnO nanoparticles improves the quantum yield from 0.5 % for untreated ZnO to 7.6% for treated ZnO nanoparticles. A deposition of an ultrathin polymer by plasma on the ZnO nanoparticles was achieved.



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**[ LPM-525 ] Design of oxide and oxy-nitride structures doped with rare earth for white-like emission**

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In past few years light emitting devices (LEDs) have been the subject of intense research towards newer and more efficient solution in lightning sources. Special consideration has been put onto a specific silicon compatibility and its immediate integration with current and future technologies. Among the wide variety of LEDs, those based on simpler chemical structures maintain special interest given the facility of study, production and of course the addition and particular interaction with the emitters.

In this matter, we will present two types of approaches for the production and characterization of simple oxides ( $\text{Al}_2\text{O}_3$ ) and oxy-nitrides (SiON) doped with rare earths (Eu, Tb, Tm), as candidates for white-like emitters in the visible range. Using pulsed laser deposition (PLD) we've produced thin films combining the ablation processes onto different targets. We will show the design for a multi-doped RGB structure with discrete and well defined PL emissions, and a single-doped multi-layers with a broadband PL emission. The main focus will be the tunability of the photoluminescence via doping concentration on some cases and its distribution for other.



[ LPM-535 ] Blue and white light emission in Tm<sup>3+</sup> and Tm<sup>3+</sup>/Dy<sup>3+</sup> doped zinc phosphate glasses upon NUV light excitation

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Tm<sup>3+</sup> and Tm<sup>3+</sup>/Dy<sup>3+</sup> doped Zn(PO<sub>3</sub>)<sub>2</sub> glasses are prepared by melt-quenching method at 1250°C and analyzed by photoluminescence spectra and decay time profiles. The Tm<sup>3+</sup> doped Zn(PO<sub>3</sub>)<sub>2</sub> glass, upon 357 nm excitation, exhibits blue emission with CIE1931 chromaticity coordinates,  $x = 0.157$  and  $y = 0.030$ , and color purity of about 96%. Under excitations at 348, 352 and 363 nm, the Tm<sup>3+</sup>/Dy<sup>3+</sup> co-doped Zn(PO<sub>3</sub>)<sub>2</sub> glass displays natural white, bluish white and cool white overall emissions, with correlated color temperature values of 4523, 10700 and 7788 K, respectively, depending strongly on the excitation wavelength. The shortening of the Dy<sup>3+</sup> emission decay time in presence of Tm<sup>3+</sup> suggests that Dy<sup>3+</sup> → Tm<sup>3+</sup> non-radiative energy transfer occurs. By using the Inokuti-Hirayama model, it is inferred that an electric quadrupole-quadrupole interaction might be the dominant mechanism involved in the energy transfer. The efficiency and probability of this process resulted to be 0.12 and 126.70 s<sup>-1</sup>, respectively.



[ LPM-581 ] Tunable white light emission from hafnium oxide films co-doped with trivalent terbium and europium ions

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In this paper, the photo and cathodoluminescent properties of HfO<sub>2</sub> films optically activated with different atomic concentrations of Tb<sup>3+</sup> and Eu<sup>3+</sup> ions, deposited by ultrasonic spray pyrolysis technique are reported. These films were deposited on glass and silicon substrates at temperatures from 400°C to 600°C, using chlorides as raw materials. The surface morphologies of all deposited films were rough and dense, formed by ramifications and spherical particles mainly in the films deposited at higher temperatures. X-ray diffraction analysis showed that the films deposited at temperatures below 400 °C were non-crystalline, while for higher deposition temperatures these films were polycrystalline exhibiting the HfO<sub>2</sub> monoclinic phase. The photo and cathodoluminescent spectra for co-doped films showed an emission very close to white light, due to emissions associated with the characteristic electronic transitions of Tb<sup>3+</sup> (green), Eu<sup>3+</sup> (red) ions, and the blue emission associated to host lattice (HfO<sub>2</sub>). Co-doped films with Tb<sup>3+</sup> (80 %) and Eu<sup>3+</sup> (20 %) showed the best ratio of intensities for the green and red emissions. The chromaticity diagram for the emission spectra of the co-doped films showed coordinates (x = 0.3350, y = 0.3423).



**[ LPM-582 ] Erbium (Er<sup>3+</sup>) and Yterbium (Yb<sup>3+</sup>) luminescent ZrO<sub>2</sub> films deposited by the ultrasonic spray pyrolysis**

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The structural, morphological, and luminescent characteristics of Erbium (Er<sup>3+</sup>) and Yterbium (Yb<sup>3+</sup>) luminescent ZrO<sub>2</sub> films deposited by the ultrasonic spray pyrolysis are presented in this work. The films were deposited on quartz substrates at 500°C using as precursor ZrOCl<sub>2</sub>·8H<sub>2</sub>O, Er(NO<sub>3</sub>)<sub>3</sub>·5H<sub>2</sub>O, and YbCl<sub>3</sub>·6H<sub>2</sub>O. The films were characterized by X-ray diffraction, Energy Dispersion Spectroscopy and electron microscopy. The films were polycrystalline with a monoclinic ZrO<sub>2</sub> phase (00-036-04020). The EDS determined chemical composition shows a 2 to 1 O to Zr stoichiometry with small traces of Cl. SEM micrographs show a uniform but rough film with vein like texture and the presence of small spheres was also observed. The best luminescence characteristics were obtained with 1%Er and 0.5%Yb.



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[ LPM-218 ] Synthesis and characterization of microwave assisted Eu<sup>3+</sup>:Y<sub>2</sub>O<sub>3</sub> nanophosphors prepared by the benzyl alcohol route

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In this work, results about the synthesis and characterization of Eu<sup>3+</sup>:Y<sub>2</sub>O<sub>3</sub> phosphors, prepared by the benzyl alcohol route, using microwave heating, are presented. The Microwave-Assisted technique is able to get a fast heating in order to achieve the required temperature reaction in a well controlled and reproducible way. The benzyl alcohol route is not only suitable for the preparation of highly crystalline nanoparticles, but also for obtaining hybrid (organic-inorganic), materials. Hybrid Lanthanides nanomaterials, prepared by the benzyl alcohol route, have shown new and interesting optical properties that are strongly influenced by the organic-inorganic microstructure. Yttrium Nitrate (Y(NO<sub>3</sub>)<sub>3</sub>) and Benzyl Alcohol at 275 °C, with different amounts of Europium Chloride (EuCl<sub>3</sub>), (0.00, 0.25, 0.50, 1.00, 1.50 and 2.0 a/o) were used during the preparation of the Eu<sup>3+</sup>:Y<sub>2</sub>O<sub>3</sub> phosphors that were later characterized by Photoluminescence, Transmission and Scanning Electron Microscopy, Energy Dispersive Spectroscopy, X-ray Diffraction and Infrared Spectroscopy. The PL spectra showed the characteristics emission bands due to Eu<sup>3+</sup> ions transitions <sup>5</sup>D<sub>0</sub> to <sup>7</sup>F<sub>0</sub> (582nm), <sup>5</sup>D<sub>0</sub> to <sup>7</sup>F<sub>1</sub> (595nm), <sup>5</sup>D<sub>0</sub> to <sup>7</sup>F<sub>2</sub> (629nm), <sup>5</sup>D<sub>0</sub> to <sup>7</sup>F<sub>3</sub> (656nm) and <sup>5</sup>D<sub>0</sub> to <sup>7</sup>F<sub>4</sub> (709nm), respectively. The XRD patterns showed the characteristic reflections of a lamellar hybrid phase. In addition, TEM revealed the latter hybrid structure. Further characterization was obtained by SEM, EDS and FTIR.

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[ LPM-257 ] Microwave assisted synthesis and luminescent properties of Sm<sup>3+</sup> doped Yttria powders

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In this work, microwave irradiation was used as optimal heating medium to obtain Sm<sup>3+</sup> doped Y<sub>2</sub>O<sub>3</sub> powders by means of non-aqueous synthesis in benzyl alcohol. X-ray diffraction patterns of calcined powders at 1000 °C showed reflections corresponding to body centered phase of yttria. Moreover, in FTIR spectra of as calcined samples, a peak centered in 557 cm<sup>-1</sup> was observed and assigned to stretching vibration of Y-O of cubic Y<sub>2</sub>O<sub>3</sub>. Sm doped Y<sub>2</sub>O<sub>3</sub> powders were composed of particles like rods, according to HR-TEM images. Also, these powders are polycrystalline, as revealed by electron diffraction patterns. On the other hand, luminescent properties of Sm<sup>3+</sup> doped Y<sub>2</sub>O<sub>3</sub> powders are due to electronic transition  $^4G_{5/2} \rightarrow ^6H_J$  (J= 5/2, 7/2, 9/2 and 11/2) of trivalent samarium ion with (J+1/2) manifolds, corresponding to Sm<sup>3+</sup> ion in a C<sub>2</sub> site of yttria. Powders were excited with Xe lamp (407 nm) as well as cathodic ray source in a range of 3 kV to 7 kV, show in both cases, orange-red light emission due to trivalent samarium ion, which intensity of emission is function of Sm<sup>3+</sup> concentration in the samples. Quenching concentration was observed above of Sm<sup>3+</sup> concentration of 0.5% mol. Quenching of photoluminescent emission may be due to cross relaxation effect. However, quenching of cathodoluminescent emission may be due to, in fact, cross relaxation phenomena as well as Auger effect. Sm<sup>3+</sup> doped Y<sub>2</sub>O<sub>3</sub> samples showed high color purity with a CIE 1931 chromaticity coordinate of x=0.5289 and y=0.4503. Also, quantum yield measurements were carried out.



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**[ LPM-298 ] Phosphors photoluminescence of Y<sub>2</sub>O<sub>3</sub>: Er, Yb, Li and composites films with PMMA**

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In this work luminescence characteristics of Y<sub>2</sub>O<sub>3</sub>: Er<sup>3+</sup>, Yb<sup>3+</sup> and Li<sup>+</sup> phosphors were synthesized by simple evaporation method and these phosphors were embedded into PMMA films, by spin coating technique are reported. It was possible to achieve UC luminescent powders that have high intensity green, red light and for the near infrared (1.534μm) down conversion (DC) emission characteristic of the Er<sup>3+</sup> ions, observable at naked eye, under continuous excitation at 980 nm The effect of Yb<sup>3+</sup> and Li<sup>+</sup> co-doping was found to change the light emission intensity up to 470 times in the case of UC emissions. Powders incorporated in polymeric films show similar emissions, non doped films are very transparent (close to 100 %T) while films with embedded phosphors are slightly less transparent (around 95 %T).



[ LPM-381 ] Effect of the Fe<sub>3</sub>O<sub>4</sub> nanoparticles on the photoluminescent properties of SiO<sub>2</sub> thin films

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The magnetite (Fe<sub>3</sub>O<sub>4</sub>), usually exhibit ferrimagnetic properties due to its crystal structure of inverse spinel, allowing it to be a non-stoichiometric compound with an electrical high conductivity and lowest resistivity above other oxides. Furthermore, this material is a semiconductor with a band gap around of 0.1 eV. Meanwhile, silicon dioxide is an insulator material that has attractive properties like high hardness, chemical resistance, high melting point, piezoelectricity and a transparent appearance. In this work, the effect of the addition of magnetite nanoparticles on the photoluminescent properties of SiO<sub>2</sub> thin films was studied. Fe<sub>3</sub>O<sub>4</sub> nanoparticles were obtained by the coprecipitation method using a complexing agent. Sol-gel was used to synthesize the SiO<sub>2</sub> matrix and different concentrations of magnetite nanoparticles were added to SiO<sub>2</sub> precursor solution. The obtained thin films were heat treated in air at 1000 °C. The magnetite nanoparticles were characterized by DLS, SEM, XRD, Raman, FTIR, and UV-Vis. Moreover, the SiO<sub>2</sub>@Fe<sub>3</sub>O<sub>4</sub> films were characterized by photoluminescence and thermoluminescent methods. The results obtained by DLS shows a size polydispersity from about 40 to 800 nm with an octahedral morphology revealed by SEM analysis. Raman, FTIR and XRD confirmed the formation of Fe<sub>3</sub>O<sub>4</sub> phase and with a crystal size of 29 nm estimated by the Scherrer equation. Optical absorption spectra of the particles shows an absorption broad band at 350 nm typical of magnetite as reported elsewhere. Thermoluminescent shows a decrease in the behavior of the glow curves of the films without heat treatment. Finally, photoluminescence spectra show an emission at 397 nm for the heat treated films at concentrations of 3 and 6% Fe<sub>3</sub>O<sub>4</sub>, and a widening of the same band films without heat treatment at the same concentrations.



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[ LPM-532 ] Comparing kinetic parameters values of nano-structures using interactive multi-trap system model(IMTS) and non-interactive multi trap system(NMTS).

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The samples of grapheme exfoliate, grapheme flakes, Sigle Wall Carbon Nanotubes (SWNT), Multi Wall Carbon Nanotubes(MWNT) and graphite, were exposed to gamma photons from <sup>60</sup>Co of a Gammacell 651 PT irradiator with a dose rate of 150 Gy/min. All the samples were read out in only one session at the end of the experimental period. The TL reader system was a Harshaw TLD model 3500; a constant heating rate of 2 °C/sec was used and nitrogen gas was allowed to flux into the reading chamber during the read out to eliminate any spurious signals. The kinetic parameters, activation energy  $E$  and the frequency factor  $s$ , of the TL glow curves were determined using the computerized glow curve deconvolution program (CGCD) and interactive multi-trap system model (IMTS) were compared with non-interactive multi trap system. The results obtained give information about the principal mechanism responsible of thermoluminescent signal.



**[ LPM-564 ] The photoluminescence properties of Al<sub>2</sub>O<sub>3</sub>: Eu<sup>3+</sup> powders synthesized by the microwave assisted solvothermal technique**

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The photoluminescence properties of Al<sub>2</sub>O<sub>3</sub>: Eu<sup>3+</sup> powders synthesized by the microwave assisted solvothermal technique are reported. After annealing at 1000 °C, the powders present some broad diffraction peaks associated with the  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> phase, with a crystallite average size in the range of 14 nm as determined by the Scherrer formula. The photoluminescence spectra presented the characteristic peaks associated with the transitions between electronic energy levels of the Eu<sup>3+</sup> ion (main peak at 614 nm), with a dominant excitation peak at 395 nm. The effects of dopant concentration as well as that of thermal treatment on the luminescence properties of the powders were studied. Concentration quenching of the luminescence intensity was observed to occur for Eu<sup>3+</sup> concentrations above 7.5 at.%, as determined by energy dispersion spectroscopy, larger than previously reported for this type of phosphor. High concentrations of Eu<sup>3+</sup> resulted in the formation of a EuAlO<sub>3</sub> crystalline phase, which resulted dominant over the Al<sub>2</sub>O<sub>3</sub> phase when the samples were annealed at 1200 °C. The highest luminescence intensity was obtained for samples with 7.5 at.% Eu concentration and annealed at 900 °C in air at atmospheric pressure which presented a quantum yield of 37.3% when excited with 395 nm light.



**[ LPM-578 ] Rare earth ions and Ag nanoaggregates in silica-hafnia sol gel films: broadband downshifting materials for solar cells**

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Energy harvesting in solar cells may be improved by spectral conversion layers, to convert poorly absorbed frequencies of the solar spectrum into the region of maximum absorption of the cell. To this purpose, we report here the study of efficient down-converting silica-hafnia glassy or glass-ceramic waveguides, doped with Tb<sup>3+</sup>/Yb<sup>3+</sup>, which combine the spectral properties of rare earth doped materials with the optical sensitizing effects of Ag nanoaggregates. The preparation of 70 SiO<sub>2</sub> – 30 HfO<sub>2</sub> glass and glass-ceramic waveguides was carried out by sol-gel route, and it was followed by Ag doping by immersion in a molten salt bath. The films were subsequently annealed in air to induce the migration and/or aggregation of the metal ions. Results of compositional and optical characterization are given, providing evidence for the successful introduction of Ag in the films, while the photoluminescence emission is strongly dependent on the annealing conditions. These films could find potential applications as downshifting layers to increase the efficiency of PV solar cells.

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**[ LPM-584 ] Luminescence in clay nanotubes doped with europium**

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Halloysite clay nanotubes (HNTs) are natural, abundant and non-expensive type of highly biocompatible materials. In this work, luminescent materials derived from HNTs doped with Eu where successfully synthesized by a simple dopant adsorption method in aqueous solution and post diffusion by heat treatment in air. The nanotubes can physically adsorb the target dopant and induce effective doping level during heat treatment. By simply tuning the alkalinity of the solution, the luminescent and structural properties of the HNTs can be enhanced. Luminescence spectra of the resultant materials are reported displaying a wide excitation wavelength range from UV to visible light, being the most intensive centered at 395 nm; on the other hand, emission spectrum exhibits features characteristic of the Eu<sup>3+</sup> ion 4f-4f transitions. Photoluminescence intensity increases as the PH increase, showing a maximum after sintering at 900°C and at 16 wt.% of dopant initial concentration. The luminescence behavior of Eu ions provides a probe at the molecular level of the changes which occur at the tubes during synthesis. These phase transitions induced by heat and alkali treatment were also studied by x-ray diffraction and transmission electronic microscopy. The combined properties of the HNTs doped with Eu offers potential applications of the as-prepared materials for cell imaging in biological systems, sensors and luminescent fillers.

Keywords: Europium, Halloysite Nanotubes, Fluorescence.



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**[ LPM-585 ] Enhancement of the photoluminescence of succinimide – Eu(III) complexes by acid treatment**

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High luminescence is characteristic of Europium (III) complexes with succinimide (SI), unfortunately, their luminescence properties undergoes quenching in an aqueous media solutions because of the non equilibrium between the ion and the ligand, which in turn limits their potential use as biomarkers or in optoelectronic devices. In order to improve the stability and even to increase luminescence performance, in this work we describe the preparation of the Eu(III)-SI complexes by a modified procedure in which an acid treatment is given to the lanthanide ions in solution before and during ligands incorporation. The resultant complexes not only successfully conserved their photoluminescence properties in solvents as water, ethanol and chloroform but also showed an enhanced luminescence performance. Finally, the complexes, embedded in thin films of different polymer matrices were studied by photoluminescence spectroscopy, demonstrating that the complexes properties can be easily preserved through this proposed procedure and the photoluminescence spectra has an important increase by the correct acid treatment. Their excellent photoluminescent properties may recommend them as photonic conversion materials in various optoelectronic applications.



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# **MICROELECTRONICS AND MEMS (MEM)**

**Chairman: Wilfrido Calleja (INAOE)**



[ MEM-33 ] I-V characteristic of OPFETs devices in presence of carbon nanotubes into the channel

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As part of the new technology in recent decades, the organic semiconductor materials are too important to the construction and implementation of devices such as OPFETs (Optical Field-Effect Transistor), made of alternative materials such as nanostructured carbon, or polymeric, that allow technological applications of these. In this paper we present the behavior I-V characteristic of OPFETs devices, these were built based on organic semiconductor materials, such as MEH-PPV, MDMO-PPV, P3HT and RuBPY, as well as a first approximation of the contribution of MWCNTs (Multiple Wall Carbon Nanotubes) in the channel, in combination with the organic semiconductor MEH-PPV.

The OPFETs devices were constructed in two ways: depositing a MEH-PPV solution and MWCNTs on channel transistor; and built with channel of a Bulk-heterojunction from MWCNTs and the semiconductor polymer MEH-PPV, with the purpose of knowing the produced effect of the MWCNTs in the behavior I-V of OPFETs devices. The nanotubes were produced by the technique of microwave irradiation, and have diameters between 20 and 50nm; the polymers MEH-PPV, MDMO-PPV, P3HT and RuBPY were purchased from Sigma-Aldrich Mexico with catalog number 536512, 546461, 698989 and 754730 respectively.  $I_D-V_G$  characteristic behaviors are obtained for our devices with  $V_G$  in the range 0-12 volts, finding a threshold voltage of 2.5 and 3.5 volts respectively for each of the devices built, and on the other hand, for the characteristic  $I_D-V_{SD}$  con  $V_{SD}$  in the range 0-10 volts are obtained a current of saturation around the scale of milli-Amperes.

**Keywords:** OPFET, semiconducting Polymers, MWCNTs.

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**[ MEM-54 ] Electrochemical batteries made of textiles**

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In this work, we fabricated a textile battery with three layers of cotton textile sandwiched between two metal electrodes (Ag and Al). The area of the fabrics and electrodes were 42mm x 6mm. The fabrics are impregnated with silver nitrate ( $\text{AgNO}_3$ ) and aluminum chloride ( $\text{AlCl}_3$ ) solutions, to serve as dry electrolytes, and one fabric is impregnated with sodium nitrate ( $\text{NaNO}_3$ ) solution to serve as a salt bridge. When liquid is applied to the battery, the dry electrolytes become hydrated and an electrochemical reaction is generated. During the reaction, Ag loses one electron while Al gains three electrons. Because of this, the  $\text{AgNO}_3:\text{AlCl}_3$  ratio was fixed at 3:1. We studied three different set of concentrations for  $\text{AlCl}_3$  (0.5, 1.0 and 1.5 M) and  $\text{AgNO}_3$  (1.5, 3.0 and 4.5 M). For the electrical testing, the batteries were connected to a Keithley 2400 instrument to measure current and voltage. To active the battery, 80  $\mu\text{l}$  of deionized water (18  $\text{M}\Omega\text{-cm}$ ) were applied, with a micro-syringe, evenly all over the battery area. The current and voltage measurement started after 3 minutes. The batteries were electrically measured for approximately 1 hour. The fabricated batteries produce a constant voltage of 1.2-1.3 V for all the set of concentrations. The generated current decreases exponentially with the time from 24 mA to 5 mA for the maximum  $\text{AgNO}_3$  and  $\text{AlCl}_3$  concentration. Our textile battery can be fabricated using inexpensive materials and methods, which can significantly lower overall device costs. The fabricated batteries are intended to be used in wearable electronics.



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**[ MEM-276 ] Design of an Electroactive Textile Fiber for Thermoregulation**

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Many types of temperature sensors have been developed for applications to medical and industrial systems using MEMS technology. To apply temperature sensors to a wide range of applications, the flexible structure and the large sized sensing areas like the human skin are required. Flexible resin materials, such as PDMS and polyimide film, are therefore used as substrates. Such a film-based sensor can bend along one axis, and therefore can be put on a cylindrical surface.

In this work we propose an artificial electroactive textile fiber structure as a new material for MEMS, and applied it for realizing a novel type of thermoregulated fabric. The thermoregulated fabric is obtained by weaving the proposed artificial fibers like a cloth.

The fiber, which is comprised of a heater and two temperature sensors, was designed over a polyimide film and placed inside a flexible hollow tube. The design was validated by multiphysics simulation in order to obtain some operating values of the heater and also the sensitiveness of the temperature sensors.



**[ MEM-322 ] A ring based micromachined thermal accelerometer design for high shock applications**

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The MEMS accelerometers are widely used in several technological areas, including automotive, aerospace, medical, defense and communication, due to their improved sensitivity and integrability. However, moving parts, usually implemented in this type of sensors, compromise the micro sensor reliability for high shock applications. Therefore, for this case, thermal accelerometers based on the sensitivity of natural convection of heated gas molecules to gravity are preferred.

In this work, a surface micromachined thermal accelerometer composed of a heater and eight temperature sensors for high shock applications is proposed. The acceleration of the device will produce a displacement of the temperature gradient of the surrounding fluid. Since the temperature sensors are equidistant to the heater along the acceleration axis, there is a mismatch in the readings proportional to the acceleration.

The accelerometer was designed with PolyMUMPS process and optimized using finite element and analytical models experimentally confirmed by other authors. The analysis was performed using a coupled study between Joule effect and conjugated heat transfer. Also, some approximations were included to reduce fluid dynamics computation.

The heater is an octagonal ring with 10  $\mu\text{m}$  width and an apothem of 50  $\mu\text{m}$  separated from the thermal sensor by a distance of 230  $\mu\text{m}$  which achieves a sensitivity of 0.44 K/g for acceleration vectors parallel to one detection axis. Also, thermal sensors achieve a sensitivity of 1.34  $\Omega/\text{K}$  obtained in a range of 416.15 to 430.15 K. The proposal improves its detection sensitivity by incorporating additional detection axes in plane and can be integrated on chip with other devices designed for the PolyMUMPS process.



[ MEM-357 ] Dielectric constant determination of  $\text{Co}_3\text{O}_4$  phase produced by thermal decomposition

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The  $\text{Co}_3\text{O}_4$  is a stable normal spinel structure of  $\text{AB}_2\text{O}_4$  type, where Co (II) ions occupy the tetrahedral 8a sites and Co (III) ions occupy the octahedral 16d sites, generating a significant change in its chemical and electronic properties. Because of these properties are crystal size dependent, each different synthesis method used to produce it will provide unique properties. The motivation of this work is to determine cobalt spinel synthesized by thermal decomposition polarization degree and its dielectric constant. T. Wanjun and C. Donghua reported the synthesis route. The product obtained was characterized by mean of X Ray Diffraction and Ultra High Resolution Scanning Electron Microscopy to verify cobalt spinel formation and particle size distribution. The polarizability is an important characteristic for capacitors construction, so, the higher polarization higher capacitance. For dielectric constant determination, a MOS capacitor structure was considered; such that experimentally, the MOS structure was Cr- $\text{Co}_3\text{O}_4$ /PMMA-Si. The greatest difficulty is the formation of the oxide film, because  $\text{Co}_3\text{O}_4$  particles tend to form agglomerates. Different surfactants were used in combination with the action of an ultrasonic tip to break these agglomerates, and then, reach a good dispersion of particles in a dielectric polymer matrix of PMMA, which serves as support for these particles too. A homogeneous particles dispersion on the thin film is desirable for the best capacitance evaluation and then calculate the dielectric constant value. From this  $\text{Co}_3\text{O}_4$  dispersion on PMMA, it is feasible to explore capacitance values depending of particles concentration embedded in PMMA matrix. Finally, the film with the best experimental capacitance result will be used to construct an element for a capacitive transduction polymer sensor fabrication.



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**[ MEM-366 ] Design and Simulation of a Vibrating Diaphragm Micro Pump With No Moving Parts**

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One of the problems in the design of a micropump is the implementation of movable elements, because they are exposed to mechanical stresses and has the limitations of the fabrication technology also are exposed to different condition that reduce their useful lifetime.

In this work is presented the design of a micropump that use a oscillate membrane to produce the movement of the fluid and the implementation of a no-moving-parts micro valve to promote the flow in one direction and to generate a restriction on the opposite direction. The micro implemented valve has a similar behavior to a check valve but, in this case with no-moving-parts. Thus the useful time of the micropumps is improved and the complexity of the design is reduced. Considering this, the cost and fabrication time is less in comparison with other kind of micropumps that implement a different type of fluid propulsion.

The design characteristics were first validated in multiphysics simulation in order to obtain the best performance of the micro valve, and then it will be compared with laboratory results.



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**[ MEM-372 ] Flexible electronics for medical applications**

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Recent studies in electromechanical devices (MEMS) defined on flexible substrates, have shown great potential in a wide range of applications, such as robotics, in-vitro diagnostic, implantable and therapy devices. In addition, this technology compared to rigid structures offer several advantages such as: high bendability and scalability, transparency, low weight, integration with heterogeneous devices and low cost. In the medical field, flexible electronics is of great interest because living organisms, organs, tissues, etc., are intrinsically flexible and malleable; therefore, flexibility is an absolute necessity for the successful integration of electronics in biological systems. Also, using a flexible device minimizes tissue damage because they have soft surfaces that allow proper matching. The polymers have been studied as materials for MEMS, either as substrate, capping or structural films. In particular, polyimide (PI) has a long history of use in microelectronics as flexible substrate and capping material, due to its excellent thermal and electrical insulation, good mechanical strength, high chemical resistance and excellent temperature stability. Starting from a viscous source by centrifugation, PI films are deposited and after specific heat treatment (curing 370 ° C) toxic components are removed, and then this material can be incorporated into some type of MEMS microcomponent, which can be used as safe implantable device. FTIR spectroscopy has been used to evaluate the absence of toxic species on the PI layer. In this context, it was designed and fabricated some arrangements of microelectrodes for stimulating/recording, defined on a flexible polyimide substrate. The design consists of an array of 16 independent recording sites, two reference electrodes, and 20 external contacts for wiring. For the fabrication of these flexible microelectrodes, three materials are used: a 19µm thick film of PI-2611 as flexible substrate; a double metal film of 1µm thick (aluminum/titanium) for interconnecting lines, recording and wiring electrodes; and finally a thin film of PI-2610 of 1.5µm thick as capping material. A complete routine for electrical and mechanical characterization was performed on these devices including in-vitro tests for evaluate the transfer of electrical signals in a biological environment. In conclusion, we have obtained BioMEMS devices technologically reproducible, mechanically flexible, multielectrode spatially selective and at low cost fabricated. These prototypes represent some key advancement to the objective of flexible electronics for medical applications. This type of multielectrode arrangement can be used for diverse biomedical applications such as cell culture platform, for electroretinogram (ERG) recording, electrical stimulation, Patch Clamp integrated systems for signal recording, and so on.



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**[ MEM-445 ] Thermomagnetic instabilities in anisotropic type-II superconductors**

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When the pinning and Lorentz forces are comparable, it is known that an equilibrium state is established, such stability of the equilibrium is mainly driven by the temperature increases. The stability between pinning and Lorentz forces in an anisotropic type-II superconductor, subjected to a magnetic field parallel the surface plate, is investigated. Analytical expressions for both the equilibrium magnetic induction and instability field are obtained, taking into account the temperature rise effect which accompanies the energy dissipation because of the admission of magnetic flux into the material.



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**[ MEM-488 ] Anisotropic silicon etch to house CMOS compatible mechanical microstructures**

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The real sense of a microelectromechanical system (MEMS) is the interaction of electronic circuits with the mechanical transducers (microstructures) to perform a useful function. This interaction yields a better performance when the parasitic elements (resistance, capacitance, inductance and conductance) of the interconnection between electronic and mechanical devices are reduced. The monolithic integration of both, electronic and mechanical elements exhibits the lowest parasitic contribution. However, the microstructures require a wide range of thickness according to the particular application, and the resulted topography directly affect the subsequent photolithography steps. The solution, without the use of planarization techniques, is the fabrication of a trench as deep as the microstructures thickness. Inside the trench, the microstructures will be fabricated, and by the use of an additional mask, the deposited material outside the trench will be removed. To carry out the above, the etch solution must be CMOS compatible, to ensure an optimal performance of the electronic devices. In this work, the use of TMAH at 10 and 25 wt. % in H<sub>2</sub>O as etch solution, is analyzed in terms of uniformity and roughness. According to the literature, KOH provides a better surface roughness than the TMAH with a lower etch time. For this reason, different etch samples were prepared with KOH 45 wt. % in H<sub>2</sub>O, to serve as the comparison basis in order to verify the quality of the TMAH etched surface. The lower etch rate of the TMAH provide a better control in the etch depth and guarantee a reproducible step process. Also the TMAH is known to have a better selectivity with the silicon dioxide (SiO<sub>2</sub>). Thermal oxide thin films (200Å) were used and successfully masks the silicon etch process, which provides a precise control on the geometries definition due to the depreciable lateral etch.

Once the trench was fabricated, traditional photolithography techniques were adapted to define geometries of 3µm inside the trench. It was demonstrated that the geometries can be placed at the edge of the trench and the dimensions still unchanged. This is required, not for the microstructures definition at the edge (undesirable situation because of the topography, the trench loose sense), but for the correct definition of the interconnect lines starting in the surface of the wafer (electronic devices) to the bottom of the trench (mechanical devices).

All the stated above open a good way in the development of a monolithic integrated MEMS technology.



[ MEM-505 ] Surface states based field-effect transistor analyzed by TCAD-simulations

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In this work, the authors explore the performance of single-gate field-effect transistor (FET) made on n-type silicon-on-insulator (SOI) substrate. In this device a nano-channel between two insulating grooves is fabricated by simple electron beam lithography [1], this produces surface states caused by the breaking of the crystalline structure, so the carrier transport between source and drain can be controlled by the modulation of the depletion zone inside the channel by the gate, resulting in a transistor-like behavior. Our numerical results indicate that the device exhibits a characteristic FET-like relationship between the drain-current and drain-to-source voltage. These curves can be manipulated to present a DC behavior as depletion or enhancement mode FET by the manipulation of the width of the nano-channel. The performance of the device is intensely modified by the thickness of the groove that separates the nano-channel from the gate. When this distance is large (small) the electric field that modulates the depletion region in the channel is reduced (raised), this is translated in a decreased (increased) drain-current. Three-dimensional simulation in conjunction with a self-heating model are used in order to define the appropriate silicon layer thickness of the devices that improve the current-voltage response and reduce the typical thermal issues of SOI technology. For our geometries, the use of active layers > 1 μm of n-type silicon increases the thermal effect. We found that the turn-on voltage and response in this device is closely related to the surface density and/or the transistor geometry, thus the viability to design the transistor with the appropriated behavior for each application is demonstrated in the DC-injection mode. This numerical study indicates that surface states-based transistor can be applied to SOI technology, thus the transistor integration scale can be raised by the use of the nanometric scale of the device presented in this study and seems to be very attractive to extend the concept towards logic gates.

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[ MEM-551 ] Comparison in the electric characteristics of TiN/HfO<sub>2</sub>/Si(100) and TiN/HfO<sub>2-x</sub>N<sub>y</sub>/Si(100) structures in MOS like devices before and after a nitridation process

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In this paper we present a study of the electrical properties TiN/HfO<sub>2</sub>/Si(100) and TiN/HfO<sub>x</sub>N<sub>y</sub>/Si(100) thin films processed at the Laboratory of Processing and Characterization of Nanofilms (LPCN) located at Cinvestav-Querétaro. Silicon (100) substrates were cleaned with a RCA method. The high k oxide was grown by atomic layer deposition (ALD Savannah Cambridge 100) using tetrakis (dimethylamino) hafnium (TDMA-Hf) as Hf precursor and water (Type 1) as an oxidant precursor [1]. The nitridation of the dielectric was done using a remote plasma source (LITMAS) integrated to the sputtering system employed for growing the titanium nitride layer, avoiding, in this way, contamination between the Hf<sub>x</sub>O<sub>y</sub>/TiN interface. Angle resolved X-ray photoelectron spectroscopy (ARXPS) was used to calculate the thickness and composition of the films. The spectra were obtained with a TermoFisher-VG instrument equipped with a monochromatized X-ray source.

A photolithographic process was used to define the patterns of MOS-like devices. The electric characterization of capacitance (C-V) and current flow (I-V) were performed using an Agilent LCR precision meter E4980A and an Agilent semiconductor parameter analyzer 4155C. Capacitance calculations were used to obtain the HfO<sub>2</sub> dielectric constant, resulting in values between 15 and 20 which are close to the expected value for hafnia nanofilms.



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**[ MEM-556 ] Deposition of LiNbO<sub>3</sub>/PCL films on silicon photonics chip**

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Microring resonators are photonic devices where light can be confined into very small volumes, using looped optical waveguides coupled to a bus waveguide. These devices may provide high photonic lifetime and low energy consumption for fast optical signal processing. Moreover, these devices can be readily integrated in 2D platforms, More importantly, in CMOS platforms in the so called Silicon Photonics.

Lithium niobate (LiNbO<sub>3</sub>) is a ceramic material with diverse properties such as ferroelectric, piezoelectric, pyroelectric, acousto-optic, electro-optic, and nonlinear optics. Several discrete photonic/optoelectronic devices have been obtained based on this material with large electro-optic and non-linear coefficients have enabled the fabrication of optical modulators, optical processors, frequency doublers and mixers. However, the small refractive index contrast in these materials and the very particular technology required for its technology seriously restrict the miniaturization and integration of these devices.

Therefore, combining the Si photonics technology, the large electromagnetic density of microring structures and the non-linear and electro-optic properties LiNbO<sub>3</sub> is of great interest. One expect the optimization of effects such as second harmonic generation, difference frequency generation, optical rectification, and sum frequency generation for applications in classical and quantum information processing. Also counts with advantages of fast tuning speed high tuning accuracy, bi-direction wavelength shift, high material stability, and no heating interference to the neighboring devices.

In this work, we investigate the deposition of LiNbO<sub>3</sub> nanoparticles on a silicon photonics chip.



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# **NANOSTRUCTURES (NSN)**

**Chairmen: Máximo López (CINVESTAV-DF)**  
**Jaime Santoyo Salazar (CINVESTAV-DF)**  
**Esteban Cruz Hernández (UASLP)**



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[ NSN-13 ] Control of Adsorption Properties of Deposited Nanoparticles by Electric Potential

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It was experimentally demonstrated in our work that one can control the adsorption properties of deposited nanoparticles of different chemical composition by providing them with the electric potential of different polarity and value from an external voltage source.

Experiments were performed in the ultrahigh vacuum setup equipped with a scanning tunneling microscope, Auger and mass spectrometer, additional accessories. The residual gas pressure in the setup chamber didn't exceed  $P = 2 \times 10^{-10}$  mbar. The Au, Pt and organoboron (OBN) nanoparticles were deposited on HOPG surface using corresponding impregnation techniques. All reactions were studied at 300 or 700 K under  $10^{-6}$  mbar. Due to low amount of nanoparticles their state and results of adsorption were determined by means of scanning tunnelling spectroscopy.

It is shown that the rate of decomposition of ammonia by platinum and organoboron  $(C_2B_{10}H_4)_n$  nanoparticles is strongly depended on electric potential. At 300 K for Pt the rate increases by 44% under negative potential  $-6$  V and by 70% under the positive potential of 6V. A similar effect was found for organoboron nanoparticles. At 700 K the positive potential  $+6$  V on the particles increased decomposition rate by 26%, while the negative potential  $-6$  V reduced it by 37%, compared to the rate of decomposition of ammonia at the ground potential of the particles.

Au nanoparticles show change in their adsorption properties towards molecular hydrogen. At 300 K the hydrogen adsorption on gold nanoparticles is not observed under potentials of  $\varphi_1 = +5V$  and  $\varphi_2 = +1V$ , and in case of nonpositive potential ( $\varphi_3 = 0$  and  $\varphi_4 = -1$ ) the hydrogen adsorption takes place.

So the controllability of adsorption properties of gold nanoparticles and platinum and catalytic properties of organoboron nanoparticles deposited on HOPG by the electric potential of different polarity and value was experimentally proved. These experiments simulate charge transfer between nanoparticles and supporter in catalytic systems.

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[ NSN-21 ] Development of novel materials for nanotechnology-based remediation of petroleum impurities from water.

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Applications of the nanotechnology-based methods [1] for removal of oil in petroleum spills and its separation from water are presented. Oil spills during petroleum extraction and processing are frequently unavoidable and could lead to events of distinct scale, from small contaminations of ground and sea water to huge disasters [2]. In addition to classic methods of oil removal, the “nano”-techniques have been developed [3, 4], which use nano zero-valent iron (nZVI), carbon nanotubes, sponges, aerogels and magnetic nanocomposites, metal and non-metal nanostructured oxides, nitrides, salts, and zeolites. Some of these nanomaterials can be prepared by “greener” methods at lower costs and without damage for the environment. Main attention is paid to simplicity, costs and commercial availability of applied nanomaterials and their precursors, as well as to the efficiency of their applications for oil remediation.

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**[ NSN-53 ] Determination of optimum concentration of conductivity nanoparticles in chitosan nanocomposites**

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Chitosan (CS) is a natural biopolymer that has several favorable properties such as biodegradability, biocompatibility, nontoxicity and possibility to interact with different nanoparticles (NPs) which allowed to develop new nanocomposites. Properties of nanocomposites essentially depend on the high surface area of the NPs which in turn depend on the dimension and concentration of NPs. In this work, CS-based nanocomposites with high conductivity gold (AuNPs), clay nanoparticles and multiwall carbon nanotubes (CNT) have been investigated and their relationship between electrical properties and optimum concentration of NPs for application in sensors have been studied. It was shown that the percolation threshold represents a critical concentration in which a physical conductive path between NPs inclusions forms allowing the flow of current. Above the percolation concentration, NPs agglomeration takes place such that the effective surface area of the nanocomposite diminishes thus producing performance breakdown. This assertion has been confirmed by measurements sensitivity of CS-AuNPs composites for  $\text{Cu}^{+2}$  detection, sensitivity of CS-clay nanocomposite membranes for  $\text{NO}^{3-}$  detection and CS-CNT composite for vapour sensing. For all these applications the best functional nanocomposite properties have been observed at NPs concentration in the vicinity of the percolation threshold. The obtained relationship between electrical, structure and concentration of nanoparticles may prove useful in the design and optimization of polymer-based nanocomposites for different applications.



[ NSN-60 ] Graphene Nanohybrids Production by Ultrasonic Techniques

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Graphene is the thinnest known material and the strongest ever measured, it shows record thermal and electronic conductivity and stiffness, it is impermeable to gases and it has the right proportion between brittleness and ductility. As consequence, graphene has rapidly emerged as a rising star in the field of material science. In this direction, several methods have been established for graphene preparation. However, most of them remain as demonstration techniques, mainly for basic research, and for providing proof of concept devices. Instead, the recent progress in making stable graphene dispersions allows the production of graphene sheets on a more preparative scale and permits the manipulation of the layers by chemical reactions. Then, chemically manipulated graphene samples can be easily incorporated into new functional materials or can be modified for the formation of other carbon nanostructures. In this work, I will show our recent efforts toward 1) producing stable graphene dispersions;<sup>1</sup> 2) ultrasonic approaches performed in graphene dispersions that modify its chemical<sup>2</sup> and structural properties,<sup>3</sup> i.e. MWNTs production by rolling up a graphene sheet; and finally 3) some applications where functionalized graphenes mimic the oxygen evolving center in natural photosynthesis.<sup>4</sup>

**Keywords:** graphene dispersion, ultrasonication, applications

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**[ NSN-179 ] Electric field imaging and carrier diffusion length measurement on ZnO nanowires**

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Whereas nanowire (NW)-based devices offer numerous advantages compared to bulk ones, their performances are frequently limited by an incomplete understanding of their properties where surface effect should be carefully considered. Here, we demonstrate the ability to spatially map the electric field and determine the exciton diffusion length in NW by using an electron beam as the single excitation source. This approach is performed on numerous single ZnO NW Schottky diodes whose NW radius vary from 42.5 to 175 nm. The dominant impact of the surface on the NW properties is revealed through the comparison of electron-beam induced current, cathodoluminescence recorded on the same NW. Indeed, the space charge region near the Schottky contact exhibits an unusual linear variation with reverse bias whatever the NW radius. On the contrary, the exciton diffusion length is shown to be controlled by the NW radius through surface recombination. This systematic comparison performed on a single ZnO NW demonstrates the power of these complementary techniques in understanding NW properties.



[ NSN-208 ] Hydrogen diffusion in disordered Ti-V-Cr hydrogen storage alloys: NMR and DFT studies

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Studies of hydrogen diffusion play a key role in the overall understanding of fundamental properties of metal-hydrogen systems. The hydrogen diffusion coefficient in metals is a crucial parameter for many applications. Quantitative description of diffusion requires characteristics which control hydrogen motion process, including jump frequency, activation energy (determined as the saddle-point energy between adjacent wells), stereometric parameters of possible diffusion channels, influence of trapping and blocking effects etc. Although ordered metal-hydrogen systems have been extensively studied both experimentally and theoretically, the theoretical description of hydrides of disordered alloys is still challenging. The main difficulties come from a correct description of the disorder. For completely disordered metallic systems it can be done within the Korringa-Kohn-Rostoker method with Coherent Potential Approximation (KKR-CPA), one of realizations density functional theory (DFT), which proved itself very efficacious to study stability and phase transitions in hydrides of disordered alloys. However, it provides averaged characteristics only, and not the information on the local environment of hydrogen atoms. From this perspective a supercell DFT approach seems to be very fruitful but unambiguously much more time consuming. Experimental information on hydrogen diffusivity and its motional characteristics, like jump frequency and activation energy, can be obtain by different techniques, including Nuclear Magnetic Resonance (NMR). The simplest way to determine the activation energy of hydrogen motion is the diffusion measurements, as the diffusion coefficient normally obeys the Arrhenius law. The activation energy determined from NMR relaxation measurements is, on the one hand, model dependent, as it is obtained from the fitting the temperature dependence of the spin-lattice relaxation within an appropriate model, but on the other hand, it allows us to estimate in a rather more correct way the activation energy distribution.

In this contribution we report on a complimentary study of hydrogen diffusion in hydrides of disordered Ti-V-Cr alloys using different experimental NMR techniques and theoretical DFT supercell approach. These alloys exhibit rather fast hydrogen sorption kinetics and a good hydrogen absorbing capacity, up to 3.7 wt.% under a few MPa H<sub>2</sub>-gas pressure. Recently, these compounds were proposed as additives to accelerate hydrogen sorption by magnesium. And one of the aims of the present study is to propose the best composition of Ti-V-Cr alloys that can be used for efficacious hydrogen delivering into magnesium.

#### Acknowledgments

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**IX International Conference in Surfaces, Materials and Vacuum**  
**September 26<sup>th</sup>-30<sup>th</sup> , Mazatlan, Sinaloa, México**

**[ NSN-209 ] Persistent nanophosphors for solar hydrogen generation**

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Long persistence nanophosphors (LPNP) have been revisited recently for sunlight driven applications, in particular: passive illumination systems, photocatalytic water treatment, artificial photocatalysis systems, and solar hydrogen generation. Among the diverse variety of LPNP the alkaline metal aluminates and alumino-silicates present excellent persistence times, good chemical stability, and have been proved to be of utility in the above cited applications. Here we present recent results on combustion synthesis methods for the production of several aluminates doped and codoped with rare earths and transition metals. Structural, morphological, Photoluminescent, and Photocatalytic characterizations have been performed. Several of the presented compounds reveal as potential candidates for the development of new alternatives in the above cited sunlight driven applications.



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[ NSN-239 ] Electronic response of nanodevices on conducting nano-cables.

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Current trend to produce faster electronic products, has led to increase the device density and therefore to the *Electronics Miniaturization*. As a consequence, the conventional manufacturing methods are reaching their limits. Thus, innovative fabrication routes are being pursued.

Electronics obtained through the bottom-up approach may lead to devices and fabrication strategies not possible with top-down methods [1-2]. For example, the assembly of nano-circuits from nanoscale components such as nanocables (1D) and nanoparticles (0D) to form useful circuit elements could be a viable route with several challenges to overcome.

Following that route, we have started studying experimentally how a nanometric dimensions deposit of materials such as Platinum interact with a conducting nanocable (using a carbon nanotube) and how the conductivity of the cable is changed. This has been done by using an individual carbon nanotube as the conducting cable, while the nanometric deposit has been achieved with a Focus Ion Beam (FIB) and a Gas Injection System (GIS) in a dual beam microscope (Jeol JIB 4500 SEM-FIB).

As the first stage of the work we present the technical challenges to plug-in this type of nanostructures to macroscopic equipment in order to monitor their electric response. This includes the design and fabrication of electrodes with the appropriate dimensions, the manipulation and placement of an individual carbon nanotube on the electrodes, and the posterior nano-soldering process of the nanotube with the electrodes. Once assembled the system, its electric response was analyzed by the four probe method.

The second stage consisted in achieving appropriate deposits of platinum on the nanotube. Once obtained such nanometric devices on the conducting nanocable, they were analyzed by four probe method measurements once more and compared. We were able to study not only one of such deposits on the nanotube, but the presence of two of such devices in a series array along the carbon nanotube.

This should represent a starting effort towards studying crossing points in multi-terminal systems to understand and analyze a node of a network or nanocircuit.

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[ NSN-268 ] **The activation and potentiation of the sers-raman signal of adsorbates in silver nanoparticles**

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In this work, we present and discuss some results on the investigation of the activation of the surface enhanced raman signals (SERS) of two organic molecules adsorbed on the surface of silver nanoparticles (Ag-NP), which are normally used to produce Ag-NP in colloidal suspensions, that function to prevent their precipitation and agglomeration. It is found the effect of Neu5Ac dissolved in distilled water to the colloidal suspensions, is to potentiate or partially quench the resultant SERS signal, depending of either if the citrate or the thiol molecules are the species adsorbed. In order to understand these experimental results, DFT calculations of the SERS of both citrate covered and thiol covered Ag-NP, in the presence of increasing controlled concentrations of Neu5Ac dissolved in distilled water, were performed. The DFT calculations of the SERS signals of isolated citrate and propanethiol adsorbed molecules on the Ag-NP surface were done in first place. Subsequently, the effect on the raman SERS intensity was systematically calculated when one, two, three up to four molecules are adsorbed in an Ag nanocluster. Afterwards, the SERS signal was recalculated when in addition acetil-neuraminic acid (Neu5Ac) molecules were added in the presence of the already adsorbed citrate or propanethiol molecules. The theoretical results agree well with the observed experimental behavior explaining the two contrasting phenomena, the potentiation of the SERS signal of the citrate-Ag-NP and the quenching of the corresponding SERS of the thiol-Ag-NP, both under the addition of Neu5Ac molecules.



[ NSN-280 ] Less-common carbon nanostructures: Nanobuds and nanotori.

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Synthesis, properties, structural peculiarities, and applications of nanobuds and related nanostructures are discussed. Such carbon allotropes as carbon nanotubes (CNTs) and fullerenes (Fs) are known from the last decades of XX century, but their combination, called “nanobuds” (NBs) and possessing unique properties superior to CNTs and Fs alone, were discovered relatively recently. This structure seems like fusion of a cylinder with a sphere; there is a covalent bond between outer sidewalls of the nanotube and the fullerene. In this material, fullerenes are covalently bonded to the outer sidewalls of the underlying nanotube. NBs exhibit properties of both carbon nanotubes and fullerenes. According to observed properties and those predicted by DFT calculations, the nanobuds are semiconducting and stable in normal conditions, can accept adatoms and molecules. They contain a relatively chemically inert carbon nanotubes and more active fullerene species and can be compatible with a variety of other materials, in particular polymers. In addition to nanobuds for SWCNTs, the nanobuds with graphene, small fullerenes or metal nanobud-like structures are also known. Nanotori cyclic structures are also discussed.

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[ NSN-296 ] Synthesis and Characterization of  $Mn_xZn_{1-x}Fe_2O_4$ : An Optimization of Structural and Magnetic Property for Possible Applications.

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The miniaturization of the electronic systems and low cost production has been generated a wide range applications of ferrite nanoparticles. These nanoparticles have unique properties because of their crystal structure and magnetic behavior, same as photoelectric absorption, temperature and frequency variation makes this material useful for various applications like; electronics, electromagnetic interference shielding, telecommunication and biomedical. The recent researches of these nanomaterials are focused on development of lab techniques (DNA extraction & bacterial isolation), biomedical (vectors for drugs delivery, cancer treatment MRI detection, pulse detection) and electronics (magnetic sensors, EMI Shielding, RADAR).

Considering the latest ongoing researches in the field of magnetic nanoparticles we have selected the  $Mn_xZn_{1-x}Fe_2O_4$  Nanocomposites because of Mn-Zn Ferrites are the most important soft ferrite materials, also their magnetic property variation in ratio of Mn & Zn concentration (magnetic permeability), saturation magnetization, high electrical resistivity, Curie temperature, are properties in terms of high-frequency magnetic applications. This nanomaterial has got especial relevance in biomedicine because has enough biocompatibility, since can be used as magnetic carrier (Bioseparations, enzyme and protein immobilization). Those aspects above give the course to realize a surface modification (inorganic layer, organic molecules or polymers) depending on the future application. This work was carried out to explore the application of magnetic nanoparticles ( $Mn_xZn_{1-x}Fe_2O_4$ ) and study their magnetic behavior with varying doping concentration of Mn and Zn ( $x=0, 0.25, 0.50, 0.75, 0.90, 1.0$ ). These magnetic nanoparticles (MNP) were synthesized via hydrothermal method using citric acid and annealed at 1000 °C temperature for 3 hour to get crystalline Nanopowders. The confirmation of prepared MNP was done using X-Ray diffraction technique with references to JCPDS. The crystallite sizes and structure of prepared MNP were measured using Bragg's diffraction law and the Morphologies were observed using scanning electron microscope. The TEM micrographs were taken to calculate the average particle size distributions. The magnetic properties of these MNP were measured using Vibrating Sample Magnetometer (Lakeshore 7300) that explains the changes in magnetic behavior with reference to doping concentration. In conclusion, ferrites with different doping concentration acts differently in their magnetic property which proves the selectivity and performance of that materials for magnetic sensing and electronic applications, same as a possible surface modification could make it useful for biomedical applications like drug delivery and MRI.



**NSN-299 | Synthesis, characterization and photocatalytic studies of nanoparticles stabilized in/on zeolite hosts**

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There are three main uses for zeolites in industry, the most important being catalysis. The development of nanoscaled host/guest compounds include synthesis of nanomaterials into the zeolites pore voids or external surface of zeolite nanocrystals. Zeolite matrices are excellent materials to support any guest materials due to their chemical and thermal stability and inertness, insulating properties, and transparency from NIR to Far UV ranges. The zeolites can be used for the preparing of the host-guest systems within the environment of the confined nanocage.

In this work semiconductor–mordenite (MOR) composites were synthesized using two methods: by Cd<sup>2+</sup>-Zn<sup>2+</sup>-ion exchange with synthesized NaMOR (I-samples), and by direct synthesis of Zn/Cd-MOR through a sol-gel technique (D-samples). Direct synthesis was performed following the patent application [1]. Both samples were processed by sulfidation treatment in H<sub>2</sub>S flow [2]. It was shown that Cd<sub>x</sub>Zn<sub>y</sub>S<sub>δ</sub>O<sub>γ</sub> semiconductor nanoparticles grow strongly bonded, revealing a core-shell-type arrangement with a wide-open ( $a_0 = 8.33 \text{ \AA}$ ) cubic *fcc* structure. Composition, morphology, and crystalline structures of composites were studied with the combined XRD, SEM, EDS, PL, XPS, UV-Vis and HRTEM analysis. These photoactive composites are promising candidates for applications in the fields of photocatalysis. Results of the atomic, electronic, and compositional structure of Cd<sub>x</sub>Zn<sub>y</sub>S<sub>δ</sub>O<sub>γ</sub>-MOR composites reveal that the nanoparticle compositions follow a parabolic function with a broad range of stoichiometry possibilities. The higher Zn content in the ion exchanged I-[Cd,Zn]-S-MOR composite and the higher Cd content in the directly synthesized D-[Cd,Zn]-S-MOR reveal noticeable differences in the absorbance spectra.

Based on these composites, highly efficient photocatalysts containing Ag-metal and CdZnSO-semiconductor nanoparticles was successfully synthesized and tested on the photodegradation of Orange 30 dye. The Ag-CdZnSO/ZM nanocomposite showed great synergistic interaction between the surface plasmon resonance of the Ag nanoparticles, the photoactive properties of CdZnSO nanoparticles, and the catalytic properties of the zeolite, which leads to the degradation of the dye (99.5% in 90 min, from optical absorbance at  $\lambda = 440 \text{ nm}$ ) [3]. The process consists of an electron transference from the Ag nanoparticle reservoir that avoids the recombination of the high electron-hole generation by the quaternary CdZnSO nanoparticles.

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[ NSN-312 ] Monitoring Raman spectrum of CVD graphene during transfer process

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Between all production techniques of graphene samples, chemical vapor deposition (CVD) is the most promising one in large-scale production [1, 2]. After obtaining CVD grown graphene on copper foil or other metals a transfer process is needed. During this transfer process, samples are in contact with several liquids as ferric nitrate, deionized water and nitric acid, to finally put the sample onto the appropriate substrate for characterization. This transfer process has not been characterized yet, but Raman spectroscopy could be an ideal tool to this end. We do not know which perturbations sample could suffer when it is in contact with a liquid, as those mentioned before. In order to elucidate this interaction we performed in situ Raman spectroscopy during CVD graphene transfer process. This implies that Raman spectra of graphene floating on liquid surfaces was possible to obtain.

CVD at atmospheric pressure was used to synthesize few-layer graphene samples [3]. We found that this material was mainly under mechanical strain when it was on copper, this condition was partially lost when the film was translated on the different liquid surfaces. Mechanical strain produced splitting for G Raman peak of graphene. Finally but not less important, with this in situ Raman study we demonstrate that p-type graphene is obtained until the sample is in contact with nitric acid.

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[ NSN-424 ] The cathodoluminescence technique in the study of point defects in nanomaterials

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The Cathodoluminescence (CL) as a technique adapted in the scanning electron microscope (SEM) permits study locally the electronic transitions of semiconductor nanostructures and nanometric crystals doped with rare earth elements. In this work, we present several examples of the use of this technique for the characterization of point defects in GaN, SnO<sub>2</sub>, ZnO, and hydroxyapatite (HAp) nanostructures, generated by incorporation of different impurities. A CL study of GaN nanowires doped with oxygen revealed the generation of an emission of 2.68 eV that increased in intensity proportionally with their oxygen content. We have attributed this emission to electronic transitions between donor substitutional-oxygen (O<sub>N</sub>) and acceptor interstitial-oxygen (O<sub>i</sub>) state levels.<sup>1</sup> CL spectra obtained from N-doped SnO<sub>2</sub> nanowires revealed that the well known defect-related emission of 2.0 eV decreased in intensity with the nitrogen content in samples, which we have assigned to a reduction of oxygen vacancies in the SnO<sub>2</sub> nanostructures.<sup>2</sup> A CL study of ZnO nanowires permitted demonstrates that incorporation of Ag as impurity do not generate significant point defects in the *wurtzite* structure. In this work we have used the CL technique also to determinate the valence state of Eu and Yb ions incorporated in HAp nanocrystals. Monochromatic CL images obtained from Eu-doped HAp revealed that Eu<sup>2+</sup> ions are distributed homogeneously in the entire crystal volume, while the Eu<sup>3+</sup> are present mainly at the crystal edges.<sup>3</sup> CL spectra of Yb<sup>2+</sup> ions present in HAp display a series of sharp peaks centered at 3.27, 2.98, 2.85, 2.53, 2.27, 2.09 and 1.06 eV, corresponding to transitions between multiple levels produced by a trigonal distortion of the regular octahedral crystal field of the Yb<sup>2+</sup> 4f<sup>13</sup>5d configuration. Similarly, CL spectra of Yb<sup>3+</sup> ions display three emissions centered at 1.16, 1.22 and 1.26 eV, generated by interconfigurational transitions between the <sup>2</sup>F<sub>5/2</sub> and <sup>2</sup>F<sub>7/2</sub> states of Yb<sup>3+</sup> ions.<sup>4</sup>

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[ NSN-528 ] Cubic  $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$  nanostructures on  $\text{GaAs}(001)$  Substrates by RF-MBE

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Cubic  $\text{In}_x\text{Ga}_{1-x}\text{N}$  is one of the most attractive compounds of the III-nitrides family, since its direct band gap can be extended from infrared (c-InN) to ultraviolet (c-GaN), by increasing of the Indium (In) content (x). Furthermore, due to the narrower band gap of cubic nitrides (about 200 meV) compared to that of hexagonal nitrides, the visible spectral range can be covered with less In content. Here, we report the growth of c- $\text{In}_x\text{Ga}_{1-x}\text{N}$  quantum wells (QWs) with c-GaN barriers and c- $\text{In}_x\text{Ga}_{1-x}\text{N}$  films by rf-plasma-assisted molecular beam epitaxy (RF-MBE) on  $\text{GaAs}(001)$  substrates. Cubic c- $\text{In}_x\text{Ga}_{1-x}\text{N}$  QWs with thickness of 10 nm were grown using two methods of synthesis: (1) conventional MBE growth, where the growth surface is exposed simultaneously to three elements In, Ga and N, and (2) MEE growth, that proceeds by alternated periods of N, Ga and In of 4 s each one. The second method was proposed in order to improve the surface diffusion of the ad-atoms (In) at low growth temperatures and to avoid the segregation of (In) on the growth surface. While the c- $\text{In}_x\text{Ga}_{1-x}\text{N}$  films were grown by the conventional MBE growth. The SIMS depth profile allowed us to identify the formation of c- $\text{In}_x\text{Ga}_{1-x}\text{N}$  in the different nanostructures and the corresponding incorporation of In. We found that, by increasing the growth temperature from 480°C to 650°C with the same In flux ( $\text{BEP}_{\text{In}}=1.8 \times 10^{-7}$  Torr), the In content (x) in the nanostructures decreases due to processes such as desorption and segregation, from x=0.27 to x=0.1. We have obtained photoluminescence (PL) emissions at room temperature with peaks between  $E_1=2.0$  eV and  $E_2=1.0$  eV for the different nanostructures, by achieving a strong green emission from c- $\text{In}_x\text{Ga}_{1-x}\text{N}$ . The variation of the PL emission was studied at temperatures varying from 20 to 300K, we observed that the PL peak emission energy and intensity decreases for the nanostructures with increasing temperature.



[ NSN-2 ] Self-assembled InAs Quantum Dashes on GaAs(221) and GaAs(775) High-Index Substrates

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In the last decade, the semiconductor self-assembled quantum dashes (QDHs) has been widely studied in order to develop new generation optical and electronic devices. For their synthesis, the self-assembling of InAs/GaAs quantum dots (QDs) via Stranski–Krastanov growth mode, and the posterior implementation of ordered QDs coalescence methods along one spatial dimension, has been proposed. Consequently, for this approach in order to maximize the QDHs-based devices performance research about the control of the QDs size and their nucleation is required. The molecular beam epitaxial growth on high-index substrates has demonstrated to be an excellent alternative for propitiating self-alignment of QDs on corrugated surfaces. However, since both the nano-channeling and the QDs formation are promoted by strain, when they are combined the resulting physics turns out to be very complex and technologically a great challenge for researchers. In this work, the self-assemble of InAs quantum dashes on high-index GaAs(221)- and GaAs(775)- substrates has been studied. The variation of the arsenic pressure ( $P_{As}$ ) from 3.0 to 6.0  $\times 10^{-6}$  mbar during the growth of GaAs buffer layers resulted on corrugated surfaces. It is demonstrated that these surfaces conduces to the formation of QDHs whose dimensions strongly depends on  $P_{As}$ . For instance, at  $P_{As}=3.0 \times 10^{-6}$  mbar the average height, width and length of the (775) QDHs is 2nm, 30nm and 180nm, respectively; but after increasing  $P_{As}$  to 6.0  $\times 10^{-6}$  mbar these parameters changed to 4nm, 30nm and 1.5 $\mu$ m, respectively. Similar findings were observed for the growth on (211)- oriented substrates, where the length of the dashes was found to be as large as 5 $\mu$ m. The optical characterization of the samples was performed by photoluminescence (PL) spectroscopy. It was found that the PL peak energy position is blue-shifted as  $P_{As}$  is increased, which was attributed to changes in the effective QDHs size caused by the growth on the wavy GaAs surfaces. These results are very promising for the synthesis of semiconductor quantum wires.



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**[ NSN-12 ] Magnetic properties of CoCu nanostructures**

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CoCu nanoalloys have attracted interest due to the giant magneto resistance effect observed in Cu matrices, where the average magnetization per Co atom is lower than for Co films. Theoretical studies on CoCu clusters with up to 147 atoms show icosahedral geometries; these same geometrical arrangements have been obtained in the synthesis of Co@Cu atomic clusters. In this work, we investigate the magnetism in Co@Cu nanoalloys, mainly CoCu<sub>12</sub>, CoCu<sub>54</sub>, Co<sub>13</sub>Cu<sub>42</sub>, besides we considered small Co<sub>x</sub>Cu<sub>y</sub> (x + y ≤ 4) nanostructures, the study was done by using DFT techniques as implemented in VASP code into the plane augmented waves method, we used the exchange-correlation potential given by Perdew-Burke-Ernzerhoff. Our results show that for Co@Cu clusters the icosahedral structure was preferred and the magnetization of the cluster takes the same value as the isolated Co cluster; whereas for small clusters prefer planar geometries and the value of the total magnetization depends on the number of Co atoms in the cluster.

This work was done with financial support of CONACyT with "Proyecto Apoyado por el Fondo Sectorial de Investigación para la Educación" with reference number 237882.



[ NSN-29 ] The effect of metal deposition order on the synergistic activity of bimetallic gold catalysts for oxidation of carbon monoxide

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The synergism of catalytic activity is a sharp increase in the reaction rate in the presence of a bimetallic catalyst ( $M_1-M_2/\text{support}$ ) as compared with the sum of the reaction rates in the presence of monometallic analogues ( $M_1/\text{support}$  and  $M_2/\text{support}$ ). Study of the synergistic effects in CO oxidation is of obvious interest for developing new approaches to the synthesis of high-performance and stable catalysts able to oxidize CO at room temperature. Despite the substantial array of experimental data, the development of optimal synergistic catalysts is still hampered by poor knowledge of the nature of active sites and the reaction mechanism.

Herein, some monometallic Au/Al<sub>2</sub>O<sub>3</sub>, M/Al<sub>2</sub>O<sub>3</sub> (M is Cu or Ce) catalysts and bimetallic catalysts with simultaneously (Au+M) and sequentially (M/Au, Au/M) deposited metals were prepared. Oxidation of carbon monoxide in the presence of these catalysts at 50-450 °C was studied. The activity of the catalysts increases in the following series: M/Au/Al<sub>2</sub>O<sub>3</sub> > Au/M/Al<sub>2</sub>O<sub>3</sub> > (Au+M)/Al<sub>2</sub>O<sub>3</sub> > Cu/Al<sub>2</sub>O<sub>3</sub> > Au/Al<sub>2</sub>O<sub>3</sub> > Ce/Al<sub>2</sub>O<sub>3</sub>. A synergistic effect was detected at 50-250 °C: bimetallic catalysts converted up to 50 % of CO to CO<sub>2</sub>, while the monometallic samples were inactive. Increasing the reaction temperature above 250 °C results in a decreased synergistic effect, although bimetallic catalysts still possess good activity. The electronic and structural organization of the catalyst active sites before and after the reaction were studied by means of XRD, TEM, EDX, XPS, and DRIFTS techniques. The causes for the synergistic effect and the reaction mechanism in the presence of synergistic catalysts are proposed and discussed.

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**[ NSN-36 ] Electronic and magnetic properties of lowest energy structures of NiAg nanoalloys.**

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The Ni-Ag nanosystem has been studied widely, experimentally and theoretically, both results show an absence in mixing atoms, i.e., these nanostructures show core-shell geometries, Ni@Ag. This behavior is very similar at macroscopic level. In this study, we show the global minimum structures of small NiAg<sub>n</sub>, Ni<sub>n</sub>Ag nanoalloys with  $1 \leq n \leq 7$ , and Ni<sub>n</sub>@Ag<sub>m</sub> with  $n + m = 13$  and  $n + m = 55$  with an icosahedral geometries preferently all the clusters considered here show a magnetic behavior. We used the density functional theory as implemented in SIESTA code, into de generalized gradient approximation parameterized by Perdew-Burke and Ernzerhoff considering core corrections and we considered relativistic effects in the pseudopotentials.

Besides we have considered the VASP code in this study and the results did not show significative changes in the lowest energy structures and in the magnetic behavior.



**[ NSN-49 ] Mono and bi-metallic nanoparticles of Au and Au@Ag at room temperature - Optical properties and application**

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Gold and gold-silver nanoparticles (AuNPs and AuAgNPs) can be used in a variety of applications, thus efficient methods to produce them are necessary. In this paper, a competitive and efficient method for frabricación colloidal nanostructures, using non-toxic reducing agents is presented. The experimental process is carried out at room temperature to prevent possible toxic vapors that occur in different production methods of nanomaterials. Optic analysis showed two absorption bands centered in 520 nm and 480 nm, associated with surface Plasmon as function of AuNPs and AuAgNPs respectively, similar to those reported in the literatura. The nanoparticles synthesized have an approximate diameter of 10 - 20 nm, seen by the transmission electron microscopy (TEM). The presence of Au and Ag in these particles was corroborated by energy dispersive X-ray spectroscopy (EDS). Additionally, Mie y Fuchs theories were used to predict the location of the absorption bands linked to the plasmon surface in gold nanoparticles. The Surface Enhanced Raman Spectroscopy (SERS) effect was analyzed considering natural zeolite (Chabazite) as analyte, in order to determinate its possible application in soil analysis.



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**[ NSN-68 ] Controlled coating of magnetite nanocubes with SiO<sub>2</sub>**

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Cubes of magnetite in nanometric range was coating with the aim of avoid the agglomeration phenomena, including a physical barrier of amorphous silica. The cubes was obtained by sonochemical method. The methodology of nanocubes coating with silica was realized as follows: functionalization of nanocubes with PVP in aqueous solution, dispersion of the functionalized nanocubes in etanol and ammonia solution and addition of different amounts of TEOS in the solution and sonicated for 1 hour for propitiate the formation of silica. We investigate the influence of concentration of TEOS in the coating thickness. The characterization of nanostructures was performed using TEM, XRD and UV-Vis techniques. The results of this investigation brings information of the control in the thickness of silica with the objective of minimized the agglomeration effects in the magnetite nanostructures.



[ NSN-77 ] Vibrational properties of Ag and Au Nanoparticles obtained by green synthesis

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This study reports the synthesis and characterization of gold and silver nanoparticles through an ecological method to obtain nanostructures from the extract of the plant *Opuntia ficus-indica*. Colloidal nanoparticles show sizes that vary between 10-20 nm, and present various geometric morphologies. The samples were characterized through optical absorption, Raman Spectroscopy and Transmission Electron Microscopy (TEM). Additionally, low energy metallic clusters of Au<sub>n</sub> and Ag<sub>n</sub> (n=2-20 atoms) were modeled by computational quantum chemistry. The theoretical results were obtained with Density Functional Theory (DFT). The predicted results of Au and Ag clusters show a tendency and are correlated with the experimental results concerning the optical absorption bands and Raman spectroscopy in gold nanoparticles.

**Keywords:** nanoparticles; Green synthesis; Low-energy structures; Radial Breathing Modes.



[ NSN-97 ] Nanostructured CuO and ZnO adsorbents for biogas desulfurization

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Synthesis, structural characterization and chemical evaluation (desulfurization) of 1D nanostructured zinc and copper oxides were realized. The hydrogen sulfide removal was also realized using non nanostructured materials in order to compare size effects in the reaction. The materials were synthesized by wet chemical routes. CuO nanowires were obtained mixing copper chloride and sodium hydroxide precursor solutions at 60 °C. The ZnO nanorods were prepared by seed assisted nucleation in chemical bath deposition at 90 °C by 3h with hexamethylenetetramine and zinc nitrate as reactants and finally it was thermally treated at 360 °C for 2 hours. In both cases, PEG was added into solutions as stabilizer agent. Grazing incidence X-ray diffraction shows wurtzite hexagonal phase for ZnO and monoclinic tenorite for CuO with domains ranging between 180-200 and 10-30 nm, respectively. X-ray energy and wavelength dispersive spectroscopies show elemental analysis in concordance with stoichiometric phases, although the purity in non nanostructured materials were lower, ca. to 92 % w/w.

The desulfurization reactions were performed at atmospheric pressure and room temperature using a fixed-bed glass reactor (i.d.= 5 mm, L/D=30) loaded with 4 g of material for each test. H<sub>2</sub>S 100 ppm (N<sub>2</sub> as balance) was used as reactant, and it was feed at 450 ml/min (GHSV 9120 h<sup>-1</sup>). The effluent gas analysis was realized using a M-560 (Sewerin) biogas detector, coupled with electrochemical H<sub>2</sub>S sensor (0-2000 ppm, ± 2). Results show that CuO and ZnO are feasible adsorbents for hydrogen sulfide removal but they have saturated at ca. 5 min. after the reaction begins. The characterization of wasted adsorbents shows evidence of the sulfur presence (obtained by WDXRF, SEM and TEM) at amounts less than 0.2% w/w, but no phase was detected neither FTIR nor XRD analysis. An effort to explain both, the chemical nature of the sulfur species, but also the size effects was done.

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[ NSN-123 ] Preparation of Trirutile-Type Magnesium Oxide Nanostructures for their Potential Application as Gas Sensors

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The ability of trirutile-type magnesium oxide to detect concentrations of carbon monoxide (CO) and propane (C<sub>3</sub>H<sub>8</sub>) at different temperatures was investigated in this work. The synthesis of the compound was done using the colloidal method in the presence of ethylenediamine. The crystalline phase was confirmed by X-ray diffraction, possessing a trirutile-type structure with cell parameters  $a = 4.64 \text{ \AA}$  and  $c = 9.25 \text{ \AA}$ , and space group P4<sub>2</sub>/mnm. The morphology, the porosity and the particle size were analyzed by means of scanning electron microscopy (SEM), observing the presence of rods with lengths in the range of 0.2 to 1.6  $\mu\text{m}$ , approximately. For a finer microstructure analysis of the material, a transmission electron microscope (TEM) was employed. It was possible to observe the formation of nanorods with a length of 86 nm and a diameter of 23.8 nm, approximately. For the testing of the gases, pellets were produced with powders of magnesium oxide calcined at 800 °C. The pellets were exposed to atmospheres of carbon monoxide (CO) and propane (C<sub>3</sub>H<sub>8</sub>) at different concentrations and operating temperatures (23-300 °C). The results indicate that the trirutile-type magnesium oxide possesses excellent thermal stability and high sensitivity in CO and C<sub>3</sub>H<sub>8</sub> atmospheres, making it a strong candidate as a gas sensor.



[ NSN-124 ] Study of the Electrical Properties of Trirutile-Type Zinc Oxide in CO and C<sub>3</sub>H<sub>8</sub>  
Atmospheres

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In this work, the electrical properties of trirutile-type zinc oxide were measured in carbon monoxide (CO) and propane (C<sub>3</sub>H<sub>8</sub>) atmospheres. The material was synthesized by a microwave-assisted method and calcined at 600 °C. The crystal structure was confirmed by X-ray diffraction, which showed cell parameters  $a = 4.66 \text{ \AA}$  and  $c = 9.26 \text{ \AA}$ , and space group P4<sub>2</sub>/mmn. To support our material's analysis, the vibrational modes of the crystal lattice were investigated by means of Raman spectroscopy, and the microstructural features were studied by means of scanning electron microscopy (SEM). It was observed with the latter the growth of microwires and microrods on the entire surface. The material's morphology was analyzed by means of transmission electron microscopy (TEM). The length and diameter of the microrods were estimated to be of approximately 6.6  $\mu\text{m}$  and 0.9  $\mu\text{m}$ , respectively. For the testing of the material's electrical properties in the presence of gases, pellets were made with zinc oxide powders and exposed to atmospheres of carbon monoxide (CO) and propane (C<sub>3</sub>H<sub>8</sub>), at different gas concentrations and operation temperature. According to our results, the trirutile-type zinc oxide possesses high sensitivity at a temperature of 250 °C, making it a strong candidate for its application as a gas sensor.



[ NSN-151 ] Synthesis of copper oxide nanoparticles via laser ablation in liquids

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Nanoparticles, defined as those particles with diameter less than 100 nm, have been extensively investigated due to their unique physical, chemical and electrical properties which are different from those of bulk metals. Today, these materials are widely implemented as functional elements in plastics, lacquers, and ceramic products. Novel applications are targeted on medical diagnostics, sensing, electronics, optics and biophotonics. However, application prospects of conventionally synthesized nanomaterials are often complicated because of their toxicity, caused by contamination with chemical precursors or additives and reaction products which are impossible to separate from the liquid. Laser ablation of solids in liquids has shown itself as a simple technique basically free from these issues since the nanoparticles are produced owing to the mechanical interaction of dense vapor of the liquid with molten layer on the target surface. Copper oxides based materials with relevance to high temperature superconductivity and semiconducting antiferromagnetism, have received extensive investigations for their prospective applications in many fields such as powerful heterogeneous catalysts, solar energy conversion, batteries and field emission emitters.

In this project, laser ablation of a copper target under pulsed high power Nd: YAG laser, in 2-propanol, varying the wavelength, time and power, was performed in order to obtain copper oxide nanoparticles. Transmission electron microscopy (TEM), high resolution transmission electron microscopy (HRTEM), UV-visible, and X-ray diffractometry were used to analyze the resulted copper oxide nanoparticles.

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[ NSN-181 ] Analysis of negative refraction in a bimetallic-dielectric superlattice

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An interesting phenomenon observed in some periodic structures is the negative refraction. These structures called metamaterials are composed of metal and dielectric. Generally, negative index metamaterials (NIM) simultaneously possess negative permeability and permittivity or, in other cases, strong chirality. Nevertheless, the negative refraction can also be observed in anisotropic media, for instance, a metal-dielectric superlattice has negative index of refraction in the frequency interval where the effective permittivity principal values, corresponding to the directions parallel and perpendicular to the planes of the layers, have opposite signs. In this work, we consider another type of superlattice, namely, a periodic nanostructure composed of two alternating layers, one is an anisotropic bimetallic medium and the other one is a dielectric. The anisotropic material is, in fact, a homogenized superlattice, composed of two alternating metallic layers and characterized by an effective permittivity tensor. We have used Drude model to describe the frequency dependence of the permittivities for the metal components. With these metal parameters, we have calculated the components of the average permittivity tensor for the bimetallic stratified medium in the long wavelength limit [1]. Besides, the dispersion relation and the optical spectra (reflectivity and transmissivity) for s- and p-polarized electromagnetic modes in the bimetallic-dielectric superlattice were calculated and analyzed. It was found that both reflectivity and transmissivity spectra exhibit narrow pass bands with either negative or positive dispersion and are associated with two types of Fabry-Perot resonances, one in the anisotropic bimetallic material and the other in the dielectric slab. For the p-polarization geometry, the resonances inside the bimetallic layer appear above the lower plasma frequency, whereas in the case of s-polarization, such resonances are observed at much larger frequencies.

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**[ NSN-184 ] Morphological, structural and optical properties of ZnO thin solid films conformed by nanoleafs or micron/submicron cauliflowers.**

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Thin films of ZnO conformed by nano and microstructures were successfully synthesized by using pyrolysis technique. At first glance the films resulted divided in 7 zones that were morphologically analyzed. The largest and therefore the main zone was formed by nanoleafs. Studies on morphology, structure and optical properties of these nano leafs were obtained and correlated too. These studies reveal nanostructured films entirely conformed by nanoparticles of 25 nm wide and 200 nm long with energy gap = 3.26 eV and hexagonal polycrystalline structure invariant to changes in technique parameters. Preliminary studies on structural defects as a function of depth profile of the film were done. An energy diagram is proposed. This diagram summarizes all measurements done about: UV-VIS reflectance, cathodoluminescence and photoluminescence, and shows the existing paths for de-excitation processes in ZnO nano leafs. It became the confrontation model with results obtained by other research groups.



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**[ NSN-185 ] Thin films of CdS:Cu, morphological, optical, structural and electrical properties**

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Thin solid films of CdS:Cu were synthesized using a wet-chemical. Doping was by thermal diffusion. Films were obtained as a function of: precursor salts, deposition time and annealing temperature. Studies of transmittance, resistivity, photoluminescence at room temperature, X-ray diffraction, high-resolution scanning and transmission electron microscopies, were performed. The CdS and CdS:Cu films obtained had an average thickness of 130 nm and 160 nm, respectively. This study provides evidence of the greater effectiveness of sodium citrate than ammonium chloride as a complexing agent. The crystalline phase of the films was cubic and did not vary with deposition time or the precursor. Studies were consistent in showing a film made up of regularly spaced, asterisk-shaped entities of about 35 nm in size, which in turn were composed of nanocrystals smaller than 10 nm. The resulting films behaved as an n-type semiconductor with an energy gap of about 2.38 eV that varied only slightly with deposition time and the precursors' nature, but increased to 2.93 eV with Cu doping. The resistivity achieved was  $5.822 \times 10^{-5} \Omega\text{-cm}$ . The PL emission spectra showed variation in optical quality and revealed a de-excitation mechanism due to the presence of cadmium vacancies, sulfur vacancies and interstitial cadmium.



[ NSN-205 ] Growth of alumina oxide nanowires

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Alumina oxide nanowires were grown using a two-step anodization of aluminum foil as a consequence of experiment to obtain alumina oxide nanopores. These nanowires are formed using chemical etching methods. An electric field and stress are necessary to grow these nanowires, and the nano-imprinted metal surface of the aluminum foil has an important role.

A porous anodic aluminium oxide template was prepared by anodizing high purity (99.9%) aluminum film (1 cm<sup>2</sup> area, 0.5 and 0.13 mm thickness) in oxalic acid solution as an electrolyte. In order to investigate the effect of the time of first anodization on the pore diameters, four samples were prepared in different times in sodium oxalate solution diluted in 0.5 to 2M concentrations at 58°C and 10, 20, 30, 60, 120, 180 y 240 minutes of anodizing times. The samples showed structures like fibers, nanowires and nanopores with several characteristics depending on the parameters of fabrication.

Several techniques, such as Scanning Electron Microscopy (SEM), Energy Dispersive Spectrum (EDS) and photoluminescence were employed to study the structure of AAO templates and alumina nanopores and nanowires.



[ NSN-211 ] Coupling between graphene and intersubband collective excitations in quantum wells

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Recently, strong light-matter coupling between the electromagnetic modes in plasmonic metasurfaces with quantum-engineering electronic intersubband transitions in quantum wells has been demonstrated experimentally [1, 2]. These novel materials combining different two-dimensional electronic systems offer new opportunities for applications and fundamental studies of collective excitations driven by interlayer Coulomb interactions. In this work, our aim is to study the plasmon spectrum of a structure consisting of conventional two-dimensional electron gas (2DEG) immersed in a semiconductor quantum well and a graphene sheet with an interlayer separation of  $d$ . We use a simple model in which the quantum well has infinite barriers and within the self-consistent-field linear approximation both the intrasubband and intersubband plasmon modes interacting with the graphene collective excitations are obtained. Here we calculate the dispersion of these relativistic/nonrelativistic new plasmon modes taking into account the thickness of the quantum well providing analytical expressions in the long-wavelength limit.

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[ NSN-213 ] Surface structure formation of 1.0-MeV Au<sup>+</sup> ion bombardment of Ti and Ti-6Al-4V

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In the present work, we describe surface nanostructure formation produced by 1.0 MeV Au<sup>+</sup> ion implantation on two polycrystalline materials: Ti and Ti-6Al-4V. Ion implantation was performed utilizing the 3 MV Pelletron accelerator of the Instituto de Física at UNAM. Two experimental conditions were studied for both materials. In the first case a fixed angle of incidence at 45° with four different fluences was studied. In the second set of experiments; 23°, 49° and 67° angles of incidence with fluences of 10<sup>16</sup> up to 10<sup>17</sup> ions cm<sup>-2</sup>. Analysis by scanning electron and atomic force microscopies shows the formation of surface ripples with typical dimensions in the nano and micrometer range. Ripple formation at these particular experimental conditions is seen to be independent of the material, but dependent on the fluence of implanted ions. The interpretation of these structures is presented using statistical tools (Gwyddion code). These nanostructures have potential for orthopaedic implant applications.

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**[ NSN-220 ] Quantum transport in self-affine graphene-based structures**

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Two-dimensional materials offer an excellent platform to study electron transport in complex geometries [1,2]. Here, we study the electron transport in self-affine graphene-based structures. The transfer matrix approach and the Landauer-Büttiker formula have been used to compute the transmission probability and the linear-regime conductance, respectively. Specifically, we find that both the transmission probability and the conductance show self-similar patterns with well defined rules. We consider that the case of the conductance is quite important, since it is a measurable quantity, and it opens the door to test that the geometrical characteristics of a system can be manifested in physical quantities.

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2. D. S. Díaz-Guerrero, L. M. Gaggero-Sager, I. Rodríguez-Vargas and O. Sotolongo-Costa, Europhysics Letter 111, 57006 (2015).



[ NSN-226 ] Seebeck effect in Thue-Morse graphene-based structures

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Graphene is not a good thermoelectric material due to its outstanding electrical and thermal conductivities. However, if we nanostructured it, it is possible to improve substantially the thermopower factor, and with it enhance considerably the figure of merit [1]. Here, we study the Seebeck effect in Thue-Morse graphene-based structure. In particular, we focus our attention to quasi-periodicity, provided by the Thue-Morse arrangement of potential barriers in graphene (nanostructuring), on the Seebeck coefficient. We have implemented the transfer matrix approach, the Landauer-Büttiker formula and the Cutler-Mott formula to compute the transmission, conductance and Seebeck coefficient, respectively. We have found that the quasi-periodicity is beneficial to the thermopower, since the interplay between long and short order filters the electron propagation improving considerably the Seebeck coefficient.

1. P. Dollfus, V. H. Nguyen and J. Saint-Martin, J. Phys.: Condens. Matter 27, 133204 (2015).



**[ NSN-229 ] Is microwave treatment the better way for exchange? A comprehensive analysis of copper-exchanged sodium mordenites prepared by the routine and microwave methods**

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Copper-exchange zeolites are highly promising materials for heterogeneous catalysts and are used in numerous of chemical reactions, especially for reduction of NO<sub>x</sub> (de-NO<sub>x</sub> catalysts) [1]. The multiple researches revealed that their catalytic properties are governed by both the valence state of copper ions and their location and coordination in the zeolite lattice [2].

Recent development of microwave-assisted treatment of materials imparted a new impact in development of material chemistry [3]. Being simple, inexpensive, and efficient nonconventional heating methods microwaves (MWs) technique is well established in the field of alternative methods in the synthesis of emerging materials, including zeolites [3,4]. Recent study of copper-exchanged mordenites with different counter-ions prepared by ordinary conventional method and MWs technics have shown that the preparation method influences copper and water content, copper surrounding, but does not change the electronic state of copper ions [3,5]. It has been found that samples obtained from sodium mordenite exhibit the more effective exchange; moreover, the MWs procedure is more efficacious for all the type of compensating cations in the starting samples.

As far as zeolites are complex systems, their analysis requires applying of complementary methods. Together with X-ray diffraction (XRD), Energy Dispersive Spectroscopy (EDS) and Inductively Coupled Plasma - Optical Emission spectroscopy (ICP) methods, which are sensitive to the structure and composition, it is necessary to apply methods those are sensitive to the local environment of selected atoms and electronic structure. thermogravimetric analysis (TGA). We select Nuclear Magnetic Resonance (NMR), which is sensible to local environment of the nuclear probe, and X-ray photoelectron spectroscopy (XPS), which are powerful instruments to describe the local composition and electronic state of materials. XPS has become an important tool for zeolite study, because it is suitable not only for study of electronic states and coordination of copper ions in zeolites [5] but for determining elemental compositions of zeolite too. However, both EDS and XPS methods are the surface ones: XPS provides information on the electronic state and chemical composition on the penetration depth between 1 and 10 nm, EDS has a deeper access, up to 1000 nm. To study the bulk composition ICP is usually applied. Thus, knowing the compositions of the surface layers of two different thicknesses and of the volume one can



analyze their differences and the elements distribution between the surface and the bulk (including the location of exchangeable cations).

In this contribution we report on the comparative analysis of copper-exchanged sodium mordenites prepared by the routine and MWs methods. As soon as a single exchange does not lead to the complete replacement of starting sodium counter cations [3] to increase the copper content we repeat the exchange procedure several times.

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**[ NSN-231 ] Synthesis and Characterization of Nanostructured NiSb<sub>2</sub>O<sub>6</sub> Powders**

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Nanoscaled inorganic materials such as nanorods, nanowires and nanotubes, have had a huge impact on many fields of scientific research because they show interesting physical and chemical properties. The control of the particle form and size is strictly necessary for their potential applications. Therefore, new synthesis techniques are required to achieve that. In this work, we employed a microwave-assisted colloidal method for the preparation of nanostructured NiSb<sub>2</sub>O<sub>6</sub>. The colloidal solution was obtained mixing the reagents (antimony trichloride, magnesium nitrate and ethylenediamine) in ethyl alcohol, stirring for 24 h at room temperature. The solvent was evaporated by low power microwave radiation in order to obtain a solid precursor material. The thermal decomposition of the precursor led to the formation of NiSb<sub>2</sub>O<sub>6</sub> at 600 °C. X-ray powder diffraction was used to identify a tetragonal crystal structure, with cell parameters  $a = 4.641 \text{ \AA}$ ,  $c = 9.223 \text{ \AA}$  and space group P4<sub>2</sub>/mnm. Using scanning electron microscopy (SEM), microrods and microparticles were observed. To support the identification of the nanostructured particles, Transmission Electron Microscopy (TEM) was employed.



**[ NSN-232 ] Hexagonal single-crystal domains of single and few layer graphene grown from pencil graphite**

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Hexagonal-shaped single crystal domains of single layer graphene (SLG) are synthesized on copper foil substrates by thermal diffusion of graphite traces hand-drawn with a sharpened school pencil. Substrates with pencil outlined patterns are heated for 15 minutes at 1050 °C in a cylindrical oven under a flow of an Argon/Hydrogen gas mixture. We study SLG growth from patterned pencil traces drawn as single straight lines and square-shaped patterns of lines with different side lengths. Scanning electron microscopy and atomic force microscopy reveal that the graphene domains have hexagonal shape oriented according copper surface grains and defects. Raman scattering analysis show that the domains are mostly single and double layered. HRTEM and electron diffraction observation of individual isolated domains reveal they are single crystals. Variation of side lengths in squared-shaped line patterns allow to study the dynamics of lateral growth of SLG stemming from patterned lines. For short enough side lengths, SLG originating from neighboring lines crash with each other and become multiple layered and polycrystalline.



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**[ NSN-248 ] Nylon fibers with copper nanoparticles**

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This project presents the development of a composite from copper nanoparticles and nylon 6,6 nanofibers. Copper nanoparticles (CuNps) were obtained by wet chemical synthesis in presence of reducing and complexing agents. The composite was obtained from electrospinning a mixture of CuNps and nylon. Copper nanoparticle size was measured by Dynamic light scattering (DLS) with an average of 20 nm was observed. Composite fibers were characterized by infrared and Raman spectroscopy. Nylon fibers were electrospun with CuNps and without them in order to compare them. The infrared spectroscopy denoted a change in intensities from characteristic functional groups of intermolecular structure of nylon, Raman spectroscopy showed a crystalline phase  $\gamma$  of nylon, determined by characteristic reflecting bands of this crystalline phase Scanning Electron Microscope (SEM), allowed to observe a fibrillar, lineal, homogeneous morphology, with an average size of 100 nm and the presence of copper nanoparticles.



[ NSN-258 ] Growth and Characterization of MoS<sub>2</sub> Monolayers

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Monolayer transition metal dichalcogenides (TMDs) exhibit unique physical properties, specially MoS<sub>2</sub> has been largely studied over the past five years showing a huge potential in optoelectronics and nanoelectronics applications.

In this work we present a method to obtain single monolayer MoS<sub>2</sub> crystals based on Chemical Vapor Deposition (CVD) technique. MoO<sub>3</sub> and sulfur precursors are placed inside the quartz tube, 100 sccm of Ar is used as a carrier gas and the growth temperature is set at 750°C during 10 minutes. MoS<sub>2</sub> Crystals morphology are studied using Scanning Electron Microscopy (SEM) showing triangular shapes with 15 μm size. Atomic Force Microscopy (AFM) revealed a thickness of ~7.5 Angstroms expected from a typical TMD monolayer (W, 2013). Optical properties were studied by means of Raman and Photoluminescence. Raman spectra show two contributions related to E<sub>2g</sub> and A<sub>1g</sub> modes, the separation of these two modes is 20 cm<sup>-1</sup> confirming the presence of a single monolayer (al., 2014). On the other hand, photoluminescence spectrum has an intense main peak around 1.84 eV which is attributed to the MoS<sub>2</sub> monolayer bandgap, it suggests that single monolayer MoS<sub>2</sub> has a highly crystallinity (Zande, 2013).

These results show that MoS<sub>2</sub> crystals can be potentially used as photodetectors, light emitting diodes, phototransistors which are of major interest of the electronic industry.

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**[ NSN-263 ] Recycled aluminum reinforced with carbon nanotubes for its use in spatial truss structures.**

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Actual environmental situations requires actual solutions integrating technology and reuse of waste materials. This, will allow the reduction or prevention of the continuous degradation of the ecosystems and environmental problems. This investigation propose a composite made with recycled aluminum from beverage cans alloy with carbon nanotubes to provide structural properties for its use in spatial truss.

According to the SENER (Mexican Energy Secretary), the total national energy consumption in 2014 was of 8,624.26 PJ, from which 18.18% was produced by the industry. From this last percentage, the 13.5% was exclusively by the steel and iron production. Aluminum on the other hand, requires about 168 GJ/T to be produced from the mineral  $Al_2O_3$  but only 7 GJ/T to produce the same amount from scrap. Aluminum's high strength-weight ratio has been very useful in the construction, aerospace and automotive areas. Recycled aluminum made of melted cans has a hardness of 75 HV which according to Vickers Hardness Conversion Table its yield strength is also 240 Mpa and this proves stability after recycled.

Even when aluminum shows corrosion resistance qualities, isn't a material used for structural purposes. Therefore, many recent experiments have shown the benefits of the addition of nanotubes in the aluminum matrix giving to the metal higher load capacity and fatigue resistance improvement.

1 mg of dispersed multi-walled carbon nanotubes in percentages of volume of 0.05%, 0.1%, 0.5%, 1%, 2%, 5%, 7% and 10% are added to the liquid aluminum to form specific measuring samples corresponding to ASTM E-8 norm for tensile and compressive tests. Scanning electron microscopy, X-ray and transmission electron microscopy tests shows porosity percentage, aluminum structure and nanotubes distribution.

Mechanical resistance properties such as elastic modulus and real strength obtained from these test are introduced in a structural software to realize and analysis of a spatial truss with 288 elements, 85 nodes and 255 freedom degrees. Diverse loads are applied in order to get to know the deformation of the elements and nodes displacement.



[ NSN-277 ] Synthesis of SrAl<sub>12</sub>O<sub>19</sub> activated with La<sup>3+</sup>, Eu<sup>2+</sup>, Nd<sup>3+</sup> ions and decorated with carbon nanoparticles.

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In the recent years, an increasing interest is observed in the area of phosphors with visible quantum efficiencies major than 100% under the excitation of vacuum ultraviolet radiation. In this work, we studied the synthesis of strontium hexa-aluminate activated with La<sup>3+</sup>, Nd<sup>3+</sup> and Eu<sup>2+</sup> ions and containing carbon nanoparticles obtained by the spay-pyrolisis method. An efficient phosphor can be prepared by this way at reaction temperature range of 700-800<sup>0</sup>C for a 5-20 min. The effects of co-doping ions, M = La<sup>3+</sup>, Nd<sup>3+</sup>, Eu<sup>2+</sup> on the luminescent properties of SrAl<sub>12</sub>O<sub>19</sub>:M were investigated. The morphology and shape of samples were studied by SEM, AFM, and powder X-ray difracction. Optical properties were also elucidated. It was shown that the luminescence of SrAl<sub>12</sub>O<sub>19</sub>:M consists of a 5d—4f broad-band emission and of 4f—4f lines; their relative intensities are strongly dependent on temperature.



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**[ NSN-279 ] Fabrication of carbon nanoparticles vía spray pyrolysis method using metal phthalocyanines as catalyst precursors.**

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In this work, the synthesis of carbon nanoparticles was carried out vía spray pyrolysis using toluene solution with suspended zinc, copper, nickel or magnesium phthalocyanines as precursors of metallic particles serving as catalysts for carbon phase formation. The process was conducted in a range of temperatures in a nitrogen atmosphere in a quartz tube, containing borosilicate glass supports, onto which surface the nanometric layers of nanoparticles were deposited. The samples were analyzed by SEM, TEM and IR-spectroscopy; their conductivity was measured vía Kelvin technique. The properties of formed nanolayers were analyzed according to metal nature in the phthalocyanine, temperature, carrier gas speed, and other process parameters. Possible MEMS applications of thus fabricated nanolayers are discussed.



[ NSN-281 ] **Magnetic forest-like carbon nanostructures doped with silver nanoparticles as antibacterial materials for water filters.**

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In this work, forests of multiwall carbon nanotubes (MWCNTs) were functionalized using two different methods and silver nanoparticles were further incorporated in them. Characterization was made by Raman spectroscopy, Transmission Electron Microscopy (TEM), among other methods; the antibacterial property was measured using method of dilution and plating. The equipment of the 4 points was used to measure the resistivity of the nanocomposites by Kelvin method making thin films by spin coating technique. It was shown that multiwall carbon nanotubes containing silver nanoparticles possess an increased conductivity of the nanocomposite. The formed nanocomposites could be used as water-purifying materials in water filters.

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[ NSN-282 ] Formation of graphene from graphite by non-standard route in mild conditions using theraphthal and ascorbic acid.

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Graphene sheets were formed in water as a result of dispersion and destruction of graphite in mild conditions using a water-soluble cobalt octacarboxyphthalocyanine derivative theraphthal (TP) together with ascorbic acid (AA) in ultrasonic treatment conditions. The synthesis was carried out using different amounts of graphite, AA and TP, which were ultrasonicated in 30 mL flasks with DI water for 5 h in ultrasonic cleaner at 42-45°C. The fact of graphite decomposition in these conditions is out of conventional concepts on classic  $\pi$ - $\pi$  stacking interactions and/or  $\sigma$ -bonding between macrocycles and carbon phases. Destruction of graphite forming partialy oxidized graphene are explained by free radical processes in the system TP-AA in strong cavitation conditions. Partial destruction of TP slowly takes place and it is known to be accompanied by formation of Reactive Oxygen Species (ROS). TP can be first coordinated to graphite surface via  $\sigma$ - $\sigma$ -stacking through aromatic supramolecular ring or covalently through COO<sup>-</sup> group(s) in the TP molecule.



[ NSN-283 ] Non-conventional synthesis of carbon nano-ribbons by the low-temperature unfolding of MWCNTs via interaction with theraphthal and ascorbic acid.

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The treatment of MWCNTs with the water-soluble cobalt octacarboxyphthalocyanine derivative theraphthal (TP, a cancer therapy drug) under ultrasonic conditions in the presence of ascorbic acid (AA) led to the dispersion and unfolding of MWCNTs, producing ribbon-like nanostructures (NRs) at low temperatures (<50°C). The synthesis was carried out using different amounts of slightly magnetic MWCNTs, AA and TP, which were ultrasonicated in 30 mL flasks with DI water for 5 h in ultrasonic cleaner at 42-45°C. In these conditions, even at low intensity ultrasound in cleaners (20-40 kHz), partial destruction of TP slowly takes place and it is known to be accompanied by formation of Reactive Oxygen Species (ROS). TP can be first coordinated to CNT surface via  $\pi$ - $\pi$ -stacking through aromatic supramolecular ring or covalently through COO<sup>-</sup> group(s) of the TP molecule. Unfolding of MWCNTs in the conditions of TP/AA addition can be explained by the *in situ* formation of ROS in TP solutions under ultrasonic treatment and their further attack on MWCNTs surface, destroying and unfolding them forming graphene sheets and ribbons. The obtained results differ from the conventional concepts of classic  $\pi$ - $\pi$  stacking interactions and/or  $\sigma$ -bonding between macrocycles and carbon nanotubes.



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[ NSN-303 ] High resolution measurement of water levels in high vacuum environments

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Vacuum chambers (VCs) require to be free of contaminants. Unfortunately, even when the air has been suctioned from VCs, at low pressures, the stainless steel vacuum chamber outgas adsorbed impurities. Since water molecules are an important fraction of these contaminants, monitoring water levels inside VCs is required. In this work, our group proposes a measurement system, which is able to measure small concentrations of any target chemical compound, in this case water. The measurement system encompass a zeolite coated quartz crystal microbalance (QCM) and a frequency meter. In the sensory part, the zeolite is capable to selectively adsorb molecules in its porosity. When a QCM is coated with a sensitive layer –in this case zeolite capable to adsorb water molecules– there is a frequency shift corresponding to the mass loading in the surface of the QCM. With basis in the last statement, it is clear that in order to quantify the adsorbed mass, a highly accurate frequency counter/meter is required. Unfortunately, because of low level of impurities in VCs, and consequently, low mass values, the frequency shift is several orders of magnitude below the nominal frequency of the QCM. That is why the state of the art of frequency counter/meters require long time for getting good approximations. And if better approximations to the desired frequency are required, more time for measuring is needed.

The core of the proposed frequency meter is the application of the principle of rational approximations. This allows to measure any frequency value with high accuracy in a very short time. As the result, our measurement system is capable to achieve resolution of 2.7 ng, which is  $9.03 \times 10^{13}$  water molecules adsorbed by zeolite, or loaded in the surface of the QCM.



**[ NSN-304 ] Methylene Blue degradation using nanocomposites of TiO<sub>2</sub>-Reduced Graphene oxide as photocatalyst material synthesized by solvothermal method**

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The organic decontamination by photocatalytic degradation has been successfully studied. The principal characteristic is the potential in environmental application such as air and water purification, disinfection and elimination of organic pollutants. The titanium dioxide has been received high attention as photocatalyst due its thermal stability and non-toxicity, however the high band gap (3.2-3.5 eV) requires ultraviolet to be activated that reduce the efficiency under visible light. The photocatalytic activity of the semiconductors could be enhanced principally increasing the photon absorption and the separation of the charge photoinduced. Recently to obtain better photocatalyst has been combined with carbon structures principally the graphene to enhance the activity, which are focused to use in organic pollutants degradation, due to high conductivity, large area effective and chemical stability. In this work, we report the synthesis in situ of TiO<sub>2</sub>-RGO (TG) by solvothermal method. The samples are prepared using titanium butoxide as TiO<sub>2</sub> source, ethanol as solvent and HNO<sub>3</sub> as catalyzer. The solution were mixed with different content of GO (15, 30, 45 y 60 mg). The samples were processed at 200°C during 6h using a steel autoclave covered by Teflon. The photocatalytic degradation studies in Methylene Blue (MB) are done using a UV light lamp (10 W) and sunlight. To know the structure and morphology the nanoparticles were characterized by X-Ray Diffraction, Transmission Electron Microscopy (TEM) and Raman Spectroscopy. The nanocomposites shows anatase phase corresponding to tetragonal structure of TiO<sub>2</sub> nanoparticles grown in the presence of GO. There is not evidence of other phase or amorphous materials. The size of the nanoparticles depends on GO quantity. The photocatalyst studies, show the 100% degradation of MB in 45 min, while for sunlight takes 50 min, corresponding to TiO<sub>2</sub> with 30 mg of GO. The results obtained show the high potential to be applied in organic pollutants degradations in water source.



[ NSN-306 ] The structural response of mordenite during copper ion-exchange treatment

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Ion exchange is an intrinsic property of zeolites. It is associated with the presence of cations that compensate the negative charge of structural  $\text{AlO}_4$  units constructed from central  $\text{Al}^{3+}$  ion tetrahedrally surrounded by oxygen. Various applications of zeolites are directly or indirectly based on this property. Ion-exchanged zeolites can be considered as starting materials for the synthesis of nanocomposites; moreover, cations of transition metals are the active catalytic sites. Introduction of copper in the zeolite structure significantly improves the catalytic performance of the system, especially for the reduction of  $\text{NO}_x$  (de- $\text{NO}_x$  catalysts).

In this work we report our complimentary study by XRD and EDS methods of the structural response of mordenite during copper ion-exchange treatment. Copper-exchanged zeolites were prepared from  $\text{Na}^+$ -,  $[\text{NH}_4]^+$ - and  $\text{H}^+$ -mordenites with  $\text{SiO}_2/\text{Al}_2\text{O}_3$  molar ratios (MR) equal to 13, 20 and 20 respectively. The first two were supplied by Zeolist Int. The proton form was obtained by calcination the  $\text{NH}_4$ -mordenite for 2 hours at 300 °C. Starting materials were treated in 0.1N  $\text{CuSO}_4$  aqueous solution. The routine copper ion exchange was carried out under stirring at room temperature for 1 day. For the microwave-assisted exchange procedure, the zeolite-solution mixtures were heated at 100° C for 2 hours into Synthos 3000 Anton Paar microwave oven. After that, samples obtained by both methods were filtered, thoroughly washed, and dried at room temperature overnight.

Changes in the general character of the XRD patterns were not observed; no changes in the half-widths of the peaks, that is there is no deterioration of the crystallinity of the lattice. However, the cell parameters are slightly modified. Changes in parameter  $c$  are minor in size for all the set of samples; parameters  $a$  and  $b$  display greater changes. These variations correlate with the measured copper content. Mordenite have orthorhombic crystal lattice, with space group  $\text{Cmcm}$ , and cell parameters:  $\alpha = \beta = \gamma = 90.000^\circ$ ;  $a = 18.256 \text{ \AA}$ ,  $b = 20.534 \text{ \AA}$ , and  $c = 7.542 \text{ \AA}$  [1]. Main channels in the mordenites structure are directed along  $c$  axis. Due to a slight difference in the  $a$  and  $b$  axes, the channel has an elliptical cross-section. The ellipticity parameter  $K$ , selected as  $b/a$  ratio, can be calculated, and it has a definite character, that



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is,  $K$  decreases with increasing of the copper concentration. For standard material with MR equal to 10 this parameter have value of  $K = 1.12478$ .

Compression-expansion and the change of ellipticity is observed in the process of ion exchange. This is because of the influence of the ion-exchange cations, so it means that they are in the zeolite channel, not on the zeolite surface. The samples prepared both by routine and by microwave-assisted methods demonstrates very similar behavior. So, initial NaMor with MR equal to 13 have  $K = 1.12956$ . Changes of  $K$  correlates with the copper content only. The  $K$  parameter changes to 1.12585, 1.12412 and 1.12339, while Cu content increased to 1.05, 1.75 and 2.19 wt % respectively. We are observing some “kickback” effect of the parameter  $K$  with reversible decreasing of the concentration of copper during the multi-exchange process, it means that deformation of mordenite channel in the exchange process is elastic and reversible. As the parameter  $c$  remains practically unchanged, it tells us that all the mechanical effects occur in a plane perpendicular to the  $c$  axis of the mordenite channel.



[ NSN-307 ] CVD Growth and characterization of MoSe<sub>2</sub> monolayers

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Molybdenum-based transition metal dichalcogenides (TMDs) monolayers are part of a new family of 2D materials. Molybdenum diselenide (MoSe<sub>2</sub>) is a monoatomic three-layer structure consisting of two Se atom layers sandwiching a Mo layer. As MoS<sub>2</sub>, molybdenum diselenide presents an indirect – to direct bandgap cross over from bulk to monolayer with a value of 1.50eV (1) making these materials suitable for optoelectronic devices. These monolayers can be synthesized using different methods; Chemical Vapor Deposition (CVD) has been demonstrated to be a successful approach to synthesize various 2D materials (2,3).

In this work, we synthesized MoSe<sub>2</sub> monolayers using CVD, selenium powder (99.9% Sigma Aldrich) were placed 15 cm. away from center of the furnace. Si/SiO<sub>2</sub> substrates are collocated face down in the boat. The boat containing the precursor and the substrate was introduced in a quartz tube and located at the center of the reactor. The furnace temperature was raised up to 750 °C for over 10 minutes with two-heating ramps, the first ramp: 0 to 300° (30°C/min) for 10 minutes and the second ramp: 300°C to 750°C (10°C/min). After growth, the furnace cooled down unassisted. During the process 200 sccm of argon was used as a carrier gas. The growth was carried on under atmospheric pressure.

MoSe<sub>2</sub> monolayers were characterized using Atomic Force Microscopy (AFM), Photoluminescence Spectroscopy (PL), Electron Microscopy (SEM) and Micro Raman Spectroscopy. SEM shows that the crystals have triangle shape, the thickness found by AFM was around 7 Å expected from one monolayer (4). PL and Raman Spectra were collected at the center of the crystal. Raman spectra shows the A<sub>1G</sub> (out-of-plane) and E<sub>2g</sub> (in-plane) peaks characteristic of MoSe<sub>2</sub> Raman activated modes (4). Photoluminescence presents one contribution at 1.51 eV corresponding to the direct band gap of MoSe<sub>2</sub> monolayer (1).

In conclusion, we demonstrate the growth and characterization of high crystallinity MoSe<sub>2</sub> single layers grown by CVD, photoluminescence results show the potential of this material for the development of ultra-thin optoelectronic devices.



**[ NSN-308 ] Chemical co-precipitation route for synthesis of magnetite nanoparticles:  
nanostructure and magnetic properties.**

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The magnetic materials, and the magnetite in particular provides unique characteristics which could be directed to diverse areas of study i.e. environmental engineering, biomedical or mechano electrical fields. An amenable route which has not been completely explored is the colloidal route, for this case the formation of the nanoparticles is through thermo chemical precipitation in solution. This method provides advantages such as a less toxicity of reactive and sometimes it is possible to obtain a large quantity of material.

The conditions to realize the reaction was to maintain the same oxidant as media of reaction under inert atmosphere, at two different temperatures: 40 °C and 60 °C for a molar relation 2:1 for [Fe]<sup>3+</sup>/[Fe]<sup>2+</sup> for 35 min. Once finished the reaction, the materials were washed intensively, dried at low temperature and protected from the air. We focused our characterization on the materials without additional thermal treatments.

We observe a great difference between the products under the conditions used. For the higher temperature (60 °C) was possible to arrive to 6 nm nanoparticles which exhibits a X-ray pattern of magnetite. In the spectra we calculate the size of the nanoparticles using the Scherrer formula:  $\beta = \frac{K\lambda}{FWHM}$

The sample reacted at 60 °C shows only the magnetite phase. The other treatment exhibits additionally some goethite. The size of the particles was confirmed by field emission microscopy. The measurement of magnetic susceptibility at two frequencies is a criteria to know if there are particles sufficiently small, under such condition the magnetization is zero due to the time of the measurement is longer than the Néel relaxation time associated with time between two flips, in our case the measurements were realized three times and we don't observe magnetization.



[ NSN-330 ] Electronic structure and proton dynamics in layered perovskite-type  $M_2La_2Ti_3O_{10}$   
(with  $M = H, Li, Na, K, Rb$  and  $Cs$ )

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Layered perovskite-type oxides are considered as promising materials for photocatalytic water decomposition under sunlight irradiation for further hydrogen storage [1]. Moreover, they exhibit rather high mobility of interlayer cations [2]. Properties of these compounds strongly depend on the composition (cations, number of perovskite layers, stacking mode) [3, 4]. From these perspectives the study of electronic structure of these compounds, hydrogen state and its mobility in interlayer slabs are highly required.

Density functional theory (DFT) calculations could provide a comprehensive insight in hydrogen state and activation energy of hydrogen motion in the interlayer slabs, which play a major role in conductivity and photocatalytic processes in these materials. Nuclear magnetic resonance (NMR) is a unique tool to study hydrogen motion, first due to a rather wide timescale, and second due to its non-invasive nature that does not perturb thermodynamic of the studied system.

In this contribution, we report on the results of our theoretical study of the effect of ion exchange of interlayer cations  $M$  on the electronic structure and activation energy of hydrogen motion  $E_a$  in triple-layered perovskites  $M_2La_2Ti_3O_{10}$  (with  $M = H, Li, Na, K, Rb$  and  $Cs$ ). The calculations were carried out within a Full-Potential Linearized Augmented Plane Wave method as implemented in Wien2k code. The result is compared with experimental proton NMR data.

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[ NSN-331 ] Nonlocal bianisotropic metamaterial response of 3D periodic nanostructures

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We have applied a homogenization theory [1], based on the Fourier formalism, to calculate the effective tensors, namely permittivity, permeability and crossed magnetoelectric ones of the bianisotropic response for three-dimensional periodic nanostructures. The theory is rather general since it is valid for arbitrary Bravais lattice and any shape of the inclusions in the unit cell. Up till now, the theory has been used only in the long wavelength limit. Here, such a homogenization approach is employed beyond the quasi-static limit where the metamaterial response is nonlocal because the effective parameters turn out to be dependent not only on the frequency, but also on the wave vector. The direct calculation of the effective tensors of the bianisotropic response requires the inversion of huge matrices because a large number of reciprocal wave vectors are involved. In order to reduce the time of the numerical calculations, we have applied the form-factor division approach [1,2] too. In particular, we have calculated the effective permittivity and permeability tensors for 3D periodic nanostructures with magnetic inclusions and we have studied the effect of their shape and type of array on the anisotropy of the metamaterial response. We present new structures with high dielectric and magnetic contrast that behave as double-negative photonic metamaterials.

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**[ NSN-342 ] Transport properties of ZnO based p-n homojunction**

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A p-n homojunction, consisting of a p-type layer (doped ZnO film with Ag, N) and an n-type layer (ZnO film undoped), was manufactured by the technique of cathodic reactive co-sputtering. The ZnO:Ag,N p-type film was deposited at room temperature under a reactive atmosphere composed of nitrogen and oxygen, following deposit the film was annealed at 400 °C, in a reactive atmosphere of nitrogen. The ZnO film was deposited at room temperature in a reactive atmosphere of oxygen. The current vs. voltage curve shows typical rectification characteristics with a rectification current of 20 mA at 5V and a reverse current of 0.1 mA at -5V.



[ NSN-358 ] Resistance to compression of mortar with additive fluidizing and nanoparticles of SiO<sub>2</sub>

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The development of specific higher early and important saving of production resistance and time of construction is required, currently the most widely mineral additives used for improving the properties of concrete and reducing the destructive effects of agents external are silica fume and fly ash, while the nano-powders most commonly used are nano-SiO<sub>2</sub>, nano-Al<sub>2</sub>O<sub>3</sub> and nano-Fe<sub>2</sub>O<sub>3</sub>, where fluidizers have become one of the indispensable ingredients in concrete formulations, which functions as a dispersing agent for cement grains and increases the fluidity of cement mixes without additional water demanded, called plasticizing effect, being understood that the dispersing effect is closely related to its adsorption on the surface of cement, with adding silica nanoparticles increases the development of the compressive strength of mortars, small size of the particles of nano-SiO<sub>2</sub> provides a larger area, which accelerates the rate of hydration of cement and pozzolanic reactions with crystals of calcium hydroxide producing C-S-H gel, therefore, the size and amount of crystals of calcium hydroxide is significantly reduced, in this study a fluidizing and SiO<sub>2</sub> nanoparticles with the aim of improving fluidity and resistance was used to compression mortars mortar.

Keywords:

Silica, mortars, fluidizing.



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**[ NSN-367 ] Magnetic behavior of SiO<sub>2</sub> opals with embedded Fe and Ni nanoparticles**

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Using the Stöber method, silica spheres were obtained and arranged in an fcc lattice. Metallic Fe and Ni were introduced in opal voids by means of the reduction of precursor salts with different reducing agents. Magnetization curves of the as synthesized metallic nanoparticles and of the artificial opals with infiltrated nanoparticles were measured by using the vibrating sample magnetometry (VSM) technique with an applied magnetic field oriented along the [111] direction of the opal matrix. Landau-Lifschitz-Gilbert [1] equation was solved numerically, in order to reproduce the experimental results qualitatively, using Ewald summations [2] to take into account the dipolar interaction between the spatially arranged magnetic nanoparticles. The theory reproduces the general features of measured magnetization curves, in particular, there is strong dependence of hysteresis loops on the magnetic nanoparticle filling fraction. Moreover different configurations and conditions were explored theoretically in order to compare the results.

This work was partially supported by VIEP-BUAP.

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[ NSN-369 ] Growth and characterization of different types of nano and micro-structures of Zinc Oxide via simple oxidation of metallic Zinc

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Zinc oxide (ZnO) nano and micro-structures were synthesized by vapor-solid method, with the simple oxidation of metallic zinc without the use of catalyst. Different types of carrier gases and different temperatures were used for the synthesis to obtain nano and micro-structures. Measurements of scanning electron microscopy (SEM) were performed to observe the different types of morphologies obtained in the various thermal treatments. In these measurements you can be observed a wide variety of morphologies of different types of nano and micro-estructures like as trumpets, swords, rods, wires, cactus and microtubes. In the measurements of energy dispersive spectroscopy (EDS) the composition of the synthesized structures was obtained, in such measurements it can be seen that in some thermal treatments structures are obtained zinc partially oxidized. Cathodoluminescence (CL) measurements were performed to observe the variation in the luminescence of the samples. In the spectra acquired it shows that there is a shift of the emission the near band edge of ZnO ( $\sim 3.22\text{eV}$ ) toward the blue, as well as the emission band of defects in the ZnO ( $\sim 2.4\text{ eV}$ ), this variation is related to the thermal treatment which is subjected metallic zinc metallic. The difference in the optics, morphological and composition characteristics of nano and micro-structures, are dependent temperature and carrier gas used for thermal treatment.



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[ NSN-373 ] Electrocoagulation system used as an electrochemical methodology to obtain Zn nanostructures of wastewater

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Electrocoagulation (EC) is an electrolytic process for wastewater treatment consisting of dissolution of a sacrificial anode (aluminum) and cathode (copper), which is applied electric charge generating Al ions that remove pollutants. The metal industry coatings generate big quantities of wastewater which contains metals and strong acids, these waters are given treatment before being discharged into the drainage system, but no recovery of metals is contained there. Electrocoagulation produces sludge and concentrate them metals (in this case Zn), but have not been studied to determine their concentrations, the wastewater of the metal industry coatings have pH equal to 10, placed in a batch reactor (EC), 700 mL for 60 minutes, current I equal to 4 A and voltage V equal to 25 V, another 700 mL was EC for 15, 30, 45, 60 and 75 minutes and apply I equal to 5 A and 20 V. Samples were characterized by scanning electron microscope (SEM), being able to observe the agglomeration of the particles and how the microstructure change with the time. In the SEM images were observer a nanoparticle with nanorods shapes. An energy dispersive X-ray spectroscopy (EDS) were done on the nanorods shape to corroborate the Zn and O elements. With EC system was possible to generate electrochemical synthesis process in which it was possible recover nanoparticle of wastewater with Zn, to find a possible application.



**[ NSN-384 ] Structural analysis of calcium phosphate nanoparticles by Rietveld refinement and electron diffraction**

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It was studied by Rietveld refinement and electron diffraction structural behavior of calcium phosphate nanoparticles, synthesized by chemical precipitation under normal temperature and pressure. Rietveld refinement using the data applied to XRD structural parameters of the nanoparticles, its crystal size and the crystalline phases were obtained. Electron diffraction semi spherical and slightly elongated morphology, defined in relation to time and aging temperature used in the synthesis, distinguishing normal hexagonal prism morphology observed in natural hydroxyapatite crystals micrometer size was observed.



[ NSN-397 ] Physicochemical parameters for the synthesis of nanocrystalline calcium phosphate  
from tooth root

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The physicochemical parameters for making calcium phosphate tooth root are established. For synthesis precipitation methods and continuous hydrothermal were used. In the precipitation method, I was used polyethylene glycol (PEG) as solvent and Cetyl Trimethyl Ammonium Bromide (CTAB) as a cationic template in order to regulate the nucleation and crystal growth. In the hydrothermal method was performed in a system of tubular flow reactor, model R-20 (Generatoris S.A of C.V), comprising three pumps. structural characterization of the nanoparticles was performed by X-Ray Diffraction (XRD), energy dispersive spectroscopy (EDS), infrared spectroscopy (IR), Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). The continuous hydrothermal synthesis method offered the best results, obtaining nano-calcium phosphate bars 50-70 nm in length and a Ca / P ratio = 1.5-1.61, whereas the results obtained by precipitation showed the presence of amorphous phases , nanoparticles with diameter 20-25 nm and 250 nm -1  $\mu$ m nano fiber length and diameter of 5 nm-10 nm with a Ca/P ratio = 1.65-1.67, corresponding to the tooth root.



[ NSN-399 ] Nanomaterials based glycidyl polymethacrylate (PMAG) and wall carbon nanotubes multiple (NTCPM) modified by microwave

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In this paper, reported the nanomaterial obtaining of glycidyl polymethacrylate (PMAG) and multiple-walled carbon nanotubes (NTCPM) modified with citric acid (AC), through radical polymerization, to establish an interaction between PMAG matrix and NTCPM-AC. Nanomaterial obtaining by microwaves radiation used a power of 200 W and temperature 90 °C. Obtained a conversion of 90% in 5 minutes. The materials obtained were analyzed by kinetic preliminary studies of the radicalic polymerization process, for know the adequate conditions of work, especific the time. Subsequently, the interaction of NTCPM-AC with PMAG, was evidenced by techniques: spectroscopic FT-IR finding bands carbonyl group characteristic of the AC, as well as the formation of covalent analyzed by XPS, which is corroborated by the analysis SEM where there is an interaction between PMAGB morphologically and NTCPM-AC.

**Keywords:** nanomaterials , PMAG , NTCPM, microwave .



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**[ NSN-403 ] Synthesis calcium phosphate coatings Ti6Al4V**

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The method of free radical polymerization was used to synthesize hydrogels poly ( hydroxyethyl methacrylate ) ( Phema ) with HA and APNPs . hydroxyethyl methacrylate (HEMA ) , and dH2O azobisisbutironitrilo ( AIBN ) in different amounts mixed. All solutions were mixed with a vortex and subjected to ultrasound . Once solidified hydrogels , pieces of 1.5 cm diameter and 2 mm thick were cut . These pieces with dH2O were rinsed and cleaned several times with ethanol . The samples were sterilized with UV rays and characterized by X - Ray Diffraction ( XRD ) , energy dispersive spectroscopy ( EDS ) , infrared spectroscopy ( IR ) , Scanning Electron Microscopy ( SEM ) and Transmission Electron Microscopy ( TEM ) .



**[ NSN-408 ] Effect of water content on the morphology of TiO<sub>2</sub> nanotubes obtained by electrochemical etching**

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Over the past decade, the electrochemical formation of TiO<sub>2</sub> nanotube layers has been intensively studied, particularly those obtained from a fluorine-based electrolyte (F<sup>-</sup>). In this work, the relationship between the amount of water in the electrolyte and the morphology of the nanotubes is studied. Samples were prepared varying the weight percentage of water in the electrolyte ranging from 0 wt% to 5 wt%. The remainder of the electrolyte was a mixture of 0.25 wt% NH<sub>4</sub>F and Ethylene Glycol from which 2.5 g total were used. Samples were prepared by electrochemical etching of 1 hour at 60 V of a 99.99+ % titanium sheet, using the electrolytes with different water contents. Prior to the elaboration of each sample, the surface was prepared by etching under identical conditions and sonication for removal of the initial layer. Samples were characterized by scanning electron microscopy, Raman spectroscopy and UV-Vis reflectance.



[ NSN-410 ] Light localization in aperiodically modulated one-dimensional photonic crystals

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In this work we present a numerical analysis of some light localization properties for three types of deterministic aperiodically modulated one-dimensional photonic crystals: Fibonacci, Thue-Morse and Cantor structures. Using the transfer matrix theory [1] and the rational approximation [2], we calculate the optical response and the electric field magnitude as a function of the perpendicular distance to the interfaces in multilayer structures having a periodic index profile formed with bilayer units: a slab A with width and refractive index  $d_a$ ,  $n_a$ ; and a slab B with refractive index  $n_b$  and a modulated width given by  $d_b = d_0 * (1 + D * S_g)$  where  $d_0$  is the B slab's width,  $D$  is a fixed width's increment and  $S_g$  represents consecutive generations of a Fibonacci, Thue-Morse or Cantor sequence formed following the Fibonacci substitutional rule: 1  $\rightarrow$  10, 0  $\rightarrow$  1; the Thue-Morse substitutional rule: 1  $\rightarrow$  10, 0  $\rightarrow$  01; and the Cantor substitutional rule: 1  $\rightarrow$  101, 0  $\rightarrow$  000. The new structures we propose can be constructed with the available technologies for the fabrication of multilayers at a nanometric scale (see for example [3]), and can be considered for novel applications where the light localization is important as the design of multifrequency photonic quasicrystal lasers, optical cavities, etc..

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[ NSN-411 ] Nanoparticles of MnO/FeO solid solution and its magnetic properties

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The synthesis of nanoparticles of MnO/FeO solid solution was carried out by the sol-gel chemical method in order to study the effect of grain size distribution achieved on the magnetic properties when measured at low temperatures. In this work, the MnO/FeO nanoparticles were obtained using a precursor solution with 1.0538g of Iron(II)acetate, 1.4957g of manganese(II)acetate tetrahydrate and 10% W of high molecular weight PVP in water, and then the gel obtained was calcined at 1100 ° C for 1 h under nitrogen. The characterization was carried out by X-ray diffraction (DRX), RAMAN Spectroscopy, Transmission Electron Microscopy (TEM) and Vibrating Sample Magnetometry (VSM). XRD patterns exposed a MnO<sub>0.33</sub>FeO<sub>0.66</sub> as the main phase present in the nanofibers with a cell parameter  $a = 4.3665 \text{ \AA}$ . RAMAN spectroscopy exposed that the overwhelming present phase was the MnO<sub>0.33</sub>FeO<sub>0.66</sub> solid solution. Characterization of morphology carried out with TEM revealed a wide distribution of grain sizes, ranging from 10 to 100 nm. Finally, magnetic properties of calcined samples characterized by VSM, shown a strong temperature dependence of coercivity values duplicating its value when goes from room temperature to low temperature. It shows up a change in the magnetic interactions as temperature goes down because the grain size distribution of nanoparticles, being these the underlying responsible of the hysteresis loops shape and magnetization values.



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[ NSN-416 ] New High-index Orientations in the Stereographic Triangle for Self-assembled Faceting

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Energetically unstable crystalline surfaces, among their uses, can be templates for the growth of periodic arrays of one-dimensional (1D) nanoscale structures. However, few studies have explored self-assembled faceting on high-index (HI) planes inside the stereographic triangle, and extant studies have not produced any criteria for encouraging the formation of one-dimensional periodic arrays. In this work, by analyzing the MBE growth of homoepitaxial facets on (631)A GaAs, a HI plane inside the triangle, we present a criteria to produce highly uniform 1D periodic arrays on unexplored surfaces. These families of planes are those belonging to the lines connecting the energetically stable HI GaAs (11 5 2) plane with any of the (100), (110), and (111) planes at the corners of the stereographic triangle. This novel strategy can lead to new possibilities in self-assembling 1D structures and manipulating physical properties, which in turn may result in new HI- and 1D-based experiments and devices.



[ NSN-435 ] Application of Nanoparticles in Agricultural Crops and Study of Their Synergetic Effect.

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Now days, nanotechnology is catching a great attention of researchers because of their unique properties which could be employed in various areas, such as biomedical (therapy and molecular markers), environmental (water purification and plant growth) and electronics (sensors). Focusing on agriculture area, there has been several researches published using carbon nanotubes to improve the water and nutrient uptake during plant growth. Also, there are reports that nanomaterials not only beneficial for the growth but also provides an antibacterial and antifungal effect in plants. Taking into account the nanomaterials benefits and importance of sorghum (*Sorghum bicolor*) in the Michoacán region which is facing some bacterial infection from the last years and affects the production by 40-50%, we have focused our research on “*Sorghum Bicolor*” growth using multi-walled carbon nanotubes (MWCNTs) and Nano-Ferrites (NF) materials at germination stage. Here, we have focused our research on two factor; 1) growth dynamics of sorghum with the use of nanomaterials (MWCNT & NF) and 2) nutrient uptake with the use of nanomaterials individually and synergetic effect while utilized both together.

The experiment was conducted during the germination stage, for a period of 10 days using MWCNTs (5, 10, 20 µg/ml) and NF of 20µg/l concentration in the growth medium. The fresh and dry weights were taken to analyses the water availability and biomass of seedlings with/without used of nanomaterials. Scanning electron micrographs (SEM) of planted seeds were taken to study the interaction morphology with and without nanomaterials assisted germination. The elemental concentration in the seedlings were measured using X-ray fluorescence spectroscopy (XRF). Results shows that the MWCTNs have an effect in growth regulation in germination stage, it reduces germination time as well the water transport. MWCNTs and NF compounds helps to transport the nutrients from the growth media to seedlings with their conduction through hydrophobic channel and free ions availability.

**Key words:** carbon nanotubes, growth promoter, nano-ferrites, germination.



**[ NSN-440 ] Fabrication of a mis structure based on two-dimensional ZnO nanostructures by chemical routes**

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Because its physical properties, ZnO is considered a potential semiconductor compound for fabricating electronic and optoelectronic devices. In this regard, several growth techniques have been developed to ensure the required control for manufacturing commercial devices based in this material. On the pathway for improving the performance of the current devices, low-dimensional ZnO structures seem to be a promising alternative.

Here, we report the fabrication of a metal-insulator-semiconductor (MIS) structure based on ZnO nanostructures grown on the surface of an anodized aluminum substrate (ZnO/Al<sub>2</sub>O<sub>3</sub>/Al) by chemical routes. While the ZnO nanostructures were obtained through a low-temperature hydrothermal route, the Al<sub>2</sub>O<sub>3</sub>/Al substrate was obtained by electropolishing and subsequent anodizing of aluminum foil. The obtained ZnO/Al<sub>2</sub>O<sub>3</sub>/Al architecture was studied by x-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and electrical measurements. The voltage-time plot acquired during the anodizing process indicates formation of an insulating barrier (Al<sub>2</sub>O<sub>3</sub>) on the metallic substrate (Al). The SEM analysis reveals that a nanostructured layer is grown on the anodized substrate, constituted by interconnected leaf-like ZnO nanostructures with average thickness of ~100 nm. The formation of the MIS structure was observed using focused ion beam technology (FIB). The EDS analysis suggests the presence of ZnO, Al<sub>2</sub>O<sub>3</sub> and Al phase; formation of these phases was confirmed definitely by XRD. Finally, the characteristic rectifying response of a metal-oxide-semiconductor junction is observed in the acquired curves I-V and C-V of the obtained architecture, demonstrating that it is possible to fabricate a MIS heterojunctions based on ZnO nanostructures using exclusively chemical routes.

Keywords: MIS structure, two-dimensional ZnO nanostructures, chemical routes.



[ NSN-441 ] Chemisorption of adenine-alkali doped Si nanowires: ab-initio study

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A theoretical study of the interaction between Li-doped silicon carbide nanotubes and its nucleic acid base complexes in water was presented by S. Ketabi *et al.* [1]. They showed that base-Li-doped SiC nanotubes produce stable compounds, which could be useful for adenine (A) sensors, which in turn could lead to the development of biosensors. Then, it is important to investigate the electronic density of states, electronic band structures, charge transfers and chemisorption energies involved in the adenine adsorption onto nanowires in order to provide a rational understanding of this process and predict the changes in the electronic structure of the nanowires. In this work, the adsorption of adenine on a hydrogen-passivated silicon nanowire (HSiNW) is investigated using density functional theory calculations, where three interaction modes, Li (A-Li-Si), Na (A-Na-Si) and K (A-K-Si) are considered. Results show that the adsorption of single adenine molecule is favored in the A-Li-Si configuration. It is also observed that the adenine adsorption introduces new impurity states in the band gap of HSiNW. Further calculations can be performed to investigate if thymine, guanine and cytosine can be chemisorbed on alkali metal-doped HSiNW, as occurs with adenine, and then expand the applications of these nanostructures as DNA base sensors.

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**[ NSN-446 ] Supercapacitors based on carbon nanostructures**

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Nowadays, environmental pollution is a problem becoming increasingly important. Pollution is present in our country and all over the world as a result of the extreme use of fossil combustible and waste produced by millions of factories around the world. Additionally, environmental pollution has led to climatic changes. To reduce pollution and promote the correct use of clean energy free of residual contaminants, we propose the use of supercapacitors. Supercapacitors devices are able to store and release energy at much higher speeds than traditional batteries. Supercapacitors can be used in portable electronic devices, memory systems for backup, regenerative braking systems (for example, conversion of kinetic energy into electrical energy), and in the use of energy in the industry. In this work we synthesize doped fullerides, a carbon material with super-capacitance, which the bigger it is, the greater the energy storage capacity of such material is. For the synthesis of fullerides we use a technique called ultrasonication. The resultant materials were characterized by techniques such as TEM, TGA, EDX, UV-Vis, Raman and conductivity tests. Their capacitance was measured by cyclic voltammetry and electrochemical techniques were performed to determine if any charge accumulation occurs. Using the characterizations techniques previously mentioned, we have determined the product of interest called fulleride, furthermore, these materials have been able to store charge, which is very important for the manufacture of a supercapacitor.



[ NSN-447 ] Interaction of platforms carbon nanostructures with cellular systems

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Carbon is a very versatile element that is present in a variety of chemical compounds, it can be observed in nature in different allotropic forms, such as diamond and graphite. There are other carbon allotropes that have a size in the order of nanometers that have gotten a lot of attention because they have very interesting and unique physical and chemical properties. Some of these forms of carbon are: fullerene, nano-onions, carbon nanotubes, graphene and nanodiamonds. During this work graphene and carbon nanotubes were used. Graphene consists on an atom thick sheet, with carbon atoms  $sp^2$  hybridization and a hexagonal geometric arrangement. Some of the unique properties of graphene are: high surface area, extraordinary thermal and electrical conductivities, high mechanical strength and capability of functionalization. Carbon nanotubes consist on one or more sheets of graphene rolled up on themselves, which have properties as high flexibility, mechanical strength, transparency, capacity of internalization into cells without causing significant damage and like graphene, capability of functionalization. Because of these properties graphene and carbon nanotubes have been proposed as materials which can be used to synthesize innovative platforms for tissue regeneration. For the success of tissue regeneration it's necessary a platform that provides a growth environment similar to natural tissue which enables adhesion, proliferation and cell differentiation. Different platforms of graphene and carbon nanotubes have been tested with cells of different types, however, the ideal conditions that allow the application of such platforms in the field of tissue regeneration have not been found. For these reasons, in this work carbon nanostructures as graphene, graphene oxide, oxidized and nitrogen doped carbon nanotubes were synthesized and characterized by techniques such as TEM, Raman and UV-vis. Platforms of each of the materials were designed and their interactions with cellular systems such as giant vesicles were analyzed; these giant vesicles function as cell model and allow us to address the problem in a simple way. Because it is known that the differences, even just a few of them, between the properties of the nanostructures have a great influence in the interactions carried out with cellular systems, it is important to compare whether there is any difference between the interactions of the cell model and platforms that were designed for this work.



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**[ NSN-455 ] Theoretical comparison of the luminiscent phenomenon between cylindrical Single Wall Carbon Nanotubes (SWCNTs) and oval SWCNTs.**

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We present a theoretical comparison of the luminiscent phenomenon originated in SWCNTs with cylindrical geometry with respect to that which is present in SWCNTs with oval geometry. In both structures their ends are capped with hydrogen atoms with which they are functionalized. The SWCNTs exhibit interesting optical, structural and electronic properties whose behavior is intimately related with their metallic or semiconductor character. Today we know that for the case of the cylindrical SWCNTs there is a strong relationship between their diameter size which is determined by the chirality indices ( $n$ ,  $m$ ) and the emitted wavelength ( $\lambda$ ) which in turn depends on the energy band gap. Our work is focused on studying the phenomenon of luminescence of both cylindrical and oval SWCNTs structures. For the case of the cylindrical SWCNTs, they are theoretically modeled considering that such structures are made up by the conventional method of rolling up a sheet of graphene, and for the case of the oval ones we proceed similarly but now we consider an "ovalene" aromatic hydrocarbon structure, in both types of SWCNTs we varied the length of the structure and kept the size of the molecule. The computational tool that supports our work is the SPARTAN and GAUSSIAN software in which we model both types of molecular structures, using the methods of Hartree Fock (HF) and the Functional Theory Density (DFT), with a major interest in the oval SWCNTs.



[ NSN-464 ] Coarsening in the homoepitaxy on GaAs high-index substrates grown by MBE:  
theory and experiment

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Among the variety of methods available for nanostructure fabrication, self-assembly on high index (H-I) substrates by molecular beam epitaxy (MBE) is very promising because it is not limited by the resolution of lithography and does not require additional processing that may introduce defects to the nanostructures. H-I substrates usually provide energetically unstable surfaces that tend to break up into low free-energy facets and naturally form a periodic corrugation array (PCA). These surfaces can then be used as templates for growing nanostructure arrays with high uniformity and density. In this work, by the Atomic Force Microscopy (AFM) and Autocorrelation Functions analysis of corrugated surfaces of GaAs grown on (631) H-I substrates by MBE, we study the mechanisms which are behind the non uniformity of PCAs at large areas (larger than 1 square micron). Specifically, coarsening defects between adjacent facets are study via the Kuramoto-Sivashinsky theoretical model and directly compared with the experimental results obtained from AFM observations.



[ NSN-465 ] Photocatalysis in mezcal vinasse with nanostructures ZnO

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Mezcal is an alcoholic beverage native of Oaxaca state, obtained from a plant called Agave. A problem for the industry is to handle the waste obtained by the distillation processes of Agave. This work is focus on a process to treat one of these waste called mezcal vinasses by the method of heterogeneous photocatalysis. Vinasse is a highly polluted water, it contains phenols sulfates and phosphates. In order to eliminate polluting compounds, the method adds nanoparticles of ZnO as catalyst. The nanoparticles of ZnO were obtained by the polyol method, using the deionized water at 18.2 MΩ, zinc acetate and diethylene glycol like reagents. The synthesis was realized in three stages: dissolution, homogenization and precipitation. Analysis of x-ray diffraction for the nanopowders of ZnO showed wurtzite hexagonal phase with primitive space group P63cm. The size grain was calculated by Scherrer formula, with the three most intense peaks corresponding to the planes (100), (002) and (101) giving  $17 \pm 1$  nm grain size. The IR analysis shows that the method is not adequate to eliminate the polluting, however the results also shows that a new compound is synthesized, probably aldehyde.

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[ NSN-471 ] Tuning of refractive index in Al-doped ZnO films by rf-sputtering using oblique angle deposition technique

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Light reflection is one of the critical problems to solve for the performance of the optoelectronic devices, such as solar cells [1]. This is due to the Fresnel reflections that reduce the intensity of transmitted light across the TCO, thus the efficiency decreases [2]. By using antireflection coatings (ARC), the light reflection can be reduced and the cell efficiency enhanced. We obtain AZO thin films with different values of refractive index by the modification of their morphology in order to design an ARC for their application in solar cells. AZO thin films were grown on Corning 2947 glass substrates by rf-sputtering during 25 minutes. A 3 inch ZnO:Al target with 2 wt% of Al<sub>2</sub>O<sub>3</sub> was used to perform the deposition. The process pressure was fixed at 10 mTorr in argon environment. The distance between substrate and target was 5 cm and no rotation was used in the course of the growth process. Each growth were done using a different tilt angle of the substrate holder ( $\theta=0^\circ, 15^\circ, 30^\circ, 45^\circ, 75^\circ$ ). X-ray diffraction measurements were done using a D5000 Siemens X-ray diffractometer, Thickness and cross sectional morphology of the AZO nanocolumns were studied by using a using field emission scanning electron microscope (FESEM) JEOL 7600F instrument. The optical properties were obtained by an Agilent 8453 UV-Vis Spectrophotometer. The transmissions of samples were into a range of 85 and 100%. The band gap energy diminished with the substrate inclination (from 3.58 eV to 3.48 eV) presumably due to local variation of Al concentration in the material [3]. The nanocolumns tilt angle influences on light scattering that falls normal to film surface. It induces that the refractive index varies in such a way that it diminishes as nanocolumn tilt angle increases in a range from about 1.78 for no tilted substrate up to about 1.50 for 75° substrate inclination, which corresponds to 13.5° nanocolumn tilt angle. This result lets refractive index engineering in order to optimize the antireflecting effect in Al-doped ZnO films.

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[ NSN-476 ] Influence of the confining liquid medium on laser ablation of CdTe Targets

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In today's world, one of the main problems that researchers want to solve is the obtainment of energy from non-polluting methods, an example of this are the photovoltaic cells. We can find in the literature that any material that goes nanoparticle improves its properties or they are drastically changed. Some research groups have shown that adding nanoparticles of Cadmium Telluride (CdTe) to the absorber layer can increase the efficiency of solar energy conversion to electricity in photovoltaic cells, therefore, in this research we attempt to synthesize nanoparticles of CdTe using the method of laser ablation that, unlike current chemical methods, can synthesize these particles with low production cost and less polluting waste. In this work we present a study of the synthesis of CdTe nanoparticles by the method of laser ablation of solids in liquids. The results are discussed as a function of the confining solvent (water, acetone and ethanol) and the laser energy by energy used for the ablation. In today's world, one of the main problems that researchers want to solve is the obtainment of energy from non-polluting methods, an example of this are the photovoltaic cells. We can find in the literature that any material that goes nanoparticle improves its properties or they are drastically changed. Some research groups have shown that adding nanoparticles of Cadmium Telluride (CdTe) to the absorber layer can increase the efficiency of solar energy conversion to electricity in photovoltaic cells, therefore, in this research we attempt to synthesize nanoparticles of CdTe using the method of laser ablation that, unlike current chemical methods, can synthesize these particles with low production cost and less polluting waste. In this work we present a study of the synthesis of CdTe nanoparticles by the method of laser ablation of solids in liquids. The results are discussed as a function of the confining solvent (water, acetone and ethanol) and the laser energy by energy used for the ablation.



**[ NSN-478 ] CdTeS nanoparticles obtained by reactive laser ablation of a solid CdTe target in thiourea solutions**

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Alloying cadmium telluride (CdTe) with sulfur (S) to form the ternary compound CdTeS allows a band gap tuning from 1.5 to 2.5 eV depending on the amount of S substituting Te, which makes the synthesis of CdTeS ternary an interest field in materials science. Additionally, size reduction of semiconductor materials to form nanoparticles has demonstrated to modify the materials properties. A very suitable technique to obtain nanoparticles is by laser ablation of solid targets in liquid media.

In the present work, the incorporation of S into CdTe nanoparticles is investigated. The synthesis was carried out by the laser ablation of CdTe in 0.1M solutions of thiourea dissolved in water, methanol, ethanol and 1-propanol, with fixed values for laser energy, in order to study the effect of the confining solvent. Samples were structurally characterized by XRD, optical properties were analyzed by UV-Vis spectroscopy. Chemical composition was studied by EDS and morphology was observed by SEM.



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**[ NSN-481 ] Effect of laser output energy on the pulsed laser ablation of CdTe in sulfur containing solutions**

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Suspended nanoparticles exhibit unique optical, electronic and magnetic properties which make them ideal candidates as novel tools for applications in several fields of science and technology. The interest in semiconductor nanoparticles is primarily because of the differences in electronic properties they exhibit from bulk material due to their small size. CdTe nanoparticles have excellent optoelectronic properties which make it interesting for solar cells and photoluminescent devices. Furthermore, incorporation of S into CdTe allows the tuning of band gap energies. Preparation of semiconductor nanoparticles in liquid environment has been achieved using mainly chemical techniques. Pulsed laser ablation of solids in liquids has proven to be a fast and easy technique for the synthesis of nanoparticles in liquids. In this work a CdTe target was ablated within thiourea solutions at different laser energies. The nanoparticles were characterized by UV-Vis spectroscopy, X-ray diffraction, scanning electron microscopy and energy dispersive X-ray spectroscopy.



[ NSN-483 ] Synthesis of Carbon Nanostructures from Naphtha 35/60

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Properties of materials change when their sizes scale up to nanometers. Nowadays the carbon nanomaterials are strengthening the materials currently used, mostly due to they exhibit unique properties such as: mechanicals, physicals and chemicals. Hence is the importance of synthesise new materials from available sources in the nanotechnology.

The aim of this work was the synthesis of Carbon Nanostructures (CNS) from the Naphta 35/60 using a stainless steel tube AISI 304 as catalyst. The process used was chemical vapor deposition employing argon as carrier gas and a tubular quartz reactor (0.6 x 0.0254 m i.d.). The experimental conditions were 800, 835 and 850°C synthesis temperature, 30 minutes time reaction and 70 ml/min argon flow. The samples obtained were characterized through Scanning Electronic Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), Fourier Transform Infrared Spectroscopy (FTIR) and Raman Spectroscopy.

SEM depicted three kinds of CNS; the first structures were long filaments with diameters in a range of 58 - 357 nm and several micrometers length. The second type of structures were carbon sheets about 300 nm width and micrometers lengths. The last ones were irregular semi-rounded sheet clusters of hundreds of nanometers.

EDS analysis shown high carbon atomic percentages (94-97) with low presence of oxygen (2.3-5.4) and iron (0.29-0.62).

The functional groups present in the nanostructures were determined by FTIR technique. The peaks obtained correspond to C-H<sub>x</sub> stretching. Also, broad bands of stretching and deformations of C = C and weak bands of C = O were present.

Raman spectroscopy was performed for the three different structures obtaining D, G, G' bands and I<sub>D/G</sub> ratio.

The filaments structures have the D band located at 1343, G at 1579 and G' at 2695 cm<sup>-1</sup>. The ratio I<sub>D/G</sub> = 0.851.

Carbon sheets structures have the D peak located at 1355 with a shoulder peak at 1240 cm<sup>-1</sup>, the G band at 1597 and G' at 2825 cm<sup>-1</sup>. The ratio I<sub>D/G</sub> = 0.641. The irregular clusters have D and G bands at 1348 and 1599 cm<sup>-1</sup> respectively and G' at 2690 cm<sup>-1</sup>. The ratio I<sub>D/G</sub> = 0.943.

A variety of structures with different morphology were obtained due to Naphta 35/60. The filament nanometric structures were standing up. Naphta 35/60 attached with the stainless steel catalyst was an accessible, efficient and low cost source for carbon nanostructures synthesis.

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[ NSN-486 ] Green synthesis of silver and gold nanoparticles and their antimicrobial activity

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Introduction: One of the problems of medicine worldwide is the development of multidrug resistant strains of pathogenic bacteria. The use of nanotechnology by nanoparticles (NP) against pathogenic microorganisms solidifies more in the industries of medicine and pharmacology. Various methods have been used and reducing agents to synthesize silver and gold nanoparticles (AgNPs/AuNPs), including reactive chemicals that have generated undesired toxicity and human and biological systems effects. Currently, several extracts of plants have been used to prepare AgNPs and AuNPs, as an alternative.

Objective: Synthesize AgNPs and AuNPs from extracts of *Glycyrrhiza Glabra* and *Amphipterygium Adstringens* and determine its bactericidal activity against *S. Aureus*, *E. Coli*, *S. Oralis*, *Enterococcus faecalis*, *S. Mutans*, *S. Salivarius*, *S. Sobrinus*.

Materials and Methods: This was an experimental study in vitro. Bark of *Amphipterygium Adstringens* (Cuachalalate) and root of *Glycyrrhiza Glabra* were employed to get ethanolic extracts. The synthesis was performed in aqueous solution, under ambient conditions and magnetic stirring. The metallic salts precursor were AgNO<sub>3</sub> and HAuCl<sub>4</sub>.

The samples were characterized using Transmission Electron Microscope (TEM), spectrophotometry (Vis-NIR), Dynamic Light Scattering (DLS), thermogravimetric analysis (TGA), fluorescence, X-ray diffraction (XRD), Infrared Spectroscopy Fourier Transformer (FTIR ).

To determine the bactericidal and antifungal activity of NP was used Minimum Inhibitory Concentration with microorganisms already mentioned. Subsequently he conducted descriptive statistics.

Results: AgNPs were obtained spherical in shape and size less than 10 nm. AuNPs were obtained spherical in shape and size less than 5nm. AgNPs and AuNPs inhibited bacterial, confirming their biological properties.



[ NSN-494 ] Towards self-cleaning coatings based on alumina-ceria nanoparticles for application in photovoltaic panels

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The use of photovoltaic cells for the advantage of the solar energy, has allowed the use of this renewable energy and has motivated the development of technology that focuses on environmental care.[1] However, photovoltaic panels are exposed to external environmental conditions, and as a result, soiling of solar panels is generated; soiling causes a decrease in power conversion efficiency, therefore, self-cleaning coatings are needed in order to keep solar panel surfaces clean.[2] In this work, we present a CeO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub> nanoparticle system for their potential use as a transparent self-cleaning coating, and the effect of functionalization of nanoparticles with octadecylphosphonic acid on hydrophobicity effects on the surface. Systems of functionalized nanoparticles were prepared at different concentrations and dispersed in ethanol, polyurethane acted as polymer matrix. Coatings were deposited with spin coating technique on a glass substrate. The results were characterized by the water contact angle technique and by means of IR and UV-Vis spectroscopy in transmittance mode, the results indicate good transparency in the visible region, showing that the coatings have hydrophilic properties and hydrophobic in some other cases, these being the most important characteristics for a self-cleaning coating. Infrared spectra for an ODPA Al<sub>2</sub>O<sub>3</sub>-CeO<sub>2</sub> functionalized system shows main bands associated to the ODPA. Thin film UV-Vis spectra of ODPA Al<sub>2</sub>O<sub>3</sub>-CeO<sub>2</sub> in polyurethane shows that a good transparency can be achieved, together with good contact angle characteristics.

Acknowledgements:

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[ NSN-497 ] Preparation of filters based on chitosan and graphene oxide

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Chitosan (CS) is an abundant polymer in the nature. This polysaccharide is obtained through des-acetylation of chitin and presents a very high rate of reposition in the biosphere, functional properties such as biocompatibility, biodegradability and easy chemical modification, which make it an important renewable resource.

Applying nanofiller techniques with graphene oxide (GO) [1], it is possible to optimize CS properties. Taking advantage of the bacterial properties of GO combined with the properties of CS, it is possible to obtain an excellent nanocomposite with diverse ecological and biological applications.

In the current work is contemplated the production of membranes based on this material, and their application as filters for the treatment of polluted water. This membranes maximizes the mechanical and biodegradability characteristics of CS [1], which provides filters with low environmental impact and low manufacturing cost, capable of removing toxic colorants, heavy metals [2] and pathogenic agents present in water.

**Key words:** graphene oxide, chitosan, filter, nanocomposites, water treatment, nanofiller.

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[ NSN-507 ] Hierarchical ZnO nanostructures synthesized by CSVT for dye-sensitized solar cells

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A novel hierarchical ZnO nanostructured films were synthesized through the close-spaced vapor transport (CSVT) technique onto fluorine-doped tin oxide (FTO) substrates followed, in all the cases, by a thermal annealing in air at 400 °C for 30 minutes and atmospheric pressure. It was found that depending upon the oxygen partial pressure, the morphology of the films can be varied from two-dimensional microdisks to hierarchical ZnO nanostructures. The morphology and the structural properties of the products were studied by scanning electron microscopy (SEM), micro-Raman spectroscopy and X-ray diffraction (XRD). A possible growth mechanism behind the formation of different micro and nanostructures has been discussed. The hierarchical ZnO films show a coral-shape morphology with high specific surface area, high crystallinity, fast electron transport, and a pronounced light-scattering effect, which are suitable properties for their use as the photo-anodes for dye sensitized solar cells (DSSCs). In accordance to the above results, it is shown that the CSVT technique is a novel, simple, and ecological route to tailor the morphology of the photoanode, which is a crucial issue in the fabrication of highly efficient DSSC's.



[ NSN-512 ] Tailoring strain and nucleation of MBE grown InAs-InGaAs quantum dots.

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The necessity for high performance electronic/optoelectronic devices and the increasing miniaturization in the field of microelectronics has driven to research on nanostructures, encouraging the interest in the zero dimensional systems like quantum dots (QDs). Those structures are very promising for develop the next generation technologies. Some examples of applications are high-efficiency LEDs and solar cells.<sup>[1]</sup> However there still are challenges to overcome for the improvement of the QDs quality and distribution. Quantum dots are small three-dimensional islands of a low-band-gap semiconductor, which are enclosed in a wideband-gap semiconductor matrix. The QDs are commonly grown on dissimilar materials (different lattice constant and parameters) to propitiate the accumulation of strain in the interface, which is the main mechanism of the formation self-assembled QDs.

In this work, we report a study of the InAs QDs self-assembling on strain compensated GaAs/InGaAs heterostructures. The self-assembling of the QDs was carried out by the Stransky-Krastanov growth mode on a GaAs surface. In order to modify the strain prior to the nucleation of the InAs QDs, a 20 nm thick In<sub>7</sub>Ga<sub>93</sub>As layer was grown below the GaAs layer, which thickness (denoted by S) determined the strain in the growth of the QDs. The thickness of the InAs was 2.1 for all samples, and S was varied from 1 to 5 nm. At the initial stages of growth, the RHEED intensity showed changes in the InAs lattice relaxation time depending on S. In other words, the InAs critical thickness (Hc) increases with increasing S. On the other hand, ex-situ Atomic force microscopy (AFM) measurements corroborated that by increasing S both the QDs density and diameter decreases.

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[ NSN-517 ] CoSb<sub>2</sub>O<sub>6</sub> nanoparticles for the detection of polluting gases

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We present in this work a study of micro and nanoparticles of the trirutile-type oxide CoSb<sub>2</sub>O<sub>6</sub> for their potential application in the detection of polluting gases. The material was synthesized using the microwave-assisted colloidal method at different concentrations of ethylenediamine. The crystalline phase obtained at 600 °C was analyzed by means of X-ray powder diffraction, finding a trirutile type structure with space group P4<sub>2</sub>/mm and cell parameters  $a = 4.654 \text{ \AA}$  and  $c = 9.283 \text{ \AA}$ . The vibration modes of the oxide's crystal lattice were investigated using Raman spectroscopy. The micro-structure characterization of the powder's surface was done by means of Scanning Electron Microscopy (SEM), showing morphologies like micro-columns, micro-bars of rectangular geometry and micro-spheres. The sizes of the microparticles were estimated in the range of 6-146  $\mu\text{m}$ . Employing Transmission Electron Microscopy (TEM), it was possible to observe nanoparticles of irregular geometry, mesopores and nanometric tetrahedral crystals; the size of the nanoparticles was calculated in the range of 32-70 nm. Gas detection tests were carried out in the presence of air/CO<sub>2</sub> flows at temperatures of 250 and 300 °C, applying AC signals with frequency of 0.1, 1, 10 and 100 kHz. Finally, tests of the oxide's electrical properties were performed in carbon monoxide (CO) and propane (C<sub>3</sub>H<sub>8</sub>) atmospheres at different temperatures. The results show that the oxide CoSb<sub>2</sub>O<sub>6</sub> can be applied as a sensor for the tested gases.



**[ NSN-522 ] Preparation recycled PET nanofiber from post-consumer bottles by electrospinning technique**

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Currently, soil contamination is one of the main problems for the environment due to the large amount of solids disposed in nature, being bottles post-consumer PET those found in greater proportion [1], therefore it is necessary make aware to search for alternatives for recycling and re-use [2]. In this work was carried out chemical recycling of PET bottles post-consumer by the method of glycolysis, for the purpose of obtain an unsaturated polyester resin (RPET) [3]. For the preparation of the nanofibers, the RPET was mixed with a carrier polymer as Polyvinyl Pyrrolidone (PVP) using the electrospinning method [4]. For the polymer solution 10% PET (1g) and 20% PVP (2 g) in relation to the solvent which in our case was dimethyl Formamide (8.51 ml) was used. Inside the electrospinning technique, the parameters studied were the applied voltage about 15-20 Kv, output flow rate of the solution of 0.5-1 ml/h and the separation distance between the needle and the collector plate of 15-20 cm. The morphology and size of the nanofibers were observed using an optical microscope (M.O) and a scanning electron microscope (SEM). The structure of the nanofibers was analyzed by infrared spectroscopy Fourier transform (FTIR). Through the electrospinning technique was possible to obtain RPET nanofibers using the PVP, where it was observed that the nanofibers containing no defects and its average diameter ranged from 100-400 nm.



[ NSN-530 ] Raman Spectra of SWCNTs at High Temperatures: Pretreated Samples in Nitrogen Atmosphere Improve Thermal Stability in Air

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We present a combined experimental and theoretical study dedicated to analyze the structural stability and chemical reactivity of single wall carbon nanotubes (SWCNT) in the presence of air and nitrogen atmospheres on the temperature interval of 300—1000 K. The temperature dependence of the radial breathing mode (RBM) region of the Raman spectra is irreversible under the presence of air, but it is reversible up to 1000 K in nitrogen atmosphere.

Our density functional theory (DFT) calculations reveal that irreversibility is due to partial degradation of SWCNT produced by a dissociative chemical adsorption of molecular oxygen on intrinsic defects of the nanotube surface. Oxygen partially opens the nanotubes forming semi-tubes having a non uniform diameter distribution observed by Raman scattering. In contrast, heating CNT's in nitrogen atmosphere seems to lead to the formation of nitrogen-doped SWCNT's. Our DFT calculations indicate that the most common types of nitrogen doping (e.g., pyridinic and substitutional) leave practically unaffected the RBM region of the Raman spectra, in agreement with our experimental data.

Actually, by allowing to interact previously nitrogen-exposed SWCNT's with air at different temperatures (up to 1000 K) we note now that the RBM region remains nearly unperturbed, defining thus our nitrogen-pretreated SWCNT's as more appropriate carbon nanostructures for high temperature applications in realistic environments. We believe we have implemented a post-growth heat-treatment process that improves the stability of carbon nanotubes preserving their diameter and inducing a defect-healing process of the carbon wall.



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[ NSN-540 ] Synthesis, characterization, and functionalization of  $\text{La}_{1-x}(\text{SrCa})_x/2\text{MnO}_3$   
nanoparticles for hyperthermia in cancer treatment

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Nanoparticles of  $\text{La}_{1-x}(\text{SrCa})_x/2\text{MnO}_3$  were synthesized by the sol-gel method at 873 K using oxides as precursors and applying the lowest temperature treatment to crystalize by microwave irradiation. The particles were coated with silica by the Stöber method to improve their biocompatibility. The nanoparticles are going to be characterized by XRD to know if we have the orthorhombic crystalline structure, FTIR to appreciate the functional groups presents in the particles, VSM to know the Curie temperature which could be 315-317 K and SEM to see if we have less than 100 nm of size in the particles. These nanoparticles could be used in hyperthermia cell treatment.



**NSN-542 | Energy band diagram of p-n-p photovoltaic quantum wires**

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Nanostructured semiconductor materials present a great potential for application in third-generation solar cells. In particular, one-dimensional (1D) nanostructures are promising in photovoltaic applications due to the improved charge transportation and large surface area for harvesting solar light due to the geometry of such 1D arrays. In this work we present a model that describe the energy band diagram of a p-n-p type junction. This model is used to describe core-shell type self-assembled n-type GaAs quantum wires (QWR) embedded in a p-type  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  matrix. A theoretical study of the energy band diagram of single and coupled p-n-p QWR, depending on the size of the QWR cross section and the separation between them, is presented. Finally, the experimental factibility of this kind of structures for photovoltaic applications is discussed.



[ NSN-552 ] Synthesis of Metallic Nanoparticles through a Pulsed Arc Submerged System

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In the present work it is described the use of a pulsed arc submerged of high current for the controllable preparation of Fe-Bi nps. The arc was submerged in water, the nps were dragged by the flow and separated by their characteristics (magnetic, heavy and light) for their recollection. Nevertheless the properties of the heavy and the light nps were similar and the only difference between them was the recollection way.

We analyzed the structure and the morphology of the nps with SEM, EDS, XRD and obtained the absorption spectrum. We observed an average size between 5 and 20 nm, a high percent of O, a low percent of Bi in the magnetic nps and found no Fe in the heavy and the light nps. We also saw spheres under 1000 nm with Fe core and Bi cover.

Additionally we took several videos with a Phantom camera and studied the spark produced by the arc, i.e. the volume and the growth speed of the bubble provoked by the spark. The maximum volume and the maximum speed increased with the energy applied to the system and while the volume grew linearly in time, the speed needed a second degree polynomial to its adjustment. Finally we observed the bubble evolution: first it expanded, then reached an equilibrium, later it contracted and expanded again before it undid.



[ NSN-560 ] Design and application of Au and Ag nanoparticles protein bound TcG1 and TcG4  
TcG2 of Trypanosoma cruzi for diagnosing Chagas disease

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The composition of nanoparticles and biological molecules is very attractive for its various applications in electronics, optics, and new applications in proteomics, genomics, and bioanalytical and biomedical areas. It has a useful and direct application in testing bioactivity and protein antigen recognition. Bioconjugation occurs primarily through covalent bonds and electrostatic interactions. Commonly conjugation via covalent metal-thiol bonds is used directly between the noble metal nanomaterial and biomolecules or crosslinking agents such as 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC), which there is a binder with amine groups and carboxylic acid. Biosensors of gold and silver nanoparticles linked to surface proteins TcG1, TcG4 and TcG2 are efficient for detection of different lineages Trypanosoma cruzi in 6/C57BL mice experimentally infected. The experimental system for synthesizing nanoparticles consisted of a simultaneous plate, which has two regulators controlling the stirring speed and temperature. A flask three necked ball was used as reactor, at one end of the flask, a thermometer monitoring the temperature reached in the reaction system was suspended. In another neck was attached a syringe to inject reagents, in the central part connects a refrigerant to carry out the reflow process finally in the bottom of the flask ball Teflon magnetic stirrer was placed to stir chemical reagents.

Recombinant protein production, to obtaining recombinant proteins cDNAs for TcG1, TcG4 and TcG2 genes were cloned into a plasmid pET-22b (Novagen, Gibbstown, NJ) with a histidine tag at its C-terminus. All cloned sequences were confirmed by digestion of the restriction fragments and sequencing of these genes in the plasmid. Plasmids were transformed into competent BL21 (DE3), and purification of recombinant proteins were performed by affinity chromatography using chelate-metal fused polypeptide polyhistidine sequences. These recombinant proteins were merged with nanoparticles. Trypomastigotes of different strains of T. cruzi were maintained and propagated in continuous passes across monolayers C2C12 cells in DMEM with 10% fetal bovine serum (HyClone, USA) to a pH of 6.8, at 37 °C, 5% CO<sub>2</sub> in an atmosphere (85%) of saturated humidity. C57BL / 6 mice were infected with three different strains of T. cruzi lineages: SylvioX10/4 (TCI); Esmeraldo (TCII) and 3869 (TCIII), with 500 to 1000 per mouse trypomastigotes of T. cruzi strain and corresponding trying to develop in mice the three phases of the disease. All mice were taken a blood sample (10 microliters) weekly for serological evaluation for T. cruzi antibodies by ELISA assay using vs the synthesis of protein-bound nanoparticle TcG1, TcG2 and TcG4. bioactivity assays of Ag/Au-NP + TcGs biosensor system were: trypomastigotes cell culture was washed with serum of experimentally infected heat-inactivated (55 °C for 30 min in a water bath) animals, diluted (50/50 V/V in PBS) in the presence or absence of human



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complement. The following groups were formed: 1) pre-immune serum Parasites + complement (negative control); 2) Parasites + complement (negative control); 3) Parasites + serum + complement inactivated by heat (test antibodies and complement the animal); 5) biosensor system Ag/Au-NP + TcGs + serum + complement inactivated by heat (test antibodies and complement the animal); 5) Parasites + heat-inactivated serum + complement (complement control); 6) Parasites + serum + complement one positive animal (positive control). A future the same above but now via through the visible ultraviolet spectrometry technique (UV-Vis) experiment was performed. It is to measure the optical properties of the nanoparticles. Assays for enzyme-linked immunosorbent assay (ELISA): It is intended ELISA assays performed as control.



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[ NSN-563 ] Stability of the as-milled reaction products: phase transition from PbSeO<sub>3</sub> to PbSe

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In the present work, we have designed a study with the aim to understand the relative stability or metastability of the as-milled reaction products; it is to say, the sluggish step associated to the synthesis of PbSe via the high-energy milling process. A detailed discussion of phase transition pathway from PbSeO<sub>3</sub> to PbSe nanopowders, or vice versa, via coordination polyhedra is proposed. The main interest is in detecting the stability or metastability of the as-milled reaction products through the bond parameters distortion. Those results are associated with the thermal decomposition behavior of PbSeO<sub>3</sub> studied by in situ high temperature X-ray diffraction.



[ NSN-569 ] A novel W-Shape nanodiode controlled by surface states

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Surface plays an important role in the behavior of semiconductor devices when they reach dimensions in nanometric scale. States, charge, and depletion zone at surface can be manipulated in order to alter the properties of thin layers by the disruption of the crystalline periodicity in the semiconductor. The so-called self-switching diode (SSD), developed by A. M. Song [1], is made when a nano-channel between two L-shape insulating grooves is fabricated by electron beam lithography. The depletion zone caused by surface states in the grooves, lets the current flux only in one direction. In this type of rectifiers the geometrical parameters have a strong relationship on the current-voltage behavior in conjunction with the surface states density. In this work, the authors explore by numerical simulations the performance of a new type of AlGaAs/GaAs two-dimensional electron gas (2DEG)-SSD called as W-Shape. In this type of SSD the electronic transport is controlled by the use of non-linear grooves. The depletion region that blocks the carrier current, is located in the W-vortex as it was concluded from calculations of the carrier density distribution. Additionally, the use of the 2DEG W-SSDs allows to explore mechanisms of changing the carrier quantum confinement dimensionality nature of the heterostructure from one- to zero-dimensional. This means that it is possible to change the electron confinement from quantum wire- to quantum-dot like by simply changing the SDD bias voltage. This could be an interesting method to study the change of the dimension of the 2DEG without modify the physical dimensions of the semiconductor. On the other hand, the geometry modification proposed allows to reduce the undesirable reverse leakage current keeping a threshold voltage near to 0 V, requirements for SSD harvesting systems that are difficult to obtain with the use of L- or V-shapes SSDs. The thickness of the channel and grooves defines the DC response of the W-shape SSDs with optimal parameters around of 20 nm for this geometry. The numerical study shown in this work explain the first principles of the change on the density of states in the W-Shape nanochannel and their performance as rectifier.

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**Acknowledgments:**

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**[ NSN-570 ] PVP electrospun nanofiber: effect of voltage and working distance**

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By the technique of electrospinning is possible to obtain fibers of different materials with diameters in the micro and nanometric scale. In particular, the combination of new properties, make nanofibers a new class of components suitable for the design and construction of new materials. In this paper was studied the effect of voltage and the working distance (distance between the tip of the needle containing the precursor and the collector where the fibers are deposited) on the formation and diameter of polyvinylpyrrolidone fiber (PVP). Varying these conditions (working distance and voltage), was possible to obtain PVP nanofibers with diameters in the nanometer scale. An ethanol solution containing polyvinylpyrrolidone with molecular weight of 55 000 was used as precursor. As a first step were tested different working distances (5, 10, 15, 20, 25 and 30 cm). smaller diameters fibers were obtained using the distance of 25 cm. Then we proceeded to vary the voltage. Values used were 5, 7.5, 10, 12.5, 15 and 17.5 kV., Increasing the voltage (5 to 17.5 kV) was possible to control the diameter of the PVP nanofibers continuous, stable and smaller diameter fibers are presented to 12.5 kV. The samples were characterized by scanning electron microscopy (SEM). Based on the properties of the polymer solution, an explanation of the effect of voltage and working distance was given.



[ NSN-571 ] Mbe growth and characterization of AlGaAs/GaAs n-p and p-n solar cells

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When a solar cell is designed, a great number of parameters (layer thickness, doping profiles, alloys, etc) have to be considered since each of those directly affects the performance and the capability of the photovoltaic device. In order to further optimize the solar cell functioning, each of the layers that are part of the heterostructure of the solar cell must be separately studied. As an example, for the realization of intermediate band solar cells one of the most important elements is the AlGaAs:Si blocking layer, since this layer electrically isolates the interband. In the same direction, it turns to be necessary to study the absorber layer and the electrical contacts to be used to improve the performance of the solar cell. In this work, the former parameters are studied by comparing the performance of Gallium Arsenide (GaAs)-based *p-n* and *n-p* junctions solar cells grown by Molecular Beam Epitaxy (MBE). The *n-p* type solar cell structure was grown *n*-type GaAs (100) substrate following the next sequence of layers: GaAs:Si( $1 \times 10^{18}/\text{cm}^3$ )/AlGaAs:Si ( $1 \times 10^{18}/\text{cm}^3$ )/GaAs:Si ( $1 \times 10^{16}/\text{cm}^3$ )/GaAs:Be ( $1 \times 10^{17}$ )/AlGaAs:Be ( $1 \times 10^{18}/\text{cm}^3$ )/GaAs:Be ( $1 \times 10^{18}/\text{cm}^3$ ). For the *p-n* type solar cell we used a GaAs (100):Zn substrates and the sequence of layers is reversed. Preliminary results obtained in the I-V characterization under the illumination of an AAA solar simulator shows that the short circuit current,  $I_{sc}$ , open circuit voltage,  $V_{oc}$ , and the efficiency,  $\eta$ , of the *n-p* solar cell are greater than those parameters of the *p-n* junction in a factor of 23, 1, 47, respectively. In other words, the photogeneration of carriers is improved when the *p*-type layers are illuminated. Moreover, it is demonstrated that the former parameters are better, as compared with a solar cell based on a single GaAs:Si/GaAs:Be *n-p* junction. Finally, in this work, the effect of Ag/Zn/Ag, Au/Ge/Au and Cr/Au alloys as metal contacts are also compared.

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[ NSN-577 ] Study of Strained InGaAs quantum wells through stressed InAs/GaAs upper barriers

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Low dimensional systems (LDS) are nanostructures capable to confine charge carriers within three or two dimensions. LDS have been studied deeply in the last decade because their unique confinement carrier properties that can be advantageous when applied in optoelectronics devices such as transistors, lasers, amplifiers, among others<sup>1</sup>. Besides, LDS offers unique opportunities for the study of fundamental properties of semiconductors and bandgap engineering studies, by changing the size of the structures and manipulating the band-edge potential that varies from layer to layer.

In this work, the authors show an alternative to manipulate the confinement potential of InGaAs quantum Wells (QWs) by changing the in-well strain through InAs/GaAs upper barriers. It is found that the strain of the GaAs/InAs upper barrier can be modified by changing the GaAs thickness and the InAs wetting layer (WL), which is left behind after the lattice relaxation of the InAs in 3D nanostructures. In particular, it is observed that by changing the GaAs thickness from 4ML to 20ML, the InAs WL thickness increases from 0.3nm to 0.4nm. The former variations are explained in terms of the reduction of the strain close to the heterostructure surface. On the other hand, the InGaAs QW nominal thickness was fixed at 20nm. The changes in the InAs WL are related to the strained InGaAs WL, therefore, these results indicate that the strain in the QW has been increased. Finally, on the assumption that the strained InAs/GaAs/InGaAs system grew within the pseudomorphic regime, the authors supported their conclusions estimating the stress tensors via strain simulations of the heterostructures.

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[ NSN-586 ] New method of synthesis of graphene from cvd in steady state

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The Graphene is a material used in a wide range of applications due to its unique structure and excellent electronic, optical, mechanical and thermal properties. Currently, several techniques are being developed to obtain graphene, one of this techniques that has highlighted which chemical vapor deposition (CVD) technique is the most reported. The fastest progress in graphene methodology in recent years have been obtained by this way. . In this sense, the aim of the investigation in graphene is to increase the graphene production by CVD with high quality and at low cost. However, usually to produce graphene, it is necessary to use high vacuum equipment and temperatures about 1800 °C, which represents a very high cost. In this paper a new method is proposed to obtaining monolayer graphene with good quality and low cost operation. Using acetylene and nitrogen as precursors by CVD is possible to obtained monolayer graphene by CVD, instead of methane and argon. Also a mix of nitrogen:hydrogen (90:10, respectively) was used instead pure hydrogen. All the components are subjected to temperatures about 1000 °C and atmospheric pressure, on polycrystalline copper foil. The synthesis of the graphene is carried out in steady state, reducing the synthesis time around a minute. The amount of gas flow is determined taking into account the reactor volume per unit mass. The presence of graphene is shown by transmission electronic microscopy and Raman spectroscopy confirmed the monolayer of graphene.



[ NSN-588 ] Deep Level Transient Spectroscopy study of Si/Si<sub>1-x</sub>Sn<sub>x</sub>/Si Quantum Wells. Valence Band Offset determination

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A set of three Si/Si<sub>1-x</sub>Sn<sub>x</sub>/Si(001) quantum wells (QWs) (x=0.0445, 0.0649 and 0.0834) are grown by molecular beam epitaxy. Ti Schottky diodes are done on the epilayer, and they are studied by deep-level transient spectroscopy. It is observed that the holes activation energies increase monotonically with the Sn fraction (x). The QWs are solved, and the activation energies of each QW are correlated to the valence band offset (the QW barrier). The valence band offset between pseudomorphic Si<sub>1-x</sub>Sn<sub>x</sub> and Si obeys the dependence  $DE_V = 1.715x$  eV. Our results confirm the applicability of the linear interpolation for the offset between the average valence bands of unstrained Si<sub>1-x</sub>Sn<sub>x</sub>/Si heterojunction  $DE_{V\_av} = 1.17x$  eV.

This work was supported by the National Council for Science and Technology (CONACyT) of México, postdoctoral fellowship 78965, the Fonds zur Förderung der Wissenschaftlichen Forschung (FWF Vienna, Austria), the PLATON-SiN project of Forschungsförderungsgesellschaft (FFG) (Vienna, Austria), project 20550, the Deutsche Forschungsgemeinschaft grant SPP1386 RA 1634/5-1 (Germany), the Bundesministerium für Bildung und Forschung within the Centre for Innovation Competence SiLi-nano, project number 03Z2HN12 (Germany).



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# **PHOTOTHERMAL PHENOMENA (PTP)**

**Chairman: Mario Enrique Rodríguez García (CFATA-UNAM)**



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**[ PTP-31 ] Photopyroelectric measurement of thermal effusivity of liquids by a method free of fitting procedures**

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This paper describes an alternative methodology to determine the thermal effusivity of a liquid simple using the well known photopyroelectric technique, without fitting the experimental data with a theoretical model and without having to know the pyroelectric sensor related parameters, as in most previous reported approaches. The basis of the method is the fact that the ratio of the amplitudes of the FPPE and BPPE voltages is linear with respect to the thermal effusivity. The method is not absolute, because a reference liquid with known thermal properties is needed. The modified measurement cell is presented, it allows measurement without sample movement for both techniques. Experiments have been performed that demonstrate the high reliability and accuracy of the method with measurement uncertainties smaller than 4%.



**[ PTP-225 ] 1D-thermophotoacoustic theory of the ultrasound generated by laser for plane samples**

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The thermophotoacoustic theory of the ultrasound generated by laser for plane samples with impedance mismatch with the surrounding medium is developed. For this, the 1D-thermoacoustic boundary value problem for the heat diffusion equation for temperature coupled with wave equation for the pressure was solve considering a system compose by a sample immerse in a non-optical absorbent fluid. The optical absorption of the samples was modeled by the Lambert-Beer law with delta (impulse response) temporal input pulses. We found that the back-propagated and transmitted spectra are continuous and periodic, with resonant frequency equal to twice the time of flight of the ultrasonic wave through the sample thickness. By means of numerical simulation it is shown that the resulting pressure over time is composed of a main pressure peak followed by periodically, time-retarded and time-inverted pulses with diminished magnitude. We found that, the retarder time (or repetition period) is equal to the inverse of the respective resonant frequency and, in contrast with the spectra. Finally, we discuss the applicability of the thermophotoacoustics for non-destructive testing and evaluation through the analysis of the frequency back propagated thermophotoacoustic amplitude.



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**[ PTP-350 ] Resonant photoacoustics**

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In the elastic regime and under the assumption that heat conduction has a negligible effect on the emitted acoustic wave, generation and propagation of Laser-Induced Ultrasound, or Photoacoustic (PA) waves, in an inviscid fluid is described by the inhomogeneous photoacoustic wave equation. In this contribution the theory of the 1D-photoacoustics for plane samples with impedance mismatch with the surrounding medium is developed. For this, the Photoacoustic boundary value problem for the photoacoustic wave equation was solve considering a system compose by a sample immerse in a non-optical absorbent fluid. It is found that the back-propagated photoacoustic spectra, for any input pulse, is a continuous function with periodic concave down peaks; contrary the transmitted one is concave up. By the inverse Fourier transformation the photoacoustic impulse is obtained in the time domain; for finite pulses, the amplitude was obtained by impulse response in convolution with the non-delta pulse. In both cases the resulting pressure is composed of main pressure peak followed by periodically, time-retarded and time-inverted pulses with diminished magnitude. These results were experimentally verified in solid and encapsulated liquids.



[ PTP-491 ] Thermal effusivity of human blood serum

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This work studies the thermal characterization of human blood serum by obtaining its thermal effusivity from the photopyroelectric technique. Photopyroelectric detection is one of the photothermal techniques that allows the thermal and optical characterization of materials. The photopyroelectric effect is the induction of a spontaneous polarization in a piezoelectric crystal not center-symmetrical as result of a change in the temperature of such crystal. Theory and mathematical modeling of the photopyroelectric effect were presented by Mandelis and Zver [1]. Thermal effusivity is a measure of the ability of a material to exchange thermal energy with its environment [2]. It is a function of the thermal conductivity ( $k$ ), and the volumetric thermal capacity ( $\rho C_p$ ). Mathematically it is defined as  $e = (\kappa \cdot \rho C_p)^{1/2}$ . Piezoelectric effect had been used for the study of biological material even before mathematical modeling. Therefore, it can be established that the pyroelectric effect is an essential and universal property of all biological systems [3]. The study was conducted on a population of 44 male patients of a clinic in the State of Mexico of a hospital for public servants. Blood samples were centrifuged for 5 minutes at 3,500 rpm to isolate the serum from the red formula. Technical setup for the photo-pyroelectric technique consists of a laser radiation source, optical fiber cable, one pyroelectric cell, a personal computer and a lock-in amplifier. The pyroelectric transducer is a film of poly-vinyl di-fluoride (PVDF) and has a thickness of 9 microns. First, it was run with just air in order to perform a normalization. The frequency modulation of the light beam varied from 1 to 1000 Hz. Data were normalized and the theoretical photopyroelectric equation was fitted to experimental data. Photopyroelectric technique let obtain both the amplitude and the phase of the pyroelectric signal of human blood serum samples. From the fit of the theoretical expression to the experimental data, it is possible to calculate the thermal effusivity. Both, the percentage error from the statistical analysis of the test and the margin of error were obtained. In conclusion the human blood serum was characterized though the pyroelectric detection technique. The average thermal effusivity obtained was  $918.847 \text{ (Ws}^{1/2}\text{)/(m}^2\text{K)}$  with an average margin error of 3.2395 %. Spectra of signal in amplitude and phase were also obtained. Further experiments of different population are necessary to corroborate these results.

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[ PTP-520 ] Juice and Rind Characterization of *Citrus latifolia* through the Photoacoustic Spectroscopy Technique

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The photoacoustic spectroscopy (PAS) is a technique quite *ad hoc* to characterize the optical properties of materials *in situ* such as biological samples. The aim of this work has been to characterize the juice and rind of the Persian lime (*Citrus latifolia*) by means of the PAS technique. In agreement to the Mexican quality standards, the samples under study were classified into four degrees of quality. We have used PAS to obtain the absorption spectra of the juice as well as the flavedo, i.e. the outermost layer of the rind. Our PAS characterization of the optical properties includes a phase resolved method. Our results verify that in the outer rind of the flavedo, the presence of flavonoid compounds necessary to protect by itself against several agents. Meanwhile, in the flavedo's depth another biological compounds as carotenoids and chlorophylls can be found. After that, using another different photoacoustic configuration, we have measured the water vapor permeability of the albedo, i.e. the innermost, white and spongy layer of the rind. Our results show that PAS is a reliable technique to get the quality assurance of samples *in situ* of fresh fruits such as Persian limes by means of the study of some of their physical properties.

Keywords: absorption spectrum; *Persian lime*; lime juice; lime peel; water vapor diffusion coefficient.



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**[PTP-583] Modeling the photoacoustic signal during the porous silicon formation**

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In this work the kinetics of the growing of porous silicon (PS) during the etching process is studied by using the photoacoustic technique. The experimental results was modelled by an extension of the Rosencwaig and Gersho model of photoacoustic effect in solids in which we propose three thermal sources: the usual pumping modulate beam, the changes in the reflectance of the PS-backing hetero structure, and the electrochemical reaction/Joule effect during the growing. The changes of reflectance are included in the model as a laser reflections of a monochromatic light term in the internal layers of the system. The frequency of this term is related with the etch velocity of PS. It is show that the velocity for large etching times it is not constant and the model provides a method that allows to determine the changes of velocity by fitting the frequency of the photoacoustic signal.



[ PTP-5 ] Phase separation technique of photoacoustic spectroscopy for the photosynthesis study  
in aquatic liriium

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We report a study on the photosynthetic activity of Aquatic Liriium (*Eichhornia Crassipes*), using phase separation technique of photoacoustic spectroscopy (PAS) when the plant is exposed to ultrasound waves (US) in low and high power of US irradiation. We consider a ultrasonic frequency of 17 KHz; low powers from 1 to 30 Watts as well as high powers from 30 to 50 Watts. Phase separation technique was used to evaluate the decrease in absorbent centers of light in the Liriium, particularly chlorophyll "a" y "b". We study of absorption spectra by means of phase separation technique in vis-region where the plants absorb the light for photosynthesis. We choose two ranges: blue range (450-520 nm) and red range (600-700 nm) where chlorophyll "b" and "a" has higher concentration, respectively. Our results show that there is a significant decrease in chlorophyll "a" by exposing the plants to high and low power ultrasound.

**Keywords:** Photoacoustic spectroscopy, phase separation technique, photosynthesis, ultrasound.



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**[ PTP-32 ] Thermal properties measurement in rigid samples by infrared thermography and a  
3D theoretical model**

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A method is discussed for thermal characterization of rigid bodies by measuring the surface temperature distribution resulting from peltier heating and fitting it using the results of a theoretical model based on the numerical solution of the heat diffusion equations with properly initial and boundary conditions. The temperature is measured using an infrared camera that gives sequences of thermographic digital images. The experiment is resolved in time, so that three dimensional mapping (two spatial coordinates and time) is realized. The aim of the fitting is to determine the thermal properties (particularly the thermal diffusivity) of the investigated sample.



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[ PTP-317 ] Characterization of aromatic oils thermal parameters using photothermal techniques

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In this work, the thermal parameters of aromatic citrus oils: diffusivity, effusivity, conductivity and specific heat, using the photothermal technique of thermal lens and pyroelectric were determined. Thermal lens (TL) is a non-invasive and highly sensitive technique for transparent and semitransparent samples, the thermal diffusivity ( $D$ ) is obtained from the setting the critical time parameter of the experimental to the theoretical curve values, using the experimental arrangement of uncoupled mode lasers; a He-Ne test laser which was operated with a wavelength of 632 nm and a power of 0.9 mW and a laser excitation of Ar + Xe with a wavelength of 514 nm and a power of 40 mW. On the other hand, the thermal effusivity ( $e$ ) of the sample was obtained by using the pyroelectric technique in inverse configuration (IPEE) where the temperature variation in the sample is due to diffusion of heat, the periodic warming in the pyroelectric sensor, due to the modulated radiation incident on this. From the obtained values of thermal diffusivity ( $D$ ) and thermal effusivity ( $e$ ), thermal conductivity ( $k$ ) was calculated from the ratio  $e=kD^{1/2}$  as well as the specific heat ( $c_p$ ) of the relationship  $D=k/\rho c_p$ . Thermal parameters obtained were compared with the values of the thermal parameters of literature. Complementary techniques UV-vis spectroscopy and infrared spectroscopy Fourier transform (FTIR) were used to study and determine absorption coefficients depending on the wavelength and chemical bonds, respectively. Among the oils studied are: dancy tangerine oil, green mandarin, grapefruit oil, orange oil and lemon oil. The importance of this research was to determine generally all parameters related to the heat conduction of these oils for food industry, cosmetic and medical applications.



**[ PTP-319 ] Phase separation of optical absorption spectrum of mixture of turmeric and black pepper obtained by photoacoustic spectroscopy.**

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*Curcuma longa* has been characterized as a highly antiinflammatory and antioxidant due to its content of phenolic compounds such as flavonoids and carotenoids [1] so its use for prevention of some diseases [2] is recommended, however, the human body needs some help to assimilate and thus maximize their benefits and an alternative of assimilation is to combine your intake with black pepper [3], achieving a greater benefit to the organism. In the present study optical absorption spectrum was obtained by means of photoacoustic spectroscopy, of *Curcuma longa* combined with black pepper, optical absorption spectra of turmeric and black pepper were also obtained separately. Furthermore, by the method of phase separation was possible to separate the two spectra corresponding to the spectrum of optical absorption of turmeric and the spectrum of optical absorption of pepper, this due to the different relaxation times that are natural pigments of turmeric and pepper. Thus apply this method to the analysis of data, amplitude and phase of the photoacoustic signal, to separate spectral components of commercial Turmeric, allowing us to obtain the absorption spectra of individual components and comparing with the spectra of optical absorption of these components, previously obtained.

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**[ PTP-450 ] Thermal Diffusivity Measurement by Lock-in Photothermal Shadowgraph**

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An innovative application of the shadowgraph technique for obtaining the thermal diffusivity of an opaque solid sample is presented. Inspired by the orthogonal skimming photothermal beam deflection technique, this new variant utilizes the shadow projected by the sample when put against a collimated light source. The sample is then heated periodically by another light beam, giving rise to thermal waves, which propagate across it and to its surroundings. The shadow is distorted due to changes in the refraction index of the surrounding media. This phenomenon is recorded and lock-in amplified in order to determine the sample's thermal diffusivity utilizing the slope method.

The technique overcomes some of the limitations of photothermal beam deflection. Alignment is simplified given that the experimenter must only interpose the sample between the probe light source and an imaging sensor in order to project a shadow. Also, the vertical offset between the probe light and the sample's surface ceases to be a major problem as one may select the pixels closest to said surface during post-processing. This method also allows us to obtain through a single measurement both spatial and temporal information. The technique has been validated through numerical simulation and by experimentally obtaining the thermal diffusivity of a set of calibration samples.



[ PTP-473 ] Comparative optical characterization of liquids by using Photopyroelectric and UV-Vis Techniques

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The light absorption by a material produces different phenomena, that depend on their physical properties, in order to study these phenomena some techniques have been developed, among these techniques stand out the photopyroelectric spectroscopy (PPES). In PPES a modulated light beam impinges on a sample which produces a modulated heat diffusion inside of this sample, which is detected by a pyroelectric sensor, in this way it is possible to know some physical characteristics of the material in study, such as: thermal conductivity, thermal diffusivity, specific heat, optical absorption coefficient, among others. Another technique that is employed in the optical characterization is Ultraviolet-Visible spectroscopy (UV-Vis), which is conventionally used in the industry and research laboratories. Both techniques, PPES and UV-VIS, are employed in the optical characterization of liquids samples. In this work a comparative study between both techniques is proposed by comparing the optical absorption and transmission spectra of four vegetable oils: Olive, Avocado, Grape seed and Sesame. The comparative study was based on the analysis of the optical absorption bands, corresponding to the natural pigments contained in each sample, obtained by the employed techniques. The results show that the optical absorption and transmission spectra, obtained by using PPES, are in agreement with the maximum optical absorptions reported in the literature for the natural pigments contained in the oils, also PPES spectra show bigger amplitude and definition when compared with the spectra obtained by UV-Vis, in this last technique is required a specific preparation for each sample. The light absorption by a material produces different phenomena, that depend on their physical properties, in order to study these phenomena some techniques have been developed, among these techniques stand out the photopyroelectric spectroscopy (PPES). In PPES a modulated light beam impinges on a sample which produces a modulated heat diffusion inside of this sample, which is detected by a pyroelectric sensor, in this way it is possible to know some physical characteristics of the material in study, such as: thermal conductivity, thermal diffusivity, specific heat, optical absorption coefficient, among others. Another technique that is employed in the optical characterization is Ultraviolet-Visible spectroscopy (UV-Vis), which is conventionally used in the industry and research laboratories. Both techniques, PPES and UV-VIS, are employed in the optical characterization of liquids samples. In this work a comparative study between both techniques is proposed by comparing the optical absorption and transmission spectra of four vegetable oils: Olive, Avocado, Grape seed and Sesame. The comparative study was based on the analysis of the optical absorption bands, corresponding to the natural pigments contained in each sample, obtained by the employed techniques. The results show that the optical absorption and transmission spectra, obtained by using PPES, are in agreement with the maximum optical absorptions reported in the literature for the natural pigments contained in the oils, also PPES spectra show bigger amplitude and definition when compared with the spectra obtained by UV-Vis, in this last technique is required a specific preparation for each sample.



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# **PLASMA AND VACUUM (PLV)**

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**[ PLV-140 ] Optical emission spectroscopy of nitrogen plasma for growth of III-nitride compounds**

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Plasma-assisted molecular beam epitaxy (PA-MBE) of III-V nitrides has been an active field of research because GaN-based heterostructures has recently been applied to the fabrication of solar cells, sensors and UV electroluminescent devices. Nitride growth kinetics mainly depend on substrate, substrate temperature and metal/N ratio in the crystallization region. The latter depends on nitrogen active species in the plasma and has a profound effect on nitrating processes, growth mode and crystal relaxation [1,2]. In this work we perform optical characterization of nitrogen plasma generated by an inductively coupled radiofrequency source. Light emission from plasma in high bright mode was collected using an optic fiber and conducted to the monochromator, where emission spectra were recorded in the range of 200 - 1000 nm for different plasma conditions. The conditions explored cover RF power values from 150 up to 350 W and molecular nitrogen flows from 0.25 up to 1.5 sccm. Atomic nitrogen density is sensitive to the RF power applied to excite the plasma while varying the incoming flow impacts the signal of metastable nitrogen molecules. This outcome allows to distinguish conditions where some kind of nitrogen species are favored than others. At relatively low nitrogen flow rate, the RF power is mainly used to generate atomic nitrogen by molecular dissociation, while excitation power is gradually distribute between molecular excitations and generation of atomic nitrogen as flow rate is increased (0.6-1.5 sccm). Detailed model was performed to estimate the relative densities of the nitrogen species as function of excitation power and inflow molecular nitrogen gas in the range of plasma stabilization. In order to study the effect of nitrogen species on growth kinetics, two sets of InN samples were grown keeping the growth conditions fixed and only varying the plasma parameters (RF power and N<sub>2</sub> flow). The first set consist of 3 samples where the N<sub>2</sub> flow was maintained at 0.25 sccm and RF varied at 250, 300 and 350 W, respectively; the other one was composed by 3 samples which N<sub>2</sub> is fixed at 1.5 sccm with RF powers of 250, 300 and 350 W. We observed that both the surface morphology and the growth mode strongly dependent on the plasma settings. In the first set of samples, active species are mainly composed by atomic nitrogen, while in the second set of samples, metastable molecular nitrogen is the main responsible of growth dynamics during InN growth.

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[ PLV-356 ] Characterization of thin films of the ternary system V<sub>2</sub>O<sub>5</sub>-CdO-Cu deposited by laser ablation

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A series of four thin films were deposited on quartz substrates by the laser ablation technique, using a Nd-YAG pulsed laser at 1064 nm during 30 minutes. The ablated target material was synthesized by melt-quenching method using as precursors powdered vanadium pentoxide, cadmium oxide and copper at 10, 80 and 10 percent on weight, respectively. The fusion process was carried out in porcelain crucibles during 30 minutes in air atmosphere, and the thermal shock at room temperature in stainless steel molds. The amorphous conditions of the ablated material and thin films were confirmed by X-Ray diffraction patterns. By Raman Spectroscopy it was observed the presence of vibrational modes centered at 434, 495 y 710 cm<sup>-1</sup> and a broad band in 828 cm<sup>-1</sup>, corresponding to compounds such as CuCdVO<sub>4</sub>, Cd<sub>2</sub>V<sub>2</sub>O<sub>7</sub> and possible traces of CdV<sub>2</sub>O<sub>6</sub> in amorphous state. The morphology of all the obtained samples was obtained by Scanning Electron Microscopy and the elemental chemical composition by Energy Dispersive Spectroscopy. Optical properties also were studied. The band gap, were estimated from 3.23 to 3.33 eV, by optical absorption and Tauc's Method. While photoluminescent emissions, were present in both kind of materials at 2.33, 2.8 and 2.98 eV. These kind of emissions, are attributed to the presence of VO<sub>4</sub> and VO<sub>3</sub> ions from the CuCd(VO<sub>4</sub>) and Cd<sub>2</sub>V<sub>2</sub>O<sub>7</sub> compounds.



**[ PLV-412 ] Spectroscopic study of plasma emission and its relation to the properties of SiO<sub>x</sub>N<sub>y</sub> thin films during reactive DC magnetron sputtering**

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In this work we present a thorough study on the relation between the plasma physics and the properties of SiO<sub>x</sub>N<sub>y</sub> thin films grown by Magnetron DC sputtering (MS) technique. Thin films were grown on silicon (100) wafers at constant fluxes of Ar and N and varying the working pressure from 3.8 to up to 8.5 mTorr in ~1 mTorr steps. Each experiment comprised a set of layers, which consisted of exposing the substrate a given time to the sputtered material at a given working pressure, from the minimum to the maximum and back again to the minimum pressure. Between layers the substrate was covered by a shutter until the next pressure in the chamber was reached.

The emission of the plasma was interrogated in real time by means of optical emission spectroscopy (OES) observing at the target and at the substrate positions simultaneously. Emission intensity from Ar, Ar<sup>1+</sup>, N<sup>1+</sup>, Si and O transitions were followed during deposition time and ratios from some of these lines are proposed as an indirect but robust monitors of the evolution of the target poisoning process and the film composition. In addition, optical properties of the films were measured in-situ by spectroscopic-ellipsometry and then correlated with OES observations. Results show that the oxygen content within the thin film increases with working pressure and these observed changes in stoichiometry, thus changes in film optical properties, can be deduced from observed changes in the plasma emission spectrum.



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[ PLV-414 ] Hard transparent coatings deposited by laser ablation

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Deposition of Al-Si-N thin films using simultaneous laser ablation of silicon and aluminum targets in a nitrogen atmosphere was performed at 200°C substrate temperature. The Si content of the films was studied as a function of the plasma parameters (mean ion kinetic energy and plasma density), produced by the ablation of the Si target. The plasma parameters were measured by means of a planar Langmuir probe and optical emission spectroscopy. The chemical composition of the films was measured by X-ray photoelectron spectroscopy. The results showed reliance between the silicon content and the plasma density. The deposition pressure was varied producing changes in the intensity of excited species ( $N_2^+$ ,  $Si^{2+}$  and  $Al^+$ ), as seen by optical emission spectroscopy, and thus in the incorporation of those elements in the sample. For a working pressure of 0.6 Pa, hardness measurements gave a maximum of  $24.7 \pm 1.2$  GPa for a silicon content between 6- 10 at. %; furthermore, results of the optical band gap measurements showed dependence across the range of Si content in the samples, obtaining values between 2.3 eV and 4.6 eV.



**[ PLV-452 ] Effect of deposition pressure on the plasma parameters used for growth of amorphous carbon thin films by pulsed laser deposition**

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Characterization of laser produced plasmas has proven to be a powerful tool in controlling the properties of thin films deposited by laser ablation. Planar Langmuir probe characterization has been widely used to diagnose the mean kinetic energy and density of the ions present in the laser produced plasmas. It has been shown that both parameters have a direct influence on the physical and chemical properties of the grown films. Plasma parameters depend on the energy density (fluence) deposited on the target. In order to change the fluence, the output energy of the laser together with the beam spot size must be controlled. For Q-switched lasers the energy can be controlled using different delay values. The variation in delay time affects the beam spot size also, thus affecting the laser fluence on the target. Typically, for pulsed laser deposition, fluence is chosen as one of the principal experimental values for controlling films deposition without concerning about plasma parameters. Thus, making a complete characterization of the laser energy and spot size dependence on the delay time followed by the plasma characterization will allow having excellent control on pulsed laser deposition experiments. In this work the energy output of the laser and the spot size at different delay values were studied. Results show that the laser energy has a linear dependence on delay time. On the other hand, the spot size was found to decrease exponentially with increasing delay time; as a consequence, the fluence does not have a linear dependence on delay time. Finally at a fixed fluence, a carbon target was ablated in order to characterize the plasma parameters as a function of pressure using air as background gas. Four amorphous carbon films were grown under different conditions finding that their physical properties are strongly influenced by the plasma parameters.



[ PLV-479 ] Effect of temperature changes on deposition process for n-ZnO/p-ZnO:Ag,N structure

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Structures formed with n type ZnO and p type ZnO:Ag, N thin films were deposited on Si(100) substrates by DC reactive magnetron sputtering at different temperature under argon and nitrogen composition. As precursor, a Zn target with a purity of 99.99% was used and a Ag target was used in the p-type films. The effect of the temperature changes on the incorporation of nitrogen and silver and the effect on the structural, electrical and optical properties was studied, as the consequence on the interface system p-type/n-type. Energy Dispersive Spectroscopy (EDXRF) confirms the presence of Zn, Ag, O, and N in the deposited film structure. XRD results showed the hexagonal phase for ZnO, with the effect of the oxygen and silver on the ZnO:Ag,N component, as it is expected. UV-Vis and IR spectroscopy presented the tendency associated to the ZnO for IR vibrational modes and band gap, with the effect of the impurities on the structure and the changes associated to both types of characterization.



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[ PLV-503 ] Sputtering yield amplification evidence for C, Al and Si measured by ion beam analysis and the CO-SS code

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Sputtering yield is considered a fixed value, however, S. Berg et al, discovered a phenomenon which they called Sputtering Yield Amplification. The phenomenon is observed by irradiating with atoms of atomic number Z, a target with atoms with a lower Z, resulting in an increase in the sputtering yield of the target irradiated. Moreover, it has also been observed the phenomenon performing magnetron co-sputtering with a target composed of two different materials. However, there is no adequate theoretical explanation of this phenomenon.

The co-sputtering simulation freeware, CO-SS, was developed by the authors to simulate the spatial variation and composition of the deposition by magnetron sputtering and co-sputtering. In this study thin films of Al/Ti, C/W and Si/W were produced to study the modification of the sputtering yield both experimentally and by modelling using CO-SS. The 4" x 1/4" sputtering targets were of high purity Al, C and Si and the sputtering conditions for all deposits was maintained at 20 sccm of argon, a gas pressure of 30 mTorr (4 Pa) and a plasma power of 40 watts. A series of films was prepared of the pure metal or with 1, 2 or 3 small pieces (0.7 X 2.5 cm) of the second material (Ti or W) placed on the racetrack directly above the 3" x 1" glass substrates. The substrates were placed such that they received material from both the uncovered and covered parts of the racetrack. The spatial variation of the thickness and composition of the films was determined by profilometer and the <sup>4</sup>He RBS technique, respectively. The results showed the existence of the previously mentioned sputtering yield amplification of Al, C and Si.



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**[ PLV-529 ] Effect of Changes on Power Deposition for n-ZnO/p-ZnO: Ag, N Structure.**

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Thin films bilayers formed with n type ZnO and p type ZnO:Ag, N thin films were deposited onto Si(100) substrates by DC reactive magnetron sputtering at different power deposition under Argon and Nitrogen composition. As precursor, a Zinc target with a purity of 99.99% was used, in order to form ZnO, Oxygen was introduced; in the case of p type films, a Silver target was used with Nitrogen, both as impurities for this type of films. The effect of the power deposition changes induced on the incorporation of nitrogen and silver and the effect on the structural, electrical and optical properties was studied, as the consequence on the interface system p-type/n-type. Energy Dispersive Spectroscopy (EDXRF) confirmed the presence of Zn, Ag, O and N in the deposited bilayer structure. The XRD patterns confirmed the typical hexagonal phase for ZnO, with the effect of the Oxygen and Silver on the ZnO: Ag, N layer, as it was previously observed in other works for ZnO doped. UV-Vis and IR spectroscopy presented the tendency associated to the ZnO for IR vibrational modes and its band gap, appearing the effect of the impurities on the structure in the changes associated to the results of both types of characterization.



[ PLV-250 ] Influence of the mean kinetic energy of the plasma on the crystalline orientations and optical properties of ZnO thin films grown by PLD

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**Abstract.** ZnO thin films were deposited on glass substrate at room temperature by laser ablation of a Zn target in an O<sub>2</sub>/Ar atmosphere. The pressure in the chamber was kept constant at  $2 \times 10^{-2}$  Torr for all deposits. The mean kinetic energies of the ions in the plasma were calculated from “time of flight” curves obtained with a Langmuir planar probe. The influence of the mean kinetic energy on the crystalline orientations and optical properties of ZnO thin films were investigated. The XRD patterns of the ZnO films reveal the presence of a strong peak corresponding to the (101) and a weak peak corresponding to the (002) planes of hexagonal wurtzite ZnO for a low energy (35 eV). Increase in kinetic energy, to 50 eV, turns into a loss of intensity in (101) diffraction peak, and the revealing of a small broad peak at  $55.6^\circ$ , which is associated to the (110) plane of wurzite ZnO. Further increase in Zn<sup>+2</sup> mean kinetic energy results in reorientation of crystal grains deposited; as revealed by the increase in intensity of the (110) peak and decrease of the intensity of the (101) peak. Low percentages in transmission spectra were obtained for the ZnO films obtained with lower range of ion kinetic energies (35 – 50 eV); meanwhile, samples deposited at energies between 106 eV and 131 eV had a transmission in the order of 85 %. Optical band gap energy ( $E_g$ ) was calculated in the range 3.2 – 3.5 eV.



[ PLV-267 ] **Optical characterization of CdTe nanoparticles embedded in a nanoparticulate SnO<sub>2</sub> matrix**

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Cadmium telluride (CdTe) nanoparticles were grown in the interior of a SnO<sub>2</sub> transparent matrix by means of the r.f. sputtering technique. X-ray diffraction (XRD) patterns reveal that the CdTe quantum dots (QD) grow in the hexagonal wurtzite (W) phase. Diffraction data show that SnO<sub>2</sub> is constituted by nanoparticles also, with size of the same order of the W-CdTe QD. The broad bands of the XRD patterns and the Scherrer formula allowed, by assuming a spherical shape, the W-CdTe QD size calculation, which have average diameters in the range 4.8 – 14.0 nm. These data were confirmed by electron microscopy images. Optical absorbance gives information to calculate the energy of the two lowest excitonic states (band gap). The Raman spectra show a broad band in the range 100 – 200 cm<sup>-1</sup>, on which deconvolution allows separate three modes at c.a. 120, 140 and 160 cm<sup>-1</sup>. The first one at ~ 120 cm<sup>-1</sup> is identified with the A<sub>1</sub> mode of tetragonal Te. The second and third modes at ~ 140 and 160 cm<sup>-1</sup>, respectively, correspond to the transversal optic (TO) and longitudinal optic (LO), respectively, modes of CdTe at the  $\Gamma$  point of the first Brillouin zone. The positions of the LO and TO bands follow, for phonons in nanoparticles, the expected behavior if the radius of crystal decreases, taking into account that the selection rules for momentum conservation are relaxed.



[ PLV-270 ] CdTe:Sn thin films grown by pulsed laser deposition using powder as target

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Cadmium telluride (CdTe) is a II-VI semiconductor compound with a direct bandgap of 1.45-1.5 eV at room temperature and a high absorption coefficient ( $>5 \times 10^5 \text{ cm}^{-1}$ ), which means that a layer thickness of few micrometers is enough to absorb 90% of incident photons. Due to these properties, the CdTe is an ideal absorber material for high efficiency low-cost thin-film polycrystalline solar cells. CdTe films have *n*- or *p*-type conductivity; cadmium excess yields *n*-type, while tellurium excess yields *p*-type conductivity. A promising system is based on the CdS/CdTe heterostructure due to a predicted efficiency around 30%. In this system the *p*-type CdTe film acts as photoabsorbing layer to generate carriers. Recently, hybrid solar cells have emerged as very promising photovoltaic devices due to they are flexible, light, inexpensive and easy to fabricate. In this work, we report the influence of Sn nominal concentration in the target-material on the structural properties of Sn-doped CdTe films grown by PLD using CdTe and Sn powder as target-material.

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**[ PLV-318 ] Development of a computational algorithm for spectra analysis oriented to the construction of a portable and self-calibrated LIBS system**

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When you target the surface of a material with a laser short pulse, part of the energy absorbed induces remotion, vaporization and ionization of the sample. If the power is high enough, it forms a plasma plume over the material who emits light in different wavelengths. The Laser Induced Breakdown Spectroscopy (LIBS) consist in implementing optical techniques to analyse the light emitted from the plasma plume to determine the elemental composition of the sample.

A portable LIBS system is a complex and hard to do project, that has only been possible in the last decade thanks to the advancing in sensors and laser technologies. Nonetheless, one of the principals limits to their portability is the constant necessity of controlled samples and environments for their calibration. The kind of sample and environment depends of the elements you hope to find in the material. As a solution, we propose the development of a system, who is still portable, but also has the information and algorithms inside to be self-calibrated.

In this work, we present an algorithm to identify spectral lines and adjust an elemental decomposition to the spectra obtained from samples of industrial aluminium, as well as an estimation of the elemental proportions. Lines found were related to the atomic transition spectral lines reported in the NIST Atomic Spectra Database Lines Form.

The adjust parameters found help us to elaborate the necessary processes for the self-calibration of the spectra.



[ PLV-346 ] Synthesis and characterization of p-type Ag-N dual acceptor doped ZnO thin films.

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P-type ZnO was realized by dual acceptor co-doping with nitrogen and silver via DC reactive magnetron co-sputtering. As precursor material were used a Zn and an Ag metallic targets with a purity of 99.999%. Structural and electrical properties were investigated. As deposited film was amorphous however after of annealed treatment the crystallization of the films are improved and they showed the hexagonal wurzite structure of ZnO. X-Ray Energy Dispersive Spectroscopy (EDX) confirms the presence of Ag and N in ZnO:(Ag,N) film. The electrical and optical properties were explored by Hall Effect measurement, and optical transmission and absorption spectra for the films as deposited and annealed for one hour in nitrogen atmosphere. The conductivity type and electrical properties of the as-deposited ZnO:(Ag,N) film revealed a strong dependence with the N/O/Ar gases ratio in the reactive atmosphere. However after annealing, all the films presented p-type conductivity and the electrical properties were improved significantly for the films annealed at higher temperature, the best values obtained were a low resistivity of  $8.56 \times 10^{-3} \Omega \cdot \text{cm}$  and high carrier concentration  $3.17 \times 10^{19} \text{cm}^{-3}$ .



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[ PLV-398 ] Analysis of electrical and optical stability of p type ZnO:Ag,N thin films.

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P-type ZnO thin films were deposited by dual acceptor co-doping with nitrogen and silver by DC reactive magnetron co-sputtering. As precursor material were used a Zn and an Ag metallic targets with a purity of 99.999%. The film was annealed at 673 K and 723 K for one hour in nitrogen atmosphere. Energy dispersive spectroscopy (EDX) confirms the presence of Ag and N in ZnO:(Ag,N) film. The electrical properties were explored by Hall Effect measurement, and the optical transmission and absorption spectra were obtained by Uv-Vis spectroscopy. The films present p-type conductivity with a low resistivity of  $8.56 \times 10^{-3} \Omega \cdot \text{cm}$  and high carrier concentration of  $9.28 \times 10^{19} \text{ cm}^{-3}$ . To study the degradation of the optical and electrical properties of the films, they were characterized again, at six and nine months after of the deposit, in the final measurement a resistivity of  $2.21 \times 10^{-3} \Omega \cdot \text{cm}$  and high carrier concentration of  $1.43 \times 10^{18} \text{ cm}^{-3}$  were obtained, these results revealed a high electrical and optical stability.



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**[ PLV-413 ] Development of computing algorithms for spectral analysis in a Laser Induced  
Breakdown Spectroscopy system**

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Laser induced breakdown spectroscopy (LIBS) has been widely used for elemental analysis of solid, liquid and gaseous samples due to its portability and the practical null sample preparation. The main drawback of this technique is the necessity of having a calibration curve to obtain quantitative information of the sample, which in some situations is practically impossible to get. Hence, it has been developed a calibration-free algorithm which provides the composition of the sample by assuming a Boltzmann distribution of all species within the ablation plasma, where spectroscopic information of all species is required. In this work a semi-automatic algorithm to identify and deconvolute emission peaks of the plasma spectrum is presented, as well as its lorentzian function fitting. The code also relates each emission peak found in the ablation plasma to those listed in the NIST atomic spectra database, so the qualitative composition of the sample is granted. The fitting parameters along with the spectroscopic data from the database will allow to implement a calibration-free procedure in the future.



[ PLV-422 ] Influence of laser ablation plasma parameters in the synthesis of nanostructured Al-Si-N thin films

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Coatings based on Al-Si-N have attracted the attention of many research groups as they can improve the hardness, transparency and oxidation resistance of AlN coatings, depending on the Si content. This type of coatings is usually deposited using plasma assisted techniques. Pulsed laser deposition is a technique that allows the deposition of ternary systems, such as Al-Si-N, but has not been extensively used. In this study Al-Si-N thin films were deposited using simultaneous laser ablation of two targets (Al and Si) in a reactive atmosphere of N<sub>2</sub>, with a substrate temperature of 200 °C. The plasma parameters (ion kinetic energy and plasma density) were studied using a Langmuir planar probe and optical emission spectroscopy (OES). The mean kinetic ion energy and plasma density of the particles from the Al target, were kept constant at values of 200 eV and  $9.3 \times 10^{19} \text{ m}^{-3}$ , respectively. The mean kinetic energy of the particles produced from the Si target, was approximately 40 eV for all the experiments and the plasma density was varied from  $0.7 \times 10^{18} \text{ m}^{-3}$  to  $7 \times 10^{18} \text{ m}^{-3}$ . XPS measurements showed a clear evidence of a linear dependence of the Si content regarding Si plasma density, which depends on the working pressure. The optical emission spectrum generated by the simultaneous ablation, showed that the most intense characteristic emission spectral lines corresponded to Al<sup>+</sup> (281.6nm), Si<sup>2+</sup> (309.4nm) and N<sub>2</sub><sup>+</sup> (391.4nm). In order to observe changes in the emission spectra, the working pressure was varied from 0.4 to 1 Pa. It was noticed that as the nitrogen working pressure increases the characteristic spectral lines relative to the excited species of Al<sup>+</sup> and Si<sup>2+</sup>, became the most important, contrary to the case of the molecular nitrogen excited species (N<sub>2</sub><sup>+</sup>) which became less intense.



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**[ PLV-482 ] ZrN thin films deposition on Si under forming gas influence.**

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The presence of oxygen in nitrides is very determining on their physical properties. It is very important to reduce the oxygen contents on these kind of films proposed as ultra-high hardness. ZrN thin films has been prepared by DC-Sputtering deposition under the influence of forming gas, to reduce the presence of oxygen. Zr target (99.99%) purity has been used to prepare films in a Ar-N<sub>2</sub> ambient, in a small home-made deposition system, at different concentrations of forming gas (80 %N<sub>2</sub>- 20%H<sub>2</sub> mixed composition). Films were deposited on Si substrates. Energy Dispersive Spectroscopy (EDXRF) confirms the presence of Zr, Ag, O, and N in the deposited layer structure. The oxygen is correlated to the presence of gas forming. XRD confirms the ZrN cubic structure related to NaCl. Structural changes are related to the oxygen incorporation on structure.



[ PLV-493 ] Effect of plasma parameters variation on the physical properties of Cu-Ag thin films deposited by the simultaneous ablation of Cu and Ag targets

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Mixing two different metals can result in enhancement or modification of the physical and chemical properties compared to that of the individual components. In order to achieve good quality bimetallic thin films it is necessary to have accurate control of deposition conditions. Pulsed laser deposition has shown to be an adequate technique for growth of high quality materials.

It has been previously observed that ion density and mean kinetic ion energy of the laser produced plasmas have a strong influence on the properties of the deposited films, thus, modification of plasma parameters allows a precise control on the films properties together with reproducibility of experiments.

In this work CuAg thin films were grown by the simultaneous ablation of high purity Cu and Ag targets. The plasma parameters were calculated using the TOF curves obtained from Langmuir planar probe measurements. The energy and density of the Cu plasma was kept constant. The ion density of the Ag plasma was varied in order to change the incorporation of Ag into de CuAg films. The samples were characterized by X-ray diffraction, scanning electron microscopy and energy dispersive x-ray spectroscopy. The results are analyzed as a function of the Ag ion density in the plasma.



[ PLV-499 ] Effect of the increase of Sn plasma ion density on thin films deposited by simultaneous laser ablation of CdTe and Sn targets

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Cadmium telluride (CdTe) films are suitable for application in optoelectronic devices such as solar cells and X-ray detectors due to its excellent optical and electrical properties. One of the main characteristic of CdTe is that a layer of few micrometers of thickness can absorb 90% of incident photons, because it has optical bandgap around 1.5 eV and high absorption coefficient ( $>5 \times 10^5 \text{ cm}^{-1}$ ). CdTe can have both *n* or *p* conductivity, depending on the doping impurities such as Ge, Pb and Sn. The material presents interesting magnetic and optical characteristics. For that reason, the interest in producing high quality layers of CdTe has been increased in recent years. These films were grown using atomic layer epitaxy, molecular beam epitaxy (MBE) and pulsed laser deposition (PLD). The PLD technique can produce high quality layers of many different materials, with the possibility of obtaining stoichiometric films with excellent physical properties.

The objective of this work was to study the changes in CdTe films with Sn impurities as a function of the density of Sn ions present in the plasma generated during the PLD process on glass substrates. Four films were grown by the simultaneous ablation of CdTe and Sn targets. The Sn ion density was modified varying the beam spot size incident on the Sn target, while the CdTe plasma parameters were kept constant for all deposits. The ion density was measured using a Langmuir planar probe, obtaining values from  $8.1$  to  $18.7 \times 10^{11} \text{ cm}^{-3}$ . The resulting crystalline structure was analyzed by XRD, these studies showed a hexagonal structure for every film with a preferential orientation in the plane (110). The band gap was calculated using UV-Vis spectrophotometry; this showed values from 1.42 to 1.47 eV for



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different layers. The films thicknesses were measured using a stylus profilometer and their chemical composition was determined by EDS. The SEM was used to study the films surface morphology and by means of Raman spectroscopy vibrational properties were analyzed.

**[ PLV-518 ] Gallium indium nitride growth by close space sublimation (CsS) into tube furnace**

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In this work we propose a new low cost and fast growth process in order to synthesize gallium indium nitride ( $\text{Ga}_{1-x}\text{In}_x\text{N}$ ) thin films for his application in photovoltaic technology development. We used the close spaced sublimation (CSS) technique employing a tube furnace, without any vacuum system or source of gases for the synthesis process. The precursors of the samples type  $\text{Ga}_{1-x}\text{In}_x\text{N}$  are, a mixture of gallium nitride powder (99.99% purity) and indium nitride powder (99.9% purity) at different concentrations, as well as ammonia hydroxide employed as compensation source of nitrogen (N) in order to obtain stoichiometric samples with low N deficiencies. The substrate employed is p-Si (1 1 1), due to his high growth rate by this method in comparison with other common substrates employed for this kind of semiconductors. Both, the substrate and the precursors are contained inside a semihermetic graphite cell, that was placed into the tube furnace for the synthesize process, considering an effective time of 10 minutes at 1200°C. The samples exhibit PL emission at room temperature. The characterizations were carried out by EDS, SEM, Raman Spectroscopy and PL.

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[ PLV-543 ] Laser annealing of semiconductors nanocrystal thin films

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In this work we show the laser annealing effects on the structures and properties of silicon and germanium nanocrystal ultrathin films fabricated by RF sputtering. Photoluminescence (PL) peaked at 2.0 eV and 1.84 eV for silicon and germanium nanocrystals, respectively, is observed in the as-deposited films. After single-pulse laser annealing, better crystallinity and increased PL intensity are obtained. The PL peak remains around 2.2 eV for silicon and 1.89 eV for germanium. The as-deposited nanocrystalline films exhibit an amplified spontaneous emission due to the interfacial potential barrier. After being annealed is transferred to a quantum-confined core because the phase transformation could remove the interfacial barrier. High laser fluence causes damage to the films and the threshold fluence for laser ablation is around 80 mJ/cm<sup>2</sup>. Multiple-pulse laser annealing with increasing pulse number at fluences below the threshold of laser ablation can provide better crystallization and property improvement than single-pulse annealing. There are a certain number of pulses for the best multiple-pulse annealing effect before damage or laser ablation occur. Laser annealing was shown to provide the possibility of fine-tuning the nanocrystals size and concentration, which is important in photovoltaic and thermoelectric devices fabrication.



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# **RENEWABLE ENERGY: SOLAR CELLS AND MATERIALS (RWE)**

**Chairmen: Guillermo Santana (IIM-UNAM)**  
**Mario Fidel García Sánchez (UPIITA-IPN)**



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**[ RWE-30 ] Investigation of CdS/CdTe photovoltaic structure for Hybrid Sun-tracking solar energy converting system**

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Solar modules based upon CdS/CdTe semiconductor junction nowadays occupy a solid position in the market of renewable energy devices, with a well established technology using a superstrate structure and Closed Space Sublimation technique of deposition of a CdTe absorber layer. This technique is quick, cheap and efficient; however, it does not allow precise control of the deposition parameters, and thus of the characteristics of the resulting structure. For specific applications in Sun-tracking hybrid system with normal incidence of the sunlight to a solar module, we have chosen a different (substrate) structure, and the different technology allowing monitoring of the deposition parameters, namely a two-stage combination of Chemical Bath Deposition (CBD) to obtain a precursor layer, and Chemical Vapor Deposition (CVD) to convert it into semiconductor absorber. Investigation of the structure obtained with standard techniques (XRD, SEM, optical methods) as well as Kelvin Probe and XPS allowed us to determine energy band scheme of the structure and to study an effect of CdCl<sub>2</sub> treatment upon the structure's parameters. It came out that the treatment mentioned drastically improves the characteristics of a potential barrier within the structure, thus positively affecting the structure efficiency. On the other hand, the different geometry of the structure allows a new design of the cell front electrode with innovative antireflection coating leading to additional advantage of the structure studied. We expect that these results can be of interest in design of efficient hybrid Sun-tracking solar energy converting systems.



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**[ RWE-38 ] Ultrathin solar cells: application for transparent window PV**

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A new trend in processing ultrathin solar cells in the thin films photovoltaic technology for windows PV in buildings and cars roofs applications has been of scientific interest in recent years. The processing of this new technology requires a very thin layers, which tend to decrease the overall efficiency of the solar cell, therefore a compromise between transmission and efficiency of the solar cells is necessary obtained, and as the same time low production costs. CdTe-based solar cells, appear to be the most promising material, and the sputtering technique best suited to the technological requirements. In this work the challenges and advances are presented in this new trend of using solar cells of second and third generation.



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**[ RWE-50 ] Visible emission from silicon quantum dots and potential downshifting application  
for third generation solar cells**

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Silicon is one of the main semiconductors used for the electronic and optical properties. However, silicon in bulk form is an indirect band gap material and thus has the limitation to be used for various applications. In this work, a visible, and even white intense luminescence has been observed in silicon quantum dots embedded in amorphous silicon oxide by using hot wire chemical vapor deposition (HW-CVD) at a low substrate temperature of about 200°C. Using scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD) structural and morphological studies have been made. The presence of various sized luminescent particles observed in this work shows the potential of this material for the downshifting to avoid PV losses (due to the poor spectral response of solar cells to high energy light). Thin films obtained in this work could be used for absorbing the high energy photons and then to upsurge the spectral response in UV and visible region to emit them in the low energy or higher wavelength region.



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**[ RWE-57 ] Photovoltaic effect in unipolar semiconductors**

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For the first time the possibility of the photo-emf occurrence in a unipolar semiconductor proved. The theory of the nonequilibrium charge carrier transport in unipolar multivalley semiconductors is developed. It is shown that the diffusion of photoexcited nonequilibrium heavy and light electrons in multivalley semiconductors is a correlated process, like the ambipolar diffusion in the case of the electron-hole plasma. The light-induced intervalley transitions, resulting in the imbalance between the subsystems of the light and heavy electrons, give rise to the electromotive force (emf) through the mechanism of the Dember photovoltaic effect. The value of the emf occurring in the "metal-semiconductor-metal" structure is calculated in the linear approximation in terms of the light intensity as a small parameter. It is shown that the emf is determined by the conductivity of heavy and light electron subsystems, as well as by the surface conductivity of the metal-semiconductor interface.



**[ RWE-175 ] Ek -012 Thermo-photovoltaics Solar System . Heat exchange with static fluid.**

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In recent years, has increased the need for the use of clean energy and further use of solar energy, it is why the research focuses primarily on the study of solar panels seeking to increase its conversion efficiency and reduction its manufacturing cost. Similarly, it has increased both the use and research in water heating systems using solar radiation; together PVT systems successfully convert the solar radiation into two distinct modes of energy, photoelectric and thermal energy. In the literature you can be found different assemblies for PVT systems whose overall efficiency is very high; however when reviewing the conversion efficiencies of each of the energies obtained from the transformation of solar radiation, the efficiency of the photovoltaic panel regularly stays the same or in some cases is decreased, the thermal insulation system using these systems paradoxically the objective of this thermal insulation is to increase the efficiency of conversion of solar radiation into thermal energy.

This research shows the assembly the PVT system called Ek-012, which is composed of a polycrystalline silicon solar panel 250 W and a system of thermal insulation of fiberglass and polyurethane. The working fluid PVT-Ek012 system has a versatile behavior, according to the hot water needs of housing, this fluid is moving only when used in a domestic service. 90% of the time of use, the working fluid remains static, this feature makes the photoelectric power solar panel is increased by up to 12% while the hot domestic water reaches a temperature of up to 43 ° C. The substantial increase in the water temperature caused collaterally the operating temperature of the solar panel drops to 20 degrees to the normal working temperature ranging 60 ° C.

Feeding water to the system PVT.Ek-012 it is made from a water tank gravitational mode. The force generated by the height difference between the fluid in the water tank and the fluid contained within the Ek-012 system enhances the supply of hot water to the saw housing, because it is not necessary to use electricity to power a pumping system and water circulation increasing the overall efficiency of PVT.Ek-012 system.



[ RWE-216 ] **On the importance of the junction temperature on studying the charge transport properties of a solar cell: the n-InGaP/p-GaAs case**

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Often the charge transport properties of a solar cell junction are neglected, taking an empirical approach to improve its performance and missing the powerful information provided by such study, which allows a much more easy tuning of the technical process parameters to reach a better cell performance. The n-InGaP/p-GaAs Heterojunction is widely used in high performance multi-junction solar cells. Its impressive performance stems from intrinsic physical properties of both materials as high absorption coefficient, low InGaP surface recombination as well as a mature technology for both materials.

In this work we show the importance of precisely knowing the cell junction temperature through a new method to extract the charge transport parameters. The method is applied to the n-InGaP/p-GaAs solar cell, based on the use of a structure that allows, by its careful design and bias; to extract the true junction temperature, as well as to screen and separate the cell recombination current in its junction space charge region from that due to the injection-diffusion of minority carriers in its neutral regions. The studied structure was grown by low pressure MOCVD using Si and C as N and P type dopants respectively. Ohmic contacts were realized using Au-Ge and Au-Zn for N and P regions. Mesas and contact areas were done using ordinary photolithographic and wet etch processes. The hetero-junction is characterized obtaining its; true temperature, space charge saturation recombination current density, the diffusion saturation current density and its series resistance. Although the structure was designed to study the charge transport properties, it nevertheless yielded  $V_{OC} = 0.750$  V for a  $J_{CC} = 7.56 \times 10^{-3}$  mA/cm<sup>2</sup>. The details of the proposed method will be fully discussed in this presentation.



[ RWE-355 ] Phosphorus Spin On Dopant Used as n-Type Source in the Emitter Formation of c-Si Solar Cells

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In this work, the study of the spin on dopant technique used as an alternative in the n-type emitter formation in crystalline silicon (c-Si) solar cells is reported. Two processes were fabricated on low cost, 300  $\mu\text{m}$ , boron doped (5-15  $\Omega\text{cm}$ ) double side polished Czochralski (CZ) silicon wafers, in order to compare the performance of the devices. In the first process, phosphine ( $\text{PH}_3$ ) was used as n-type gas source and the emitter of the solar cells was formed in two stages of ten minutes each one, preposition and drive-in at 950 °C. In the second process, the Filmtronics Spin-On Dopant (SOD-P905) was used as n-type liquid source deposited by spinning and diffused into silicon at 950°C for ten minutes, for the emitter creation.

The active dopants and the emitter profile were obtained and the results reveal that the n-type profiles and junction depth are similar in both processes. In relation to the electrical characterization, solar cells were measured under standard terrestrial conditions ( $\text{AM1.5 } 100 \text{ mW/cm}^2$ ) using the solar cell simulator oriel New Port. We observed that there was a small discrepancy in the open circuit voltage, short current density and fill factor of the two processes, thus the efficiency were similar (8.2% using phosphine and 7.9% with SOD).

In order to improve the efficiency of the devices with SOD diffusion, a step of wet surface texturization based on potassium hydroxide (KOH) was incorporated into the fabrication process. Reflection losses were reduced from 36% (bare silicon) to 14% with surface texturization and 6.5% by the incorporation of an antireflection layer of silicon dioxide ( $\text{SiO}_2$ ). The efficiency reached in this work was improved to 12%. These results suggest that SOD-P905 can be used to produce low-cost silicon solar cells.



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**[ RWE-360 ] Electrical characterization in P3HT/CdS heterostructures and their potential applications**

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In recent years have been focused on unconventional materials for diodes as photovoltaic cells and phodiodes, polymer semiconductor materials are one of the best option because of the advantages as easy processing, cost reduction, flexibility of the material and larger-scale applications, although one of the biggest problems of these materials are their low efficiencies. It has observed that an organic/inorganic heterostructure improve this efficiencies. In this work, we have analyzed the potential applications of organic-inorganic P3HT/CdS heterostructures as solar cells and photodiodes for light detection in the visible range. CdS layer were deposited on ITO-coated glass substrates as n-type layer by the photochemical bath method employing an ammonia-free recipe. For p-type layer, P3HT was deposited on the CdS/ITO/glass substrates by the drop casting method. The photovoltaic performance was studied with respect to the power conversion efficiency from the J-V curve in dark and under illumination exhibiting average efficiencies for an hybrid solar cell. From these measurements the photosensitivity as a photodiode was determined and the response of the heterostructure as a function of illumination intensity was obtained from transient photocurrent measurements.



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**[ RWE-421 ] GaN/Si Solar Cells, a first step towards high efficiency tandem solar cells**

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Record high conversion efficiencies have been achieved (larger than 44%) with tandem solar cells of 4 or more junctions under concentrated sunlight (300-500 suns). Hence, tandem cells under concentrated sunlight promises to be one of the ways in order to reduce the PV energy cost, for terrestrial applications, in the near future. In this work, we propose to develop single junction solar cells based on III-N compounds on Silicon, as a first step to make tandem solar cells of several junctions with sub-cells of this kind (III-N compounds) on silicon. A proposal is made for a GaN/Si solar cell and its behavior is simulated numerically, showing that high efficiencies could be achieved. In the future, it would be possible to realize 2 (or more) junction solar cells with III-N and silicon subcells. At the end, we shall comment on the technological challenges to overcome for obtaining high efficiencies with this kind of solar cells.



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**[ RWE-469 ] Growth and characterization of c-GaN / GaAs solar cells**

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III-Nitrides solar cells have taken special attention in recent years due to the excellent properties such as the tunable band gap and the high absorption coefficients of Nitrides. In particular indium gallium nitride (InGaN) alloys are very promising for high-efficiency photovoltaic applications. However, the difficulty to achieve appropriate Indium incorporation, high conductive p-type layers, and low resistance ohmic contacts are the challenges for this technology. On the another hand, from the theoretical point of view, the integration of cubic phase III-nitrides with III-V compounds presents attractive advantages for solar cells applications. III-nitrides / III-V tandem solar cells have the potential to vary the band gap to completely cover the solar spectrum without the incorporation of built-in electrical fields presented in hexagonal III-Nitrides produced by spontaneous and piezoelectric polarization. However, no reports have been showed in the literature. Moreover, from the technological point of view, the cubic phase presents the possibility of simple cleaving instead of mesa dry etching process and no p-GaN layer is needed.

Here we report our recent study of cubic-phase GaN/GaAs solar cells grown by molecular beam epitaxy on GaAs substrates. The objective of this work is to demonstrate the feasibility of a metastable cubic GaN device. The GaN/GaAs solar cell structure is described as follow: a Zn-doped GaAs substrate was used as p+ back surface field (BSF). Over the GaAs substrate, an intrinsic GaAs absorbent layer was grown thick enough to absorb sunlight, but thin enough to keep low the series resistance of the device. Finally, on the top a n-type cubic GaN window layer was doped with Si to achieve an electron concentration in the order of  $10^{18} \text{ cm}^{-3}$ . The characterization was carried out by HRXRD, SIMS, PL, I-V and spectral response. From SIMS abrupt GaN/GaAs interfaces were observed, and the doping concentrations were confirmed. PL clearly presents the GaN emission and the absence of other luminescence contributions as deep level crystal defects. HRXRD revealed a high crystal quality and the reduction of hexagonal inclusions. I-V curves showed good reverse rectification properties of the diode in the darkness, and the photovoltaic effect was observed under illumination of standard AM 1.5. From spectral response analysis, the best response was found at a wavelength of 600nm.



**[ RWE-527 ] Design and synthesis of ZnO transparent contacts for InGaN solar cells**

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Zinc Oxide (ZnO) has attracted attention as one of the materials for the antireflection coating of solar cells because it has good transparency, an appropriate refractive index ( $n = 2$ ) and because it is possible to increase its electrical conductivity by doping.

In this work, theoretical calculations of the reflectivity of aluminum doped ZnO (ZnO-Al) thin films as antireflective transparent layers for application in InGaN solar cells are presented. Experimentally, ZnO-Al thin films deposited by RF sputtering were studied as an electron transport layer on InGaN thin films grown by MBE.

According to calculations, InGaN thin films coated with ZnO-Al exhibited an increase in the external quantum efficiency (QE) of at least 5% in the spectrum between 300 to 850 nm under AM1.5G irradiation compared to samples without coating. Optical and electrical characterization of InGaN thin films coated with ZnO revealed a drastic reduction in reflectivity compared to samples without coating according to UV-Vis spectrophotometry data analysis, and for lowest reflectivity samples, an electrical resistivity of about  $2 \times 10^{-3} \Omega\text{-cm}$  in the ZnO layer was achieved.

Structural, optical, electrical and chemical properties were evaluated by means of XRD, Raman spectroscopy, UV-Vis, Hall effect, EDS, XPS, and SIMS.



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**[ RWE-549 ] There are conditions in Mexico for a photovoltaic solar industry? CdTe Case  
Review&**

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Even still, in the near future, given the Mexican commitment to reduce carbon dioxide emissions; they would be presenting magnificent opportunities driven and supported by the federal and state governments to develop renewable energy, in particularly solar photovoltaic.

In conclusion, several proposals are presented in order to trying for establishing a plan for the near and long term future time.

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[ RWE-579 ] Heterogeneous catalysts for more efficient biodiesel production

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The alarming trends in energy demand and the finite nature of fossil fuel reserves have motivated the search for energy sources more sustainable. In this regard, biodiesel can provide a significant contribution in the energy independence. The most common method for producing biodiesel is via triglyceride transesterification from vegetable oils and animal fats in the presence of short-chain alcohols and homogeneous acid or base catalysts. Heterogeneous catalysts are most efficient in transesterification reaction due to many advantages such as easy catalyst separation and reusability, improved selectivity, reducing process stages, no water formation or saponification reaction, included under green technology and cost effective. In this work, different catalysts were synthesized microwave-assisted hydrothermal process and ultrasonically assisted hydrothermal synthesis. Then, catalysts were evaluated as potential catalytic materials. The structure and microstructure of the catalysts were characterized using X-ray diffraction, scanning electron microscopy and N<sub>2</sub> adsorption. Synthesized materials were tested as a basic catalyst for the production of biodiesel from transesterification reaction. The influence of some parameters was investigated, such as the reactant concentrations (molar ratios), reaction time, temperature and re-use of the catalyst. Specially, the use of Na<sub>2</sub>SiO<sub>3</sub> is a good option to test as catalyst transesterification reaction in the reutilization with high yields. The maximum FAME conversion efficiency was ~99% at 1 h of reaction time and 3wt% of catalyst. The cyclic behavior revealed that the catalyst had a relatively stability. The production of biodiesel through heterogeneous catalysts is a good option to reduce cost and pollution.

*Keywords:* Biodiesel, heterogeneous catalyst, silicates.

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**[ RWE-62 ] Proposed graded emitter design for efficient HIT solar cells using dichlorosilane in PECVD equipment.**

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In the present study, we have shown the potential of graded emitter region for the new type of HIT of solar cells using the conventional plasma Enhanced Chemical Vapor Deposition (PECVD) equipment. Polymorphous silicon thin films were obtained from dichlorosilane and hydrogen as precursor gases. By varying different deposition conditions, it was possible to vary the band gap from 1.66 to 2.0 eV. Crystalline fractions of the thin films were studied using Raman spectroscopy. On the other hand, for inspecting the optoelectronic properties, relationship of the photosensitivity with the RF power and the behavior of diffusion length has been extensively studied. By the implementation of this new design, in the near future we could increase the efficiency of solar cell devices.



[ RWE-96 ] CdS thin films grown on flexible PET-substrates by CBD

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Cadmium sulfide (CdS) thin film deposition has attracted increased attention to materials research scientists due to a predicted efficiency of 30% in the CdS/CdTe solar cell system. CdS is a wide bandgap *n*-type semiconductor with value of 2.42 eV, it crystallizes in hexagonal and cubic phases, being the wurtzite hexagonal the stable phase. Over the last years, flexible substrates have demonstrated a great potential to be used as flexible solar cells, flexible displays among other applications. Particularly, polyethylene terephthalate (PET) substrate has been used for photovoltaic devices because it provides higher electrical conductivity, light weight, transmittance in visible range, low cost and good flexibility. CdS thin films were grown on flexible polyethylene terephthalate (PET) substrates by chemical bath deposition. Three samples were grown on PET substrates at deposition times of 60, 90 and 120 min. X-Ray diffraction results showed that films are composed of crystalline structures together with non-crystalline CdS. The crystalline contribution has the CdS hexagonal phase, which was confirmed by TEM results. A strong green photoluminescence emission was observed in all the samples, this emission is associated to near band edge transitions for CdS. The calculated bandgap values by UV-Vis are in excellent agreement with PL emission. EDS results showed that CdS-nanocrystals films grown with excess of Cd.

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**[ RWE-100 ] Photovoltaics windows based on CdS/CdTe heterostructure**

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Currently the research seeks to solve environmental issues by implementing new forms of energy. The solar windows have been a successful option that enables solar energy to be obtained. The paper seeks to manufacture the CdS/CdTe translucent deposit that allows the partial transmission of sunlight, which in turn converts the rest of the light into electrical energy. The CdS/CdTe solar cells are one of the most promising photovoltaic materials: as the heterostructure has a predicted theoretical efficiency of 30% [1]. However the experimental efficiency achieved is around 21.5% [2], which thus indicated that there is still much scope for research in this particular field using the aforementioned device. For the usual processing for the cell, a CdTe film of up to 8  $\mu\text{m}$  thick is required, which represents an inconvenience, considering that Te is a scarce element [3]. Nevertheless CdTe is a semiconductor with a bandgap of 1.45 eV and a high absorption coefficient ( $>10 \text{ cm}^{-1}$ ) [4], so only certain micrometers are required to absorb 90% of the incident light. Having considered this aforementioned aspect, these problems shall be solved through the employment of an ultra-thin CdTe film ( $<2 \mu\text{m}$ ), through the RF Sputtering technique that allows it to achieve this thickness.

In this work, are shown the preliminary results that have been obtained from the CdS/CdTe prototype photovoltaics windows processing and the results shall be consequently discussed with particular regard to growth parameters.

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[ RWE-108 ] Comparison of enthalpies of  $MgxM1-xH2$  alloys (M= Al, Ni, Zn;  $1.0 \leq x \leq 0.8$ )

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In this work we use Density Functional Theory (DFT) to obtain the enthalpies of formation of three magnesium alloys, magnesium-aluminum, magnesium-nickel and magnesium-zinc, for different magnesium concentrations  $x = 1.00, 0.98, \dots, 0.80$ . We build bulk crystal structure and then we cleave the bulk in the direction of the plane (110). Hydrogen molecules on this surface are added to obtain their enthalpies. We compare results of enthalpies before hydrogen molecule is added and after hydrogen molecule is added, and we conclude that magnesium-aluminum alloy is the most stable. We use generalized gradient approximations (GGA) in CASTEP module, of the molecular simulation program Materials Studio 6.0, to obtain our results.

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Keywords: Magnesium-aluminum alloy, magnesium-nickel alloy, magnesium-zinc alloy, formation enthalpies.



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[ RWE-109 ] Electronic density of states in bulk and surface (110) OF Mg<sub>1-x</sub>M<sub>x</sub>H (M=Al, Ni, Zn) alloys

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Metal hydrides are promising materials used for hydrogen storage in solid phase. One metal with this characteristics is Magnesium (Mg), with about 7.6 % of hydrogen (H<sub>2</sub>).

In this work we realize a comparison between the electronic density of states of three magnesium alloys, magnesium-aluminum (MgAl), magnesium-nickel (MgNi) and

magnesium-zinc (MgZn). We build crystal structure of bulk and then we cleave in the direction of the surface (110), where hydrogen is added on this surface. We use Density

Functional Theory (DFT) to obtain electronic density of states before hydrogen molecule is added on the surface (110) of the alloy. Then we add hydrogen molecule on the

surface (110) and obtain their electronic density of states. We compare our results and conclude that MgAl is the best alloy for hydrogen storage, because the gap of their

density of states decreases about 10 eV.



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[ RWE-173 ] Properties of indium sulfide thin films onto flexible substrates by chemical bath deposition

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The importance of alternative energy sources has increased in significance both energy supply and ecological conservation reasons. An example of this, is solar energy, where a natural resource has been used through photovoltaic devices. In recent years, solar cells based on cadmium and selenium have been developed. However, the use of these materials have being questioned due to their toxicity. In order to elaborate nontoxic solar cells, alternative materials have been studied. Indium sulfide is a semiconductor compound with photovoltaic applications because of their structure, transparency and wide band gap. There are several techniques to growing thin films, one of the most widely used is the chemical bath deposition (CBD), which can be scalable to obtain films onto super substrates at low cost. Moreover, flexible devices have drawn attention for their light weight and there are easily to carry and fold. The flexible photovoltaic devices offer an alternative energy source at low cost, and flexible large surface area. There is much demand for these products because they have many applications: Clothing, sport bags and tents.

The main objective of this research is to obtained indium sulfide films with suitable properties to use in solar cells. Grown parameters was been controlled, such as temperature and deposition time, citric acid was added as complexing agent to reduce the activity of indium ions and to adjust the pH. The growth of these films were be made on flexible substrates. Structural characterization was performed by HR-TEM and Raman spectroscopy. Optical properties were determined using UV-Vis spectroscopy, where it was obtained transmittance and band gap. Finally, electrical properties were known through Hall Effect technique.

**Keywords:** *Chemical Bath Deposition, Indium sulfide films, Flexible substrates, Nontoxic solar cells.*

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**[ RWE-176 ] Hierarchical TiO<sub>2</sub> Nanostructures in Lead Halide Perovskite Solar Cells**

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Here, we report the use of hierarchical TiO<sub>2</sub> nanostructures (HNs) to reduce the charge recombination at FTO/TiO<sub>2</sub>/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> interface. The TiO<sub>2</sub> HNs were fabricated by a second-step hydrothermal modification method. Briefly, TiO<sub>2</sub> nanorod (NR) trunks with optimal lengths of 540 nm were used as seed to grow TiO<sub>2</sub> nanobranches with lengths of 45 nm and diameter of 13 nm. Different device configurations were fabricated with TiO<sub>2</sub> seed structures (compact layer, NR and HNR) and different perovskite growth method, by comparing mixed-halide CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>-xCl<sub>x</sub> perovskite (Sing-MAICl) and lead iodide CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> perovskite (Seq-MAI). Perovskite solar cells (PeSCs) based on HNs-CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> achieved the highest power conversion efficiency of 10.5% compared to PSCs with other TiO<sub>2</sub> nanostructures. This result can be ascribed mainly to lower charge recombination as determined by impedance spectroscopy, improving the efficiency of the overall device.



[ RWE-193 ] Toward an improvement of CdCl<sub>2</sub> thermal treatment for CdTe thin films

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CdTe thin films were grown by RF magnetron sputtering and annealed with CdCl<sub>2</sub> methanolic solution. Different CdCl<sub>2</sub> solutions were prepared with 0.15 g, 0.20 g, 0.25 g, 0.30 g, 0.35 g of CdCl<sub>2</sub> in methanol and deposited on the CdTe thin films by airbrush spraying. After the solution was sprayed, samples were thermally annealed at 387 °C in air. Since the annealing temperature and time, and CdCl<sub>2</sub> concentration are crucial to improve optical and electrical properties of CdTe, samples with 0.30 g CdCl<sub>2</sub> concentration were annealed at 365 °C, 375 °C and 387 °C to study the temperature effect. The structural and optical properties of CdTe thin films were investigated as grown and after annealing by UV-Vis spectroscopy, X-Ray diffraction and scanning electron microscopy techniques. Hence, the results of the optical and electric properties of CdTe thin films leads us to the best conditions for the thermal treatment with CdCl<sub>2</sub> suitable for our CdTe thin film solar cells.

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**[ RWE-194 ] Prototype of a CdS/CdTe ultra-thin solar cell.**

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The objective of this work is to develop CdS/CdTe ultra-thin solar cells by magnetron sputtering. This technique is attractive because produce conformal thin films and CdS and CdTe can be sequentially deposited without breaking the system vacuum. One advantage of the magnetron sputtering over wet deposition methods is the absence of waste solutions and disposal of these residues. The effect of the deposition parameters (substrate temperature, power, pressure and Ar flow) and their impact on the solar cell efficiency was studied. The CdS and CdTe film thicknesses were in the order of 60-70 nm and 500 nm, respectively. Different post-deposition parameters were required in the CdS/CdTe thin-films to improve the efficiency of the solar cells. The solar cells were fabricated with the structure glass/SnO<sub>2</sub>:F/SnO<sub>2</sub>/CdS/CdTe/contacts. This solar cell showed photovoltaic response. The ultra-thin films were characterized using X-ray diffraction, optical transmission, scanning electron microscopy, photoluminescence and SIMS. The current-voltage characteristics of the solar cells were measured under dark and light conditions.

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[ RWE-212 ] Photocatalytic hydrogen production by water/methanol decomposition using  
Au/TiO<sub>2</sub> and RGO/TiO<sub>2</sub>

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Titanium dioxide (TiO<sub>2</sub>) was synthesized by the Sol-gel method and it was modified by the incorporation of reduced graphene oxide (RGO) forming RGO-TiO<sub>2</sub> composites and Au nanoparticles (Au np), these metal nanoparticles were deposited by different methods, first via insitu sol-gel route and also photodeposition. The powders were crushed and annealed at 500° C for 4 h. The materials were characterized by DRX, BET surface analysis, DRS UV-Vis spectroscopy and the results show that the obtained materials presented type IV, isotherms, characteristic of mesoporous materials. By XRD the formation of the TiO<sub>2</sub> anatase phase was confirmed. The photocatalytic evaluation for hydrogen evolution was performed using a mixture of methanol/water (1:1 vol.) under ultraviolet light irradiation ( $\lambda=254$  nm). Preliminary results shown the Au np/TiO<sub>2</sub> at 5 wt. % exhibited an enhanced photocatalytic activity with a rate of  $72 \mu\text{mol}\cdot\text{h}^{-1}\cdot\text{g}^{-1}$  , which was 2.6 times higher than the one obtained for bare TiO<sub>2</sub> ( $27 \mu\text{mol}\cdot\text{h}^{-1}\cdot\text{g}^{-1}$  ). More experiments are being performed and will be presented to obtain the optimal metal loading and the optimal RGO sheets in the composites for hydrogen production, under UV light and also under visible light irradiation.



**[ RWE-217 ] Tailoring the properties of BiFeO<sub>3</sub> for photovoltaic applications through First-principles calculations**

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Recently, the Anomalous Photovoltaic Effect (APVE) in ferroelectric materials has been directed to solar energy harvesting. The anomaly is manifested by the appearance of a steady state current in a short-circuited ferroelectric sample illuminated with radiation with wavelengths corresponding to its absorption range. However, this range is the principal limitation for the efficiency of absorption in the visible spectrum, since the bandgap for ferroelectric materials is typically, over 3 eV. In particular, the multiferroic BiFeO<sub>3</sub> (BFO) has an experimental gap of ~ 2.7 eV, which makes it a promising material for photovoltaic devices and a candidate for processes devised to lower the bandgap.

Considering the above restrictions, we show the results of the calculations of electronic and optical properties of BiFeO<sub>3</sub>, (Bi<sub>0.9</sub>La<sub>0.1</sub>)FeO<sub>3</sub> and Bi(Fe<sub>0.9</sub>Co<sub>0.1</sub>)O<sub>3</sub> which were investigated using density functional theory (DFT) with generalized gradient approximation (GGA) plus the Hubbard correction (U). The Berry phase calculation of the polarization was performed by finite differences of polarization. The electronic structure shows that BiFeO<sub>3</sub> has an indirect (very close to direct) band gap of 2.48 eV.

Finally a photovoltaic device of a single ferroelectric layer was designed and simulated to show the potential for applications for these materials.

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**[ RWE-286 ] Theoretical study of TiO<sub>2</sub> films as buffer layer on CdS/CdTe solar cells.**

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In this work we report a theoretical study on the effect of a TiO<sub>2</sub> thin film as front contact buffer layer (BL) in CdS/CdTe solar cells. Typically, a ZnO BL with thickness around 100 nm is used, however, this layer shows high absorption of light in the blue region, limiting the photogenerated current on the solar cell. In a previous experimental work we showed that a 15 nm thickness TiO<sub>2</sub> layer acts as a BL but also improves the photogenerated current. Here we show our results on the simulation of the two kind of solar cells (with ZnO and TiO<sub>2</sub> buffer layer) performed by the AMPS-1D software. Simulations showed that efficiency is highly dependent on the TiO<sub>2</sub> thickness, and that the higher electrical resistance of the TiO<sub>2</sub> ( $10^7 \Omega\text{-cm}$ ) in comparison to the ZnO ( $10^3 \Omega\text{-cm}$ ) allows to decrease the thickness of the TiO<sub>2</sub> BL until 15 nm, which cannot be made with the ZnO BL. Similar efficiency of 12% was achieved by using 15 and 100 nm thickness for TiO<sub>2</sub> and ZnO BLs, respectively, in agreement with the experiment. Simulations also show that solar cells fabricated with the TiO<sub>2</sub> BLs present an improved stability against temperature in contrast to solar cells using the ZnO BL, losing a smaller fraction of the starting efficiency (at room temperature) as the operating temperature is raised. This improvement is related to the increase of the fill factor. These results demonstrate that TiO<sub>2</sub> BLs can be used for high efficiency CdS/CdTe solar cells.

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[ RWE-325 ] Effect of Chemical Compounds Formed After Activation with  $\text{CHClF}_2$  and  $\text{MgCl}_2$   
in CdS/CdTe Solar Cell.

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In this work we study the chemicals compounds that formed in the surface of the CdTe solar cell after activation with  $\text{MgCl}_2$  and  $\text{CHClF}_2$  and their effect on the electrical properties. The structure of solar cell was ITO/ZnO/CdS/CdTe/Cu/Mo. ZnO, CdS, and back contact films were deposited by reactive RF-Sputtering while the CdTe film was deposited by conventional CSS. The activation was performed with  $\text{MgCl}_2$  saturated solution and  $\text{CHClF}_2$  gas. The annealing was performed at 400 °C in dry air for 30 minutes. Activation effects are more noticeable with  $\text{MgCl}_2$ . The FE-SEM image and the XRD analysis showed MgO formation on CdTe surface. The solar cell activated with  $\text{MgCl}_2$  and  $\text{CHClF}_2$ , had an efficiency of 12.5% and 12.8%, respectively; open circuit voltage, short circuit current and fill factor were 831 and 817mV, 23.31 and 23.6 mA/cm<sup>2</sup>, 64.5 and 66.6%, respectively.

**ACKNOWLEDGEMENTS:** This work has been supported by CONACYT-SENER (México) under project CeMIE-Sol 207450/P25. The authors gratefully acknowledge D. Huerta and Wiliam Canul for technical support, and L. Pinelo for its secretarial assistance.



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**[ RWE-327 ] pH Influence on the Physical and Chemical Properties of SnS Thin Films Prepared by CBD.**

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In this work the effects varying the bath pH (from 5.5 up to 8.5) in the SnS thin films deposited by CBD is reported. Tin chloride and sodium thiosulfate were used as precursors, ammonium citrate as complexing agent and NaOH to stabilize the pH. The samples were characterized by phototransmission, FE-SEM, EDS, XRD and XPS were performed to study optical properties, morphology, structure and chemical composition of the deposited films as the bath pH changes. The SnS thin film is well crystallized and only one phase is observed by XRD. The FE-SEM, EDS and XPS show that increasing the bath pH, the films are thinner and the tin oxides are formed. The SnS film deposited in a bath at 6.5 pH appears as the most promising absorber for solar cells, since it exhibits a good crystallinity with a preferential orientation (111), as well as a good direct allowed transition of  $1.2 \pm 0.1$  eV.

**ACKNOWLEDGEMENTS:** This work has been supported by CONACYT-SENER (México) under project CeMIE-Sol 207450/P26. The authors gratefully acknowledge D. Huerta and Wiliam Canul for technical support, and L. Pinelo for its secretarial assistance.



[ RWE-340 ] Oxygenated cadmium sulfide (CdS:O) used as a window layer in thin film solar cells

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In this work we present the effects of oxygenated cadmium sulfide (CdS) for application as a windows layer in solar cells of Cadmium telluride (CdTe) and Copper Zinc Tin Sulfide (CZTS). CdS:O thin films were deposited by reactive RF-Sputtering with a CdS ceramic target with 99.99% purity by using a gas mixture of Ar+O<sub>2</sub>. Deposition was performed at room temperature with working pressure of 25 mTorr, a sputtering power of 40 Watts and varying the oxygen concentration in a range of 0% to 1.4%. Preliminary results show that it is possible prepare CdTe solar cells with a structure ITO/ZnO/CdS:O/CdTe/Cu/Mo where the CdTe film was deposited by conventional CSS and using a CdS:O window layer by varying the thickness and the oxygen concentration. Solar cells were characterized using measuring the external quantum efficiency (EQE) and current density vs. voltage (J-V) curves. EQE spectra show the spectral response in short wavelengths range increase when the oxygen concentration rise. However, that the best solar cell was obtained using a CdS:O with 1.1% of oxygen concentration, with a efficiency of 13%. We are working to test the CdS:O to integrate into CZTS solar cells.

**Keywords.** Oxygenated cadmium sulfide (CdS:O), CdTe and CZTS

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**[ RWE-383 ] Design for an electricity generation pilot facility from microbial fuel cell hybrid based systems**

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Microbial fuel cells (MFCs) allow simultaneous water treatment and electricity generation. Scalability of MFCs has been a long studied issue mostly because the need of optimization of the cell subsystems such as the anode, proton permeable membrane and cathode. Additionally, the electricity generation depends on a constant content of organic material and also the reachable currents are still low. Anodic electron transference suffers from biofouling, large resistances caused by hydrophobic material and poor interaction of bacteria consortium. Proton permeable membranes also present clogging and biofouling as well as ion permeation from cathode to anode chamber, thus reducing cell efficiency. Air cathodes are limited by the oxygen reduction reaction kinetics or by the use of expensive precious metal catalysts. Many alternatives such as functionalized anodes, clay and ceramic membranes and photoregenerative or redox cathodes have been devised not only to increase MFC efficiency but to add functionalities such as photocatalytic degradation of dyes or cathodic metal concentration. In this work we present a conceptual system of a plant with capability of treatment a volume of 0.05 m<sup>3</sup> wastewater from the main building of CICATA Altamira. The system pumps and performance sensors will be powered by a commercial photovoltaic system. The plant will serve as a test laboratory for MFC optimization as well as for other combined technologies such as photocatalysis, metal concentration, advanced sorbent testing, energy storage and so on. Financed by SIP multidisciplinary project 20161804/0294, 0299 and 0304. Support from Innovation Projects SIP 2016 is also acquainted.



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**[ RWE-388 ] Simple process for the manufacture of copper iodide thin films**

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Actually, exist a great interest in the semiconductor fabrication with a charge transport capacity as a support for the performance at solar cells. This work present an easy way to development thin films of copper iodide which have a p type behavior with a viability on big scale process. Also shows the optical properties of the thin films analyzed by Uv-Vis and photoluminescence, as well as, compositional studies by X-ray diffraction and surface by scanning electron microscopy.



[ RWE-395 ] Influence of laser scribing of ITO in CdS/CdTe PV mini-modules

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In this work the influence of laser scribing of ITO (P1) on the PV mini-module efficiency is discussed. The ITO thin film is deposited on glass substrate, and it is used as a substrate to fabricate the PV mini-module. The scribing is made by using a pulsed laser of 532 nm. After the laser scribing the glass/ITO is cleaned, then thin films of ZnO/CdS/CdTe are deposited. Next the structure is annealed into atmosphere of Ar-O<sub>2</sub>-CHClF<sub>2</sub> at 400 °C for 20 minutes. Finally a back contact of 5 nm of Cu and 400 nm of Mo are deposited. The ZnO was deposited by reactive sputtering in Ar-O<sub>2</sub>. The CdS, Cu and Mo are deposited by sputtering in Ar atmosphere. While CdTe thin film was deposited by conventional CSS. Each cell of the PV mini-module was tested by scribing a small cell of 0.4 cm<sup>2</sup>. Preliminary result indicates that cells were around 10.0±1.5% and PV mini-modules were around 4.5±2.0%. The electroluminescence image indicates that there are scribing lines that produces some short circuits, and it is one cause of losses, we are studying the effects on the electrical parameters of PV mini-modules. Also the electroluminescence images shows some small zone into the cell that can be considerate as a defect, it is underway. The J-V curves of the testing cell shows high shunt resistance and low series resistance, indicating that the main cause of losses in PV mini-module coming from scribing of ITO (P1).

**Keywords.** PV Mini-module, CdTe, electroluminescence.

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**[ RWE-418 ] Comparative pv-performance of prototype cigs solar cells**

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In this work we report of CIGS solar cells with CdS as a window material grown on glass substrates through the chemical bath deposition technique (CBD), in an ammonia free process which uses amino acids (glycine, alanine and serine) as complexing agents and using the Sputtering technique. All the films were crystallized under a hexagonal wurtzite type structure with preferential orientation in the plane (002). The morphology analysis showed that the resulting films were formed by highly compacted hemispherical shaped aggregates homogeneously distribute along the substrate with sizes lower than 100 nm and well defined grain boundaries. Cross-section micrographs from scanning electron microscopy revealed that the thickness of the resulting films were in the range from 100 to 130 nm. These CdS films were optically transparent with transmittance average values of 55-74% and band gap energies of 2.43-2.53eV. The variation of the characteristics of these films are consequence of the molarity of the precursors and the kind of amino acid used in the process. Usually, the window layer of CIGS (copper-indium-gallium-(di) selenide) solar cells are fabricated with CdS thin films grown by CBD method with ammonia as complexing agent. The CIGS films were grown in a coevaporation systems with the used of 4 K-cells providing a controlled atomic flow of each element in time and temperatures in order to obtain a high quality chalcopyrite compound that is used in processing CIGS high-efficiency solar cells. In this work, we show preliminary results of our CdS thin films as window layers in the structure of CIGS solar cell, as well our PV performance of the devices.

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**[ RWE-466 ] Synthesis and characterization of hafnium carbide using concentrated solar energy**

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Hafnium Carbide (HfC) is an ultra-high temperature ceramic with melting point of 3900°C, has good thermomechanical and thermochemical properties and has several applications such as cutting tools, aerospace industry and emitters.

HfC was synthesized using concentrated solar energy in the solar oven IER-UNAM, via carbothermal reduction, which leads to the development of a production process low CO<sub>2</sub> emissions. Hafnium tetrachloride and pectin were used as precursors of hafnium and carbon respectively, obtained at a temperature HfC 1500°C, under argon. The structure and morphology of HfC obtained was analyzed with FTIR, XRD and TGA/DSC. The results show that it is possible to use concentrated solar energy for synthesis of HfC's and reduce emissions.

Keywords: Concentrated solar energy, Solar furnace, Hafnium carbide, Carbothermal reduction, UHTC.



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**[ RWE-474 ] Improving conditions thermal housing stake of a subdivision of the city of Oaxaca**

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**Abstract**

This document proposes to improve thermal housing conditions in the Villas Monte Albán neighborhood in Oaxaca City. To accomplish this, a personal identity card housing card is assigned to each unit to assess the current conditions. Subsequently a qualitative and quantitative analysis was made; the qualitative is to evaluate the thermal perception of users through a questionnaire and the quantitative analysis is to conduct a climatological analysis of the site in order to know the weather conditions of housing and make a comparison with the firing thermal confort. Later, a thermal monitoring will be conducted in hot and cold conditions. Finally improvements will be determined to achieve optimal thermal confort and energy savings and these will be validated by a thermal simulation study.



**[ RWE-492 ] Characterization of CdS/CdTe solar cells as a function of the CdTe thickness and back contact deposited by laser ablation**

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Due to the demand of a clean and durable energy source, research on solar cells is in constant growth. Cadmium Telluride (CdTe) thin films are now one of leading materials for the development of cost-effective photovoltaics thanks for its high optical absorption coefficient and chemical stability, along with a direct band gap of 1.5eV (close to the ideal value for photovoltaic conversion efficiency). The theoretical efficiency of CdTe thin films solar cells is expected to be 30%. One of the factors that affect cells efficiency is the quality of CdTe thin films. It has already been reported that laser ablation of CdTe targets produces high quality layers at room temperature.

In this work CdTe/CdS solar cells have been obtained. The CdS layer has been growth by chemical bath deposition keeping deposition conditions constant for all the samples. The CdTe layers were grown by laser ablation, it has been proved that controlling the plasma parameters (mean kinetic ion energy and density) thin films with homogeneous surfaces, low roughness, porous free and reduced grain boundaries can be growth.

The CdTe layers were deposited monitoring the plasma density and the mean kinetic ion energy using a Langmuir planar probe, to ensure that all the conditions are the same in every deposition. The CdS and CdTe layers were characterized by UV-Vis, SEM and EDS independently. Using the same plasma parameters, the deposition time was varied in order to grow CdTe films with different thicknesses. Different back contacts were deposited by laser ablation. The photovoltaic response of the solar cells was analyzed as a function of the CdTe thickness and back contact.



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**[ RWE-500 ] Synthesizing and characterization of thin films of a nanostructured thermoelectric material based on silicon and its alloys with Ge, H and Ar.**

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Energy consumption grows increasingly as technology progresses. Currently, the energy comes mainly from fossil fuels, but its high level of pollution has led science to develop alternative energy sources, seeking efficiency and low economic and environmental cost. One way to reduce this energy consumption is by recycling, such as transforming heat energy into electrical energy.

Processes in which the main source of energy is based on burning fuel, machinery and electrical and electronic devices where heat is residual energy and devices with high operation temperatures can improve its energy efficiency by capturing residual heat and converting it into useful electrical energy, a process called "thermoelectric conversion"; This is where the application of devices such as thermoelectric generators (TEG's) comes into play.

Most thermoelectric materials used in TEGs are based on Te and rare earths. Tellurium is the ninth of the rarest elements on earth and it's predicted it would disappear in 2020 with current use; this is why it's important to find cheap thermoelectric materials with high efficiency and Te free. That is why the use of a cheap and abundant material is proposed: silicon in form of nanostructured amorphous silicon and its alloys with H, Ge and Ar, deposited by PECVD: a versatile technique that allows us to adjust the properties of the materials obtained, depending on deposit conditions such as temperature, pressure, gas flux and gas ratio.

The resulting nanostructured material has been electrically characterized; its nanostructures have improved its conductivity by five orders of magnitude, working at temperatures as high as 250°C. Due to the difficulty of obtaining the thermal and thermoelectric properties of a thin film the TERM-PRU-MA1 microchip was designed, containing structures that allow us to characterize a thermoelectric material thin film.



**[ RWE-504 ] Hydrophilic Coating of TiO<sub>2</sub>-SiO<sub>2</sub> with Self Cleaning Properties and its possible application on Solar Panels**

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One of the most used devices among renewable energy generation systems are photovoltaic panels that use sunlight to generate electrical energy. There are factors that influence the performance and efficiency of the photovoltaic module, one of them is the environmental condition of the used space. The solar panels are exposed to the environmental features and interact with the weather conditions; the result is a soiling panel, principally by dust, organic material, etc. When the panel gets dirty its efficiency decreases and the performance is limited. That is why it is important to develop materials that prevent or even avoid the soiling of the panel and an interesting alternative is the development of self cleaning coatings [1-3]. Therefore, in this work is presented the development of coatings based on commercial nanoparticles functionalized with silane agents and afterwards dispersed in an ethanol-water medium. Acrylic acid was employed as polymer matrix and the coatings were deposited on glass substrates using spin coating technique. The results obtained showed that the coatings have hydrophilic and hydrophobic properties, that is to say, present self cleaning features, making them suitable for application on photovoltaic panels.

Keywords: hydrophilic, hydrophobic, self cleaning, nanocomposite.

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**[ RWE-523 ] Processing and characterization of the Sb<sub>2</sub>Te<sub>3</sub> AS p+ material**

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The Antimony Telluride (Sb<sub>2</sub>Te<sub>3</sub>) is used like material p+ on CdTe solar cell. This work presents results about the deposit and characterization of Sb<sub>2</sub>Te<sub>3</sub> growing by Sputtering-DC. The Sb<sub>2</sub>Te<sub>3</sub> was deposited varying the power of magnetron to 60 W, the substrate temperature between 100 and 300 C and the deposition pressure to 20 mbar. Some characterizations are carried out on Sb<sub>2</sub>Te<sub>3</sub> such as profiler, EDS and morphology. Then we find in the EDS analyses that if the pressure increase the quantity of Te in the substrate decrease, when the increase the temperature to 300 C the quantity of Te increase near to 3.77 keV and appear a structure type "sheath" of Sb<sub>2</sub>Te<sub>3</sub>. So for CdTe solar cells application is convenient grow Sb<sub>2</sub>Te<sub>3</sub> by Sputtering-DC to low pressure and relative high temperature near 300 C.



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**[ RWE-524 ] Processing and characterization of the back contact Mo in 100 CM<sup>2</sup> for photovoltaic applications**

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The Molybdenum (Mo) is used like back contact on CdTe solar cell. This work presents results about the deposit and characterization of Mo growing by Sputtering-DC. The Mo was deposited varying the power of magnetron to 300 W, the substrate temperature between 100 and 250 C and the deposition pressure to 15 mbar. Some characterizations are carried out on Mo such as profiler and resistivity. We find when the pressure increase the grown ratio of Mo in the substrate decrease, when the temperature increase to 250 C we found a slide grown ratio of Mo. We found that the resistivity it's correlation with the Mo thickness. So for CdTe solar cells application is convenient grow a thickness near to 750 nm of Mo and the lowest value obtained for the resistivity was  $10^{-5}$   $\Omega$ -cm by Sputtering-DC to low pressure and relative temperature near to 250 C. We obtained a photovoltaic module prototype with a uniform back contact Mo with efficiency close to 4% in cm<sup>2</sup>.



[ RWE-548 ] Hydrogen Generation across by Copper Doped Titania

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Titanium dioxide has attracted great attention in the fields of environmental purification, solar energy cells, photocatalysts, gas sensors, photoelectrodes and electronic devices. In addition, their high chemical stability, environmental friendliness, easy availability, and cost effectiveness makes TiO<sub>2</sub> an ideal candidate as a photocatalyst. The previous research works provided some promising methods to enhance the photoactivity of TiO<sub>2</sub>, involving metal or non-metal ions doping and co-doping. But nevertheless, the effect of doping on the activity depends on many factors, e.g. the method of doping, and the type and the concentration of dopant. The synthesis of TiO<sub>2</sub> by the sol-gel method has proven to be a very useful tool for photo-induced molecular reactions to take place on a titanium dioxide surface. There are special variables that affect the photo-induced reactions, including particle size, phase composition, incident light and preparation method.

In this work, we compared results for hydrogen generation using materials such as copper doped TiO<sub>2</sub> prepared by sol-gel method, and sol-gel assisted by microwaves. We identified anatase phase in samples Cu doped TiO<sub>2</sub>. These materials were probed like photocatalysts in hydrogen production as main aim. Moreover, we observed that the incorporation of copper ions into the TiO<sub>2</sub> structure seems to enhance the photoactivity of the system, and with it, was improved hydrogen production.



**[ RWE-568 ] Effect of the TiO<sub>2</sub> crystalline structure on the CdTe-based solar cell performance.**

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In this work we report a theoretical study on the effect of the crystalline structure of TiO<sub>2</sub> thin films employed as front contact buffer layer (BL) in CdTe-based solar cells. A key issue to rise the solar cell efficiency is to improve the optical and electrical properties of the front contact buffer layer. Here we used a TiO<sub>2</sub> thin film buffer layer because of its high resistivity both in crystalline and amorphous phases, which permits to decrease the thickness of the layer without losing efficiency due to shunting effects, but increasing the spectral response in the short wavelength range. We have performed the simulation of the solar cells by means of the AMPS-1D software and the ITO/TiO<sub>2</sub>/CdS/CdTe solar cells structure was employed. We conducted several experiments by changing the physical properties of the TiO<sub>2</sub> buffer layer according to the amorphous, anatase, a rutile phases; the differences in the bandgap, transmittance and resistivity where took into account. The effect of the thickness was studied, obtaining a better performance when the thickness is decreased in all cases. However, the wide band gap of the amorphous phase improves the spectral response. Efficiencies around 14 % where demonstrated with this buffer layer.

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[ RWE-580 ] SnS thin films prepared by Chemical Spray Pyrolysis with potential application in solar cells

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Tin monosulfide (SnS) is a promising Cd-free candidate as absorber layer in Thin Film Solar Cell technology. In this work SnS thin films were synthesized by chemical spray pyrolysis (CSP) technique using a 0.2 M equimolar precursor solution of tin chloride and thiourea at substrate temperatures of 350, 370 and 390 °C, and pressure of 0.5 and 1.0 kgf/cm<sup>2</sup>. Characterization of synthesized films was performed by X-ray diffraction, Raman spectroscopy, scanning electron and atomic force microscopy, transmission, reflection and absorption measurements, and electric characterization techniques. Films present an orthorhombic phase, p-type conductivity, a direct optical energy band gap of 1.3 - 1.7 eV and a high absorption coefficient ( $\geq 10^4$ /cm). We found that the variation of the carrier gas pressure induced n-type electrical conductivity on SnS films, which may allow an *in-situ* serial fabrication of the SnS homojunction without the need of additional doping materials.

**Keywords:** SnS thin films, absorber material, chemical spray pyrolysis, n type conductivity.

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# **SCIENCE DIVULGATION (SCD)**

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**[ SCD-45 ] Avances y retos en el uso de las celdas solares en sistemas fotovoltaicos**

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En 2015, se instalaron módulos fotovoltaicos con una capacidad de generación de electricidad de 38,7 GW alrededor del mundo y se espera que más de 100 GW de sistemas fotovoltaicos se instalarán en el año 2020, que representará aproximadamente el 3% de la demanda total de electricidad para ese año.

Para alcanzar este objetivo, es necesario considerar los costos de los sistemas fotovoltaicos, que se relaciona con los materiales y técnicas utilizadas en los procesamientos de las celdas y accesorios de los sistemas, las eficiencias de las celdas y además garantizar los lugares en que se instalarán los sistemas. Más sistemas fotovoltaicos requieren más tierra y por lo tanto limitaciones para usarla en otras aplicaciones como la agricultura y la vivienda.

Por lo tanto, el procesamiento de celdas solares con una relación eficiencia/costo lo más alta posible y la energía fotovoltaica integrada en edificios constituyen los mayores retos para resolver un futuro uso masivo de las celdas solares en sistemas fotovoltaicos.

La conferencia abordará estos aspectos haciendo un análisis de los mismos, la situación mundial en el desarrollo fotovoltaico y el contexto en que México se inserta.



[ SCD-120 ] Celda de combustible como sistema de energía renovable y sustentable

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Las celdas de combustible convierten permanentemente sustancias químicas en electricidad a través de una serie de reacciones electroquímicas. Son similares a las baterías de los automóviles que producen corriente eléctrica. El problema con las baterías, es que su tiempo de vida útil es limitado y terminan disfuncionales. La celda de combustible, es un sistema muy sencillo, típicamente está compuesto de un ánodo y un cátodo, donde se introduce principalmente hidrógeno y oxígeno respectivamente. En ellos se presentan dos reacciones químicas; oxidación del combustible ( $H_2$ ) en el ánodo y reducción del oxígeno en el cátodo. Entre estos dos componentes se encuentra un tercero, el electrolito, encargado de conducir los iones de oxígeno al electrodo anódico para su reacción y producción de electrones que pasan por un circuito externo conductor. Asociado a la electricidad producida, también se genera agua 100% pura y calor, que se producen como resultado de las reacciones químicas en el ánodo y cátodo al utilizar hidrógeno. Las celdas de combustible tienen una eficiencia de hasta el 60% y, con algunas modificaciones tecnológicas al utilizar sistemas de co-generación, pueden alcanzar hasta un 80%. En comparación, las turbinas tienen una eficiencia de entre el 40 y el 50%, y todavía es más baja en los motores de combustión interna de entre el 10 y el 25%.

El uso de celdas de combustible reducirá la dependencia del petróleo en el mundo. La contaminación, que principalmente esta compuesta de  $CO_2$  y produce el efecto invernadero, se vería reducida drásticamente, debido a que el combustible utilizado (hidrógeno), no generaría emisiones contaminantes, y se obtendría muy probablemente de gases como butano, propano y metano. Cabe resaltar el uso del metano, que, de entre otras fuentes, puede obtenerse de la descomposición orgánica de los rellenos sanitarios, pirólisis de biomasa o residuos agrícolas, y utilizarse de manera directa en una celda de combustible. Actualmente, en el mercado existen diversos tipos de celdas de combustibles, sin embargo, las celdas de óxidos sólidos (SOFC), son los sistemas de generación eléctrica más atractivos por su alta eficiencia y durabilidad en operación. Además, son mejoradas día a día y podrán ser introducidas en muy poco tiempo para reducir el costo de la producción de energía eléctrica libre de contaminantes. Se pueden fabricar desde pequeños dispositivos de 0.2 W hasta centrales de 50 MW. Las investigaciones actuales, pretenden desarrollar componentes para este tipo de celdas que funcionen a temperaturas menores a los 1000°C.



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**[ SCD-158 ] Principales escenarios ambientales y su relación con las migraciones humanas**

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El análisis de los cambios ambientales y su incidencia con las migraciones humanas es relativamente reciente, en 1992 se agudizan los estudios sobre la migración y sus vínculos con el medio ambiente, destacando importantes desafíos para la seguridad humana y el desarrollo sustentable. El calentamiento atmosférico está acelerando la degradación de ecosistemas propensos a la deforestación, salinización, erosión de suelos y desertificación incidiendo en la seguridad humanidad al exponerse a inundaciones, sequías, olas de calor, terremotos, maremotos, entre otros; lo que provoca migrar temporal o permanentemente, causando repercusiones al ambiente tanto del lugar de origen como el lugar de destino. El propósito de éste trabajo es analizar los posibles escenarios ambientales que se relacionan a las migraciones humanas, como la migración temporal y permanente provocada por cambios ambientales graduales; la migración por actividades en gran escala; la migración y sus repercusiones sobre el ambiente; la vulnerabilidad humana ante la migración y los conflictos jurídicos vinculados a la migración. Se ha concluido que es indispensable una gestión efectiva de la migración en consideración a causas ambientales para garantizar la seguridad humana, su bienestar y propiciar condiciones de desarrollo sustentable.



**[ SCD-187 ] Depósito por baño químico para el desarrollo de películas delgadas semiconductoras de materiales alternativos**

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La creciente demanda energética de hoy en día junto con los acelerados desarrollos tecnológicos demandan con mayor intensidad, la preparación y caracterización de nuevos y mejores materiales, entre los cuales los semiconductores siguen recibiendo particular atención, sobre todo en la forma de película delgada debido a sus múltiples aplicaciones en diferentes dispositivos tales como sensores, transistores, celdas solares, celdas fotoelectroquímicas, entre otros. Por ello, el campo de la Ciencia de los Materiales ha puesto un especial interés, por un lado, en el desarrollo de películas delgadas semiconductoras de materiales alternativos que estén formados por elementos poco tóxicos y de alta abundancia, con propiedades adecuadas para una aplicación determinada. Y, por otro lado, que la preparación de estos materiales sea a través de metodologías de depósito que proporcionen películas de buena calidad, que sean sencillas, de bajo costo y que provoquen un efecto nocivo mínimo en el ambiente, con la finalidad de no contribuir con la problemática ambiental.

Existen varios métodos para depositar películas delgadas semiconductoras, entre estos destaca el depósito por baño químico (DBQ), ya que es un método muy conveniente para hacer depósitos sobre una amplia variedad y tamaño de sustratos (área grande), bajo condiciones no especiales de presión y temperatura (presión atmosférica y temperatura  $\leq 90$  °C). Las películas obtenidas con baño químico son consideradas de buena calidad, uniformes, bien adheridas al sustrato, reproducibles y comparables con las producidas por otros métodos de depósito más sofisticados. Utilizando DBQ, se han logrado obtener películas delgadas de un gran número de calcogenuros de metales (CdS, CdSe, Bi<sub>2</sub>S<sub>3</sub>, PbS, Sb<sub>2</sub>S<sub>3</sub>, CuS, ZnSe, In<sub>2</sub>S<sub>3</sub>, etc) y también películas de hidróxidos y óxidos tales como Sb<sub>2</sub>O<sub>3</sub>, CdO, Cd(OH)<sub>2</sub>, Cu<sub>2</sub>O, NiO, Co<sub>3</sub>O<sub>4</sub>, solo por mencionar algunos. No obstante, a pesar de los beneficios que presenta el depósito por baño químico, existe aún cierta controversia sobre su implementación, principalmente a gran escala. Esto es porque para llevarse a cabo, se parte de soluciones acuosas que contienen metales que en su mayoría son considerados tóxicos, por ejemplo en los depósitos de películas de CdSe y PbS. De esta manera, se considera un reto importante la implementación del baño químico para el desarrollo de películas delgadas de materiales alternativos.

En años recientes, se ha presentado un aumento significativo en las investigaciones sobre películas delgadas de materiales alternativos para dispositivos de interés tecnológico, principalmente en las áreas fotovoltaica y fotoelectroquímica. Dentro de estos materiales se encuentran calcogenuros de cobre y estaño, óxido de titanio, compuestos de hierro, calcogenuros de antimonio y compuestos ternarios y



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cuaternarios de los mismos elementos. Todos ellos cumplen con las características de ser abundantes y con baja toxicidad y, si a estas cualidades se les une la opción de poder desarrollarlos mediante una ruta sencilla y viable como lo es DBQ, el interés por su investigación se incrementa aún más.

En el presente trabajo se mostrarán los fundamentos y detalles básicos involucrados en el método DBQ, con lo que se pretende dar un panorama general de su viabilidad y alto potencial para su uso a gran escala. Además, se mostrarán algunos resultados relevantes de películas delgadas de materiales alternativos desarrollados por este método que se encuentran bajo estudio, que ya han sido aplicados o que se busca su aplicación.



**[ SCD-188 ] Incorporación de la nanotecnología de depósito por capa atómica para contribuir a la solución de diferentes problemas de la industria mexicana**

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Uno de los grandes problemas de México, es la existencia de un enorme atraso tecnológico en comparación con los países de primer mundo. Un ejemplo muy claro de esto lo podemos observar en un área tan importante en la actualidad como lo es la nanotecnología, en donde a pesar de que está presente cotidianamente en las actividades científicas y tecnológicas de nuestro país, todas las herramientas tecnológicas utilizadas para llevarla a cabo, desde las etapas de investigación y desarrollo hasta la incipiente industria mexicana basada en dicha área, son de origen extranjero y no se vislumbra que en un futuro próximo se desarrolle tecnología propia para cambiar esta situación. En este sentido, realizar proyectos que tengan el objetivo de desarrollar tecnología avanzada con miras a tener un impacto inmediato en la sociedad, resulta indispensable para la comunidad científica mexicana.

Una de las tecnologías que se ha posicionado entre las predilectas de la comunidad científica y tecnológica internacional dedicada a la investigación en la escala nanométrica, es el depósito de películas delgadas por capa atómica (*Atomic Layer Deposition, ALD*). Con esta nanotecnología se han abordado una gran cantidad de problemas de muy diversas áreas, que van desde la protección de superficies contra la corrosión hasta la fabricación de dispositivos electrónicos. En México, el interés en esta metodología se ha concentrado principalmente en la parte de los dispositivos electrónicos, mostrando un aumento significativo en la última década. Hoy en día existen varios centros de investigación y laboratorios nacionales que cuentan con un sistema ALD con características específicas de acuerdo a diferentes necesidades. De esta manera, se puede argumentar que en nuestro país se está acumulando una buena cantidad de experiencia en el ramo y que se ha alcanzado un grado de madurez suficiente para considerar dar el siguiente paso: la expansión hacia otras aplicaciones con potencial para ser transferidas a diferentes industrias en un plazo más corto.

En este trabajo se discutirán los fundamentos, las potencialidades y las áreas de oportunidad que tiene esta nanotecnología. Además, se mostrarán el trabajo que se está haciendo con ALD y la infraestructura con que se cuenta en el Centro de Investigación en Materiales Avanzados unidad Monterrey. Finalmente, se discutirá también una visión de cómo podemos incluir a la juventud mexicana para que participe activamente en este tipo de iniciativas.



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**[ SCD-230 ] ¿Agua, material estratégico?\***

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La humanidad podría resistir y adaptarse si los combustibles desaparecieran súbitamente; pero no resistiría el quedarse sin agua adecuada para consumo humano. La tierra debe su apodo de planeta azul, a la gran cantidad de agua disponible sobre su superficie y por supuesto es el sostén de las diversas forma de vida que en ella florecen.

La evolución que llevo lugar a la aparición del hombre sobre la tierra ha generado tensiones diversas sobre ella. Desde extinción de especies de animales o plantas hasta la contaminación del aire y el agua. La contaminación atmosférica, por ejemplo el exceso de gases precursores de ozono, genera un circulo vicioso debido a que provoca aumentos en la temperatura de la tierra y cambia la acidez de los océanos. El aumento en la temperatura debido a cambios en la atmosfera, previsto a principios del siglo XIX, solo ha cobrado notoriedad recientemente; propiciando la propuesta de soluciones científicas para mitigar los efectos de los contaminantes.

En esta plática discutiremos el estado actual de las propuestas de remediación y utilización del agua para mitigar algunos de los efectos adversos del desarrollo tecnológico. La plática se centrara alrededor del uso de semiconductores en procesos de fotolisis del agua para descomposición de contaminantes orgánicos, generación de hidrogeno y aprovechamiento de CO<sub>2</sub> para generación de biocombustibles.

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[ SCD-256 ] Películas delgadas para aplicaciones como recubrimientos duros

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La utilización de películas delgadas data desde la era en que el hombre descubrió que martillando el metal podía obtener películas extraordinariamente delgadas que usó con fines de ornamentación y protección. Actualmente las películas delgadas tienen aplicaciones que van desde los usos industriales hasta los cotidianos. La manufactura de recubrimientos duros ha representado un impacto en el mejoramiento de propiedades superficiales de herramientas y dispositivos para uso industrial. Una opción que ha mostrado grandes mejoras en este sentido, son los recubrimientos de películas delgadas de nitruros y carburos de metales de transición, así como los sistemas multicapas de estos materiales. Recientemente, se ha propuesto al nitruro de tantalio (TaN) y carburo de tantalio (TaC) como capas en la formación de superredes junto a otros nitruros de metales de transición, con la finalidad de obtener materiales superduros. El objetivo de este trabajo es dar a conocer las condiciones experimentales adecuadas para depositar recubrimientos de películas delgadas de  $TaN_x$  y  $TaC_x$ , así como multicapas de ambos materiales con altos valores de dureza, encontrando la relación de esta propiedad mecánica con la composición química, estructura y morfología de los recubrimientos depositados.

#### Agradecimientos

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**[ SCD-305 ] Tecnología Nacional PolyMEMS INAOE: Electrónica Moderna con Aplicaciones en Ingeniería Biomédica**

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Actualmente la Electrónica moderna se desarrolla en base a la tecnología de los chips, la ingeniería de software y la ciencia de materiales principalmente.

Los Sistemas MicroElectroMecánicos (MEMS, MicroSistemas) surgen como una nueva tecnología con aplicaciones interdisciplinarias a partir de la ya consolidada industria de los circuitos integrados (CI's) o Microelectrónica. Esta nueva tecnología ha dado cauce al desarrollo de sensores y actuadores que se fabrican en combinación con bloques de CI's para el procesamiento de las señales eléctricas (Sensores inteligentes). Desde sus inicios, los MEMS presentaron aplicaciones restringidas hacia áreas de electromecánica: pero posteriormente, con el desarrollo de diversos materiales compatibles con los chips, los Microsistemas se han diversificado hacia áreas tales como biología, óptica, fluídica, medicina, magnetismo, entre otras.

Hasta la fecha, los prototipos MEMS totalmente integrados con amplio uso industrial son enfocados hacia aplicaciones específicas, algunos ejemplo son los acelerómetros para protección en colisiones, los cartuchos para inyección de tinta en las impresoras y recientemente los circuitos para control de frecuencia en sistemas temporizadores.

En un contexto general de investigación y desarrollo, los MEMS representan un amplio campo de estudio. En otro contexto de interés público, los dispositivos (Microcomponentes) MEMS para aplicaciones médicas (BioMEMS) representan un campo de estudio estratégico porque se proyecta como un mercado con potencial muy alto. La tecnología de BioMEMS permite el desarrollo de Microcomponentes con posibilidades de interacción con el cuerpo humano, utilizando materiales inertes o de alta pureza química por los requisitos de biocompatibilidad. Los primeros dispositivos BioMEMS fueron fabricados en 1970 consistiendo de sensores de presión arterial micro-maquinados en silicio. En la actualidad, los trabajos de investigación en BioMEMS han derivado en una gran variedad de procedimientos en síntesis de materiales y métodos de fabricación, que utilizando técnicas de miniaturización de fluidos han conducido al desarrollo de la tecnología denominada "Lab on a chip". Este tipo de tecnología incrementa la precisión en el análisis bioquímico, posibilitando nuevas capacidades de análisis clínico de tipo ambulatorio.

En esta conferencia se abordan proyectos de desarrollo de BioMEMS, utilizando la Tecnología nacional PolyMEMS INAOE<sup>®</sup>, los cuales por sus características de innovación y bajo costo resultan de alto interés público.



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**[ SCD-309 ] Colores estructurales de la naturaleza**

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En 1887 Lord Rayleigh [1] sugirió que el paso de la luz de cierta frecuencia podría ser bloqueado por un material con una estructura periódica de un tamaño de red similar a la longitud de onda de la luz incidente, debido a la interferencia destructiva con las ondas reflejadas por las interfaces de la estructura en el material. Los tamaños de parámetros de red entre 380 y 750 nm, esto es menores que 1 micrómetro (estructuras nanométricas) corresponden a las longitudes de onda del violeta hasta el rojo. En la década de los 80, en el siglo pasado, Eli Yablonovitch [2] propuso y fabricó los primeros cristales fotónicos, como son ahora conocidas estas estructuras periódicas con bandas de frecuencias que no son transmitidas por el cristal fotónico en una, dos y tres dimensiones. Estos materiales tienen múltiples aplicaciones, como filtros, reflectores, sensores y otras. Sin embargo desde siempre en la naturaleza, la interacción de la luz con complejas estructuras regulares nanométricas de origen natural nos regala hermosos efectos visuales, entre ellos colores en alas de mariposas, caparazones de insectos, alas de aves, y escamas de los peces. En 1919 Lord Rayleigh [3] también sugirió la posibilidad de que estos brillantes colores fueran producidos por las estructuras regulares, esto es, colores estructurales. Desde mediados del siglo XX, usando microscopía electrónica, se ha hecho mucha investigación para encontrar la relación entre las estructuras de origen animal y el color, sin embargo el entendimiento de todos los procesos físicos involucrados en los efectos ópticos observados continúa siendo un tema de investigación actual [4], sobre todo por las posibles aplicaciones derivadas de la imitación de las estructuras naturales.

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**[ SCD-345 ] Modificación no covalente del grafeno con moléculas de amina**

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En los últimos años el grafeno se ha convertido en uno de los materiales más investigados por sus increíbles propiedades tanto térmicas y electrónicas, por mencionar algunas. Estas investigaciones han revolucionado muchas industrias pero aún con muchas propiedades positivas este material todavía tiene deficiencias, por esta razón, la comunidad científica se ha dedicado a la búsqueda de formas de que el material llegará a ser óptimo en cualquier sentido. Así, se han hecho trabajos para modificación de la superficie del grafeno, que pueden ser divididos en modificaciones no covalentes y covalentes. Con esto en mente este trabajo se centra en la modificación no covalente del grafeno con moléculas de aminas aromáticas, en el que se propone un método que es amigable con el medio ambiente y explica este tipo de modificación a una mejor comprensión.



**[ SCD-347 ] Diodo emisor de luz y su desarrollo en un sistema de depósito de vapor químico usando precursores metalorgánicos (MOCVD)**

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Desde la invención y comercialización del foco incandescente, atribuida a Thomas Alba Edison, el foco no había sufrido una modificación tecnológica relevante que mejorara su desempeño. Desde hace unos pocos años se cesó su fabricación para dar lugar a los llamados focos ahorradores. No estábamos acostumbrando a ellos y su luz blanca – llamada también luz fría– cuando de pronto nos encontramos con las luminarias fabricadas con LEDs ultra-brillantes. La gran mayoría de las personas tiene un concepto mental de lo que es un led – suelen referirse a él como “foquito”– pero pocos saben que la abreviación significa diodo emisor de luz. Los LEDs son dispositivos electrónicos a los que estamos tan acostumbrados que su presencia pasa casi desapercibida. Suelen encontrarse como indicadores de encendido y apagado de los aparatos electrónicos comunes como el equipo de sonido, equipo de cómputo, en reproductores de discos o el televisor. Pero si quisiéramos iluminar una habitación con estos leds no alcanzaríamos a generar suficiente intensidad luminosa para lograrlo con éxito. Pero ¿Cómo es que un modesto indicador luminoso se convierte en una fuente de luz capaz de iluminar grandes áreas? En este trabajo se presenta una reseña de la evolución del diodo emisor de luz enfocado en el sistema MOCVD. Este tipo de sistema ha sido construido en el Centro de Investigación en Dispositivos Semiconductores (CIDS) bajo la dirección del Dr. Godofredo García Salgado, asesoría del Dr. Víctor Sánchez Reséndiz y colaboración del Dr. Crisóforo Morales Ruíz y M.C. Francisco S. Ramírez González. Es importante hacer notar que es el primer MOCVD que se encuentra funcionando en nuestra Universidad (BUAP) y en el Estado de Puebla. El objetivo de nuestras investigaciones es contribuir en el desarrollo de dispositivos electrónicos mediante el estudio del crecimiento de los materiales en un sistema MOCVD.



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# **Semiconductors (SEM)**

**Chairmen: Sergio Jimenez (CINVESTAV-Qro)**  
**Salvador Gallardo Hernández (CINVESTAV-DF)**



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**[ SEM-61 ] Nature of the thermoelectric power in bipolar semiconductors**

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Thermoelectrics draws increasingly the attention of researchers because it can provide with methods to generate environmentally clean energy and solid-state cooling. However some problems of the thermoelectricity physics still remain unsolved. In this paper a new approach to thermoelectric phenomena, as a linear transport process of non-equilibrium charge carriers is presented. The role of non-equilibrium carriers, as well as the ones of surface and bulk recombination, has shown to be crucial even within the linear approximation. Electron and hole Fermi quasilevels that appear in a thermal field are calculated for the case of a thermoelectric current flow through a circuit and the corresponding boundary conditions are obtained. It is shown for the first time that the Fermi quasilevel of one of the subsystems of quasi-particles can be a non-monotonous function of spatial coordinates. General expressions for the thermoelectric current, the thermo-electromotive force (thermo-emf) and the electrical resistance of bipolar semiconductors have been obtained. Also for the first time, both surface recombination and surface resistance were taken into account in thermoelectric phenomena.



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**[ SEM-178 ] Nonlinear charge transport in bipolar semiconductors due to electron heating**

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It is known that when strong electric field is applied to a semiconductor sample, the current voltage characteristic deviates from the linear response. In this work, we propose a new point of view of nonlinearity in semiconductors which is associated with the electron temperature dependence on the recombination rate. The heating of the charge carriers breaks the balance between generation and recombination, giving rise to nonequilibrium charge carriers concentration and nonlinearity.



[ SEM-186 ] Effect of synthesis temperature in the properties of TiO<sub>2</sub> obtained by molten salt method

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TiO<sub>2</sub> is one of the most studied semiconductor for application in devices such as solar cells or in processes such as photocatalysis because of its optical properties and which it is not a toxic material. This material has been synthesized by different methods, mainly by sol-gel synthesis and hydrothermal, however it is possible to obtain by other methods, for example, molten salts. On the other hand, the conditions of each method influence the shape (spheres, tubular, etc.) and particle size. One of the most important conditions is the synthesis temperature because it is strongly related to the crystal structure of the material and particle size.

In this work, we present the influence of temperature synthesis in the structure, shape and band gap of TiO<sub>2</sub>. This material was synthesized by the method of molten salts, varying the synthesis temperature. Analysis of X-ray diffraction (XRD) was performed to identify the phases present and Scanning electron spectroscopy (SEM) and transmission (TEM) to determine the size and shape of the particle. Furthermore, UV-Vis spectroscopy was performed to obtain the absorption curves and determine the influence of synthesis temperature in the band gap of TiO<sub>2</sub>.

**Keywords:** TiO<sub>2</sub>, molten salts synthesis, band gap.



[ SEM-195 ] Temperature dependence of electrical parameters of PEDOT:PSS/ZnO Schottky barrier diodes

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This work reports the temperature dependence of the electrical parameters of PEDOT:PSS/ZnO Schottky barrier diodes grown on glass substrates with a maximum processing temperature of 80°C. The electrical parameters were extracted from current-voltage-temperature characteristics (302-373<sup>0</sup>K) using the thermionic emission and Cheung's methods. The obtained Richardson constant and effective barrier height were 5 A-cm<sup>-2</sup>-<sup>0</sup>K<sup>-2</sup> and 0.74 eV, respectively. The diode ideality factor was 1.5 and the series resistance was 36 Ω. All these electrical parameters turned out to be temperature independent, which is associated to the presence of both transport mechanisms electron-hole recombination in the depletion region ( $n = 2$ ) and thermionic emission ( $n = 1$ ). The Richardson constant slightly deviate from theoretical values due to the presence of interface defects create by the ZnO film etching from the acidic PEDOT:PSS solution. The conductive polymer PEDOT:PSS, as a Schottky contact to ZnO, arise as an alternative to the expensive noble metals such as: Pt, Pd, Ag, AgO<sub>x</sub>, IrO<sub>x</sub>, PdO<sub>x</sub> and PtO<sub>x</sub>.



**[ SEM-242 ] Impact of the stacking sequence in the atomic content of CZTS deposited by chemical bath**

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The development of high efficiency solar cells with  $\text{Cu}_2\text{ZnSnS}_4$  (CZTS) thin films depends on the synthesis of films with kesterite as unique phase. Because of the secondary phases which usually occur, it is a challenge to prepare CZTS films with kesterite as unique phase. For this reason, a systematic study of the deposition process to reach optimal elementary relations, which are in the ranges of  $\text{Cu} / \text{Sn} = 1.7-1.8$  and  $\text{Zn} / \text{Sn} = 1.2-1.3$ , is essential. In this work, a methodological study of the six possible stacking sequences of ZnS, CuS and SnS binary systems is presented. The impact of their different sequences upon atomic content and microstructure was investigated by scanning electron microscopy (SEM) and X-ray diffraction (XRD). On the basis of experimental evidences, the most appropriate deposition route for CZTS formation is proposed.



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**[ SEM-274 ] Properties of TiO<sub>2</sub>:Eu<sup>3+</sup> nanofibers**

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The design and preparation of one-dimensional nanostructural materials, such as nanorods, nanowires, or nanofibers have attracted great attention because of their potential unique properties and applications. There are several techniques to make these materials, electrospinning technique as a simple and low-cost method for making nanofibers has been utilized in the preparation of many one-dimensional nanostructural materials. In recent years, there has been a growing interest in the fabrication of semiconductor oxides nanofibers such as WO<sub>3</sub>, ZnO, and TiO<sub>2</sub> nanofibers by this technique. Rare-earth ions have

been chosen for study as dopants because they are extremely useful in optical applications due to their sharp, near monochromatic emission lines. The research on the luminescent properties of the rare-earth elements hosted in several crystalline matrices, such as fluoride glasses, metal organic complexes, and a variety of semiconductor materials, is strongly

motivated due to their technological applications in optoelectronics devices and flat panel displays. In this work we study the dependence of the structural, chemical, morphological and luminescent properties of TiO<sub>2</sub>:Eu<sup>3+</sup> nanofibers as function of the annealing temperature. Nanofibers have been prepared by electrospinning of a mixture solution of europium acetylacetonate, Eu(C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)<sub>3</sub>/ titanium tetraisopropoxide (Ti (OiPr)<sub>4</sub>)/poly(vinyl pyrrolidone) (PVP). The samples were annealing to different temperatures under Nitrogen atmosphere. The morphology has been studied by Scanning Electron Microscopy (SEM) and crystalline structure was analyzed by X-Ray Diffraction (DRX). The luminescent properties were measured using Photoluminescence at room temperature. The results shown, that the origin of the luminescence could be associated at the presence of Eu<sub>2</sub>O<sub>3</sub> in the samples.

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[ SEM-323 ] Optical constants of ZnO and ZnO:Zr thin films grown by rf sputtering technique

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ZnO and Zr doped ZnO thin films were grown onto glass slides by the radio frequency sputtering technique utilizing targets from a mixture of ZnO and ZrO<sub>2</sub> powders. The doping level was in the range of 1 to 5 at. %. Normal incidence transmittance and near normal incidence reflectance spectra were used to determine the optical properties of the films. The experimental data were analyzed with the commercial software FilmWizard by modeling the samples as an air-film-substrate system. The optical constants of the substrate were determined from measurements performed on an uncoated substrate whereas the complex dielectric function ( $\epsilon$ ) of the films was represented with a generalized form of the harmonic Lorentz oscillator. By an analysis of regression of the model-calculated and experimental data the film thickness and the parameters defining the dispersion of  $\epsilon$  are determined. The results are discussed in terms of the complex refractive index of the films  $N=n+ik$  where  $n$  is refractive index and  $k$  the extinction coefficient. Samples doped with 1, 2 and 5 at.% of Zr show a small variation of  $n$  with respect to pure ZnO. For the films with 3 and 4 at.% of Zr  $n$  is, respectively, larger and smaller than for ZnO. A wider bandgap ( $E_g$ ) was obtained in Zr doped ZnO films than in the film of pure ZnO. The results are critically discussed in terms of the quality of the fitting due to a non uniform thickness.



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**[ SEM-396 ] structural, nanoelectrical and optoelectronic characterization of ZnOAl films  
prepared by spray pyrolysis**

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In this work zinc oxide (ZnO) was deposited by spray pyrolysis method with constant synthesis parameters (temperature, time, concentrations, etc.) with five different percentages of aluminum doping against zinc molar ratio. Samples were analyzed by scanning electron microscopy which showed the ZnO surface changes as increased doping and roughness. X-ray diffraction showed the ZnO preferential growth in zincite phase and Rietveld analysis that the dopant enters instead of Zn, but depending on the lattice site, the habit growth changes drastically from hexagonal plates to nanopencils, truncated pencils and hexagonal columns. Texture analysis confirmed this changes in crystal growth habit and correlations with Urbach disorder parameter and electrical properties are made. By atomic force microscopy surface topography of samples it was studied using the conductive mode and to measure current driving mechanism grains depending the amount of dopant in the case of ZnO. ZnO was also studied by diffuse reflectance spectroscopy and sheet resistance was measured by two points. The band gap and the relative position of the donor states reflect the amounts of Al incorporation while electrical properties are directly related with the crystallographic position. Financed by SIP Multidisciplinary Project 20161804/0291.



[ SEM-437 ] Study and characterization of GaAs films grown by a low cost technique

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Technological interest of GaAs in optoelectronics and microelectronics, has been developed several techniques for obtaining films. But some of these techniques have a high cost and use toxic and pyrophoric compounds how trimethyl gallium ((CH<sub>3</sub>)<sub>3</sub>Ga) and arsine (AsH<sub>3</sub>). However there are other alternatives, such is the case of the CSVT technique (Close Space Vapor Transport) [1], [2], this offers a possibility to grow GaAs films at low cost [3]. In this work presents the study and characterization of GaAs films deposited on silicon and quartz substrates, in a temperature range of ~730 to 480 ° C, from the CSVT technique, using a HFCVD reactor system. The films were characterized morphologically by SEM and can be observe the change in size due temperature change. Structurally characterization was carried out by X-ray diffraction in grazing incidence mode. From the diffraction patterns was determined the obtaining of GaAs polycrystalline films with a Zincblende structure, with guidances at (111), (220) and (311). EDS information show that the chemical composition on the films surface that is closely stoichiometric.

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**[ SEM-451 ] What's up Mr. Schottky?**

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In 1930 and 1932, the early years of quantum theory, the model of electron tunneling from metals into semiconductors was developed by Frenkel, Joffe, Wilson, Nordheim and Zener. Yet the experimental observation had to wait for the development of materials technology of semiconductors, and was made in 1959 by Holonyak, Lesk, Hall (R.N.), all working for the General Electric Company, and one year later by Esaki and Miyahara; Leo Esaki shared the Physics Nobel Prize in 1973 with Ivar Giaever and Brian Josephson for their contributions that involved electron tunneling. Further investigations in this topic led to precision tests of the “old” tunneling model in the middle and late 60’s and several applications were developed. The nature of the junction between a metal and a semiconductor was very well pictured by what is called a “Schottki barrier”. It seemed that not much were left to investigate. But Mr. Schottki and his barrier came back into the world scene of frontier physics in the early 2010’s when two astonishing reports of novel devices applications made their way into the scene. Firstly in 2012<sup>1</sup>, a graphene Schottki diode (in which the key is an atomically sharp interface between graphene and hydrogenated silicon) with a tunable barrier height appeared as a great platform for the study of interface transport mechanisms as well as for several applications (photodetection, high speed communications, solar cells, etc.). On the other hand it was clear that non-volatile memories made of ferroelectric tunnel junctions (FTJs) with applications on smart phones and robots needed improvement. Then in 2013<sup>2</sup>, a report is made announcing the enhancement of the tunneling electroresistance effect (TER) by two orders of magnitude by incorporating a semiconductor, Nb doped SrTiO<sub>3</sub>, as an electrode in a FTJ: Pt/BTO/Nb:STO, also a great platform for theoretical studies and applications.

The underlying physical mechanism of these two finding is very important from the technological as well as from the scientific point of view. This two aspects of novel electron tunneling into semiconductors research will be addressed in this talk.

So, Mr. Schottki still has many rabbits in his hat. Only God knows when or how they will appear!

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**[ SEM-502 ] Synthesis and characterization of MoS<sub>2</sub>-MoSe<sub>2</sub> Van der Waals heterostructures**

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During the last years, two dimensional materials (2D) have become one of the most dynamic field in materials research. Like graphene, many materials can be either exfoliated or synthesized to obtain single layers including the possibility to form heterostructures. Among all these new materials, monolayer transition metal dichalcogenides (mTMDs) particularly Molybdenum based mTMDs are intrinsic semiconductors with well-defined direct bandgap values making them suitable for optoelectronic devices, such as photodetectors, photovoltaics and light-emitting devices with novel characteristics or unique functionalities

In this work we present the synthesis and characterization of a 2D heterostructure system composed by both, lateral and axial MoS<sub>2</sub>-MoSe<sub>2</sub> Van der Waals heterostructures. The structures were epitaxially grown using a simple and controllable technique based on a CVD two-step process. Micro-Raman and PL spectroscopy and imaging show spatially contributions of different vibrational modes and luminescence of the two materials over the structures. In particular, photoluminescence spectra show that the emission can be tuned in a large spectral wavelength range from 1.55 to 1.85 eV. Crystallinity of the MoSe<sub>2</sub>-MoS<sub>2</sub> heterostructures was studied by transmission electron microscopy (TEM). Finally, we studied the presence of trions and thermal quenching mechanism of neutral excitons in the MoS<sub>2</sub>/MoSe<sub>2</sub> vertical heterostructures.



[ SEM-506 ] Macroporous 3D-TiO<sub>2</sub> thin film functionalized with palladium nanoparticles and its sensing properties to reducing gases

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Macroporous quasi-ordered tridimensional titanium oxide (3D-MTiO<sub>2</sub>) thin films were synthesized by the sol-gel-technique using micro-spheres of Poly(methyl methacrylate) (PMMA) as a template. The PMMA template was removed by thermal annealing in air at atmospheric pressure and 450 °C. The as-obtained 3D-MTiO<sub>2</sub> films exhibit a semi-ordered structure with high surface to volume ratio in which the wall thicknesses are around 50 nanometers. The 3D-MTiO<sub>2</sub> films were functionalized through the deposition of palladium nanoparticles on its surface using a palladium chloride-based aqueous solution. Then, the functionalized films were used as the sensitive element for the fabrication of a conductimetric gas sensors. The sensors were characterized using several reducing gases (acetone, alcohol, ammonia, and xylene) considering the range of temperatures of 300-400°C and gas concentrations in the order of parts per million in volume (ppm), through conductance transient measurements. The results of the sensors characterization reveal high response to acetone and alcohol; in addition, the optimal sensors operating temperatures correspond to 350 and 400 °C, respectively. In all the experimental conditions, it was found that the sensors response and recovery times fall in the range of seconds. This work demonstrates the high potential of quasi-ordered semiconducting metal oxides for sensing purposes because this process provides a better control of the porosity; and thus, the diffusivity of the gas species in the volume of the nanostructured film, undoubtedly permits the design of sensors with high performance and high repeatability in the fabrication process.



[ SEM-558 ] Electrical Optical and Structural Properties of Polycrystalline Silicon / ZnO:Al /  
Glass to form emitter layer in thin film solar cells

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Transparent conductive oxide ZnO:Al films on glass covered with a thin layer of polycrystalline silicon (poly-Si) were deposited by RF Sputtering and Nickel Induced Crystallization Epitaxy method respectively. To optimize the electro-optical properties of the ZnO:Al films, substrate temperature, pressure and the RF power were varied. The transmission and the haze factor were recorded in the visible range. Resistances of the order of  $13 \Omega/\square$  and transmission higher than 80 % were obtained. they were annealing at 580 °C during 24 hrs, its properties remains stables. Then on the top of the ZnO films a thin layer of a-Si:H was deposited by PECVD and crystallized following the NIC method, XRD analysis showed a polycrystalline film oriented in the (220) plane.

The poly-Si thin films obtained from nickel-induced crystallization presents average grain sizes between 70-100  $\mu\text{m}$  and estimated thickness of 300 nm. To study the thermal stability of the ZnO films the bare ZnO:Al film and ZnO:Al covered with poly-Si, were subjected to two types of heat treatment, one at 580 °C for 24 h in a conventional furnace and another at 850 °C for 200 s in RTA furnace. The electrical properties of bare ZnO:Al films were degraded after thermal treatment, the sheet resistance increases up to an order of magnitude compared to the values measured without annealing. However the samples of ZnO:Al films coated with poly-Si, showed a lower sheet resistance for the case of conventional annealing and up to an order of magnitude lower for the RTA process, indicating that the poly-Si prevents its electrical properties are degraded and an improvement of the electrical properties of ZnO:Al was observed. The results obtained are of great interest in the study of the thermal stability of ZnO:Al at post-processing annealing temperatures in fabrication of emitter layer in polycrystalline silicon thin film solar cells technology.



**[ SEM-6 ] Destruction of Fano Resonances in bilayer graphene-based systems: The role of the bandgap induced by an applied electric field**

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Fano resonances are an exotic property of bilayer graphene [1]. An electric field applied perpendicularly to the graphene sheets can induce an energy bandgap [2], and in principle this gap can affect the Fano resonances. In this work, we study the conditions under which the Fano resonances are preserved or destroyed due to the influence of an applied electric field. We implement a four band-band Hamiltonian to properly describe the opening of the bandgap and the non-parabolicity of the bands. In particular, we study the transmission properties of a two barrier system using the transfer matrix approach.

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[ SEM-26 ] Electronic and phononic properties of GaSb quantum wires: a theoretical approach

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In the last years semiconductor nanowires (NWs) have been extensively studied for the development of field effect transistors, solar cells, lithium batteries and sensors. Specially, NWs based on GaSb are of great interest for applications in fiber optic communications since the emission of these materials is in the range of mid-infrared, and also in field effect transistors where the nanowire serve as the conducting channel, for these applications a correct understanding of the vibrational properties is fundamental, however, there are seldom theoretical investigations about this matter. In this work we use the methodology of the Density Functional Theory to study the vibrational properties of GaSb nanowires with different diameters grown on the [111] crystallographic direction, where all surface dangling bonds are passivated with H atoms. To model the NWs we used the supercell scheme [1,2] and the Local Density Approximation, the changes in phonon dispersion relations shows a shift to lower frequencies of the optical modes compared to their bulk counterparts while the electronic band gap shows an increment when the diameter decreases, both according to the quantum confinement scheme.

#### Acknowledgments

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[ SEM-40 ] GaN buffer layer obtained from GaAs nitridation used in GaN epitaxial growth by  
OMVPE

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We present gallium nitride (GaN) epitaxial growth by a homemade organometallic vapor phase epitaxia (MOVPE) system. The epitaxial layer was growth using a two steps growth process in the same system. In the first step, the system was used as rapid thermal annealing (RTA) in order to obtain a buffer layer by nitridation of crystalline gallium arsenide (GaAs) (111)B. An atmosphere of Hydrogen and Ammonia gas was used to nitride the GaAs wafer at 900 °C for 5 min. The second step consisted in the GaN epitaxial growth using trimethyl gallium (TMGa) as organometallic precursor and NH<sub>3</sub> at 900 °C for 30 min. Photoluminescence spectra shown cGaN and hGaN band-band emission (360-380 nm) without contributions around 500 nm (yellow band). The x-ray diffraction (XRD) characterization shows that the obtained material is GaN with a preferential cubic presence. Scanning electron micrographs show a rugose surface and an isolated island formed of microstructures as needles.



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[ SEM-143 ] Comparison structural, morphological, optical and electrical properties of CdSe thin films growth by two different techniques

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Growth of CdSe thin films deposited on glass substrates by Chemical Solvent evaporation and Tape casting techniques was studied. The chemical solution in the experiment were prepared with CdCl<sub>2</sub> and Se as precursors and it was used in both techniques. The solution was prepared by colloidal synthesis assisted by ultrasonic vibration approach. The samples were subjected to annealing process at 150° and 250°C in air environment. Morphological, structural, optical, and electrical measurements were obtained from each CdSe films group. After annealing at 250°C meta stable cubic phase, found initially, was transformed in to stable polycrystalline hexagonal phase for both sets of samples is shown. Lower mean values in the crystallite size (4.5 nm) were obtained from the films grown by SE-CdSe compared to those obtained by TC-CdSe (8.24 nm). The band gap energy values ranged between 1.73 – 1.83 eV for SE-CdSe, meanwhile for TC-CdSe kept constant at 1.82 eV. SEM images shows that as deposited CdSe films are uniform and homogeneous, and almost covering the entire substrate surface. After the heat treatment great changes in its surface morphology are observed with the appearance of elongated hexagon shaped nanorods. The electrical resistivity is found to decreases with both annealing temperature and crystal size. These changes are attributing to the crystal size effects in the semiconductor films.



[ SEM-146 ] Obtaining of Te semiconductor films by sputtering technique and its application as p<sup>+</sup> type layer in photovoltaic cells

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The solar energy is one of the energy sources that can be harnessed on earth through photovoltaic materials, which can transform it into electric energy. Semiconductor materials in the thin film technology have allowed the exploitation of this energy source with the development of solar cells. CdTe (cadmium telluride) is a material that can be used as absorbent layer in solar cells due to its chemical and optoelectronic properties. Has a value of band gap,  $E_g=1.5$  eV and a high coefficient of absorption ( $>5 \times 10^5$  /cm), which means that a high yield can be expected over a wide range of wavelengths. About 30% of the efficiency is estimated for the CdS/CdTe heterostructure [1]. To generate a p-type conductivity is necessary an excess of Tellurium or introduce impurities to the surface with other elements such as Cu, which is inefficient because this element can diffuse into the material and affect the cell operation [2]. One of the main aspects to improve in these solar cells is the back contact, a back contact is one on which current flows in a solar cell and this should allow the free flow of carriers through it [3]. CdTe is a material with a high electron affinity, making it difficult to doping and obtaining a good electrical contact on this. In this work, Tellurium films were grown on glass and CdTe substrates by RF magnetron sputtering technique. The characterization by X-ray diffraction and raman spectroscopy was carried out in order to determine the crystal structure of Te thin films and the electrical characterization was made by effect Hall measurements; the results are discussing in terms of growth details.

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**[ SEM-174 ] Optical and electrical characterization of Li doped PbS thin films.**

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Lithium (Li<sup>+</sup>) doped Lead sulfide (PbS) thin films were prepared chemical bath method. The concentration of Lithium in the precursor solution of Lead Sulphide was varied from 3mls to 6mls. The structural properties of as deposited films were characterized by X-ray diffraction. XRD patterns indicated the presence of cubic phase PbS with preferential orientation along (111) plane. Optical absorbance in visible region of the film increases with dopant concentration. The optical measurements reveal that the PbS:Li thin films possess direct band gap and the band gap energy increases with an increase of Li<sup>+</sup> concentration. Thin films were found to be 1.8, 2 and 2.1 eV respectively. The dc conductivities of PbS and PbS:Li thin films are measured in temperature range 10–40 K. It is observed that the thermal conductivity increases at with an increase of Li content in PbS system. The experimental data suggests that the conduction is due to thermally assisted tunneling of the charge carriers in the localized states near the band edges. The activation energy and optical band gap are found to increase with increasing Li concentration.



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**[ SEM-177 ] Studies on the Resistivity of transparent ZnO Thin Films prepared by Sol Gel, doped and co-doped with Aluminum, Indium and Boron.**

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ZnO is a versatile material, that has been under intensive investigation for a long time since 1950s. The material is attractive not only for being non-toxic, but also for being cheap. Transparent ZnO thin films prepared by diverse methods have demonstrated to be conductive enough to be applied in a wide range of electronic devices. Also, transparent ZnO conducting films doped with diverse variety of elements are commonly reported in literature. In this work we prepared ZnO films by the sol gel method, doped and co-doped with Aluminum, Boron and Indium. The aim of the work is to discuss results on the resistivity of the films, as measured with an electronic device designed and developed by us. The films were prepared with 0, 1, 2, 4, 6, 8, 10 and 12 at. % ratio of impurities to Zn.

The films were deposited on glass substrates by spin coating, from a solution of zinc acetate with different doping levels, and thermal treatments at 200, 300, 400 and 500<sup>0</sup> Centigrade were made.

The built device to measure resistivity is based on the use of an operational amplifier (opamp) configured as integrator. When a constant input voltage is applied, a linear output voltage is obtained, and the slope of this line is given in terms of values of the resistance, the capacitance and the input voltage. Through a digital analog converter and a microcontroller programmed in C language, the output voltages and capacitor discharge times were monitored and sent to a computer, to be analyzed using a Java program. From these calculations the resistivity of the material is finally obtained.

The various behaviors of the electrical resistivity of the material in terms of the doping levels are discussed. Details of the preparation of the sol gel films, as well as details of the construction of the electronic dispositive to measure resistivity are also given in this work.



[ SEM-190 ] Lipid bilayer formation within pores in macroporous silicon

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Electron paramagnetic resonance (EPR) spectroscopy was used to study the pore filling of macroporous silicon (MPS) with lipid vesicles (liposomes), added with a spin label. MPS samples were obtained by electrochemical anodization of p-type boron doped crystalline silicon wafers, in darkness. The resulting macroporous films have thickness of around 30  $\mu\text{m}$ , and pore sizes of 1.0-1.2  $\mu\text{m}$ . The samples were functionalized by several methods in order to turn hydrophilic the inner surface of the pore network. Then, the pore structure was filled with an aqueous solution of 100 nm unilamellar liposomes of the phospholipid DMPC plus 2 mole percent spin label 5-doxyl stearic acid (5-SASL). EPR spectra were acquired in X band at 30°C after different incubation procedures. Spin label spectra are sensitive to the orientation of the magnetic field  $B$  relative to the  $p$  orbital of the nitroxide, which for 5-SASL is parallel to the hydrocarbon chains. While liposomes have isotropic spectra, the spectra of lipids inside porous samples for  $B$  parallel to the pore axis are different from those for  $B$  perpendicular to the axis. The spectra could be well simulated with an admixture of the spectrum of liposomes, plus a simulated spectrum corresponding to that of a cylindrical distribution of lipid bilayers. This means that cylindrical lipid bilayers were formed covering the inner surface of the pores, although some liposomes remain inside the pores. Diverse protocols were explored in order to optimize the lipid covering of the pore walls, and to achieve an adequate lipid hydration. A 2D photonic crystal made of MPS can be used as a sensor for changes in the dielectric function of the filling material. We propose the use of such devices to study effects of confinement on DMPC phase transition, which occurs near room temperature.



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[ SEM-249 ] Synthesis and characterization of Zn/ZnO core-shell structures obtained by thermal evaporation and condensation technique

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An urchin-like Zn/ZnO core-shell structure was synthesized and deposited directly on a glass substrate by using a thermal evaporation and condensation technique using a mixture of zinc and zinc oxide powders at 650 °C for 60 min. and nitrogen as carrier at atmospheric pressure. This material contains a Zn sphere core, and the shell is composed of numerous single-crystalline ZnO nanowires radially protruding from the central Zn core. The core-shell structure was characterized in structure, morphology and composition by X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS). These studies indicated that the growth of hollow ZnO urchins, involves the vaporization of Zn powder, solidification of liquid droplets, surface oxidation, sublimation, and self-catalytic growth of one-dimensional nanowires. These Zn/ZnO core-shell structures can be a promising candidate for anode material in solar energy conversion devices.

Keywords: Core-shell structures, Thermal Evaporation-Condensation technique.



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**[ SEM-275 ] Effect of metal work function on the properties of TiO<sub>2</sub> thin films deposited by reactive RF Sputtering.**

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Titanium Dioxide is a promising photocatalyst for its strong oxidation potential and its moderate potential reduction due to the generation of electron - hole pairs in the valence band (VB) and conduction (BC). The excited electrons in the BC reduce oxygen in super oxide radical, and holes in the BV oxidize water molecules into hydroxide radicals. These radicals are potent intermediates in the decomposition of organic molecules. In addition, the TiO<sub>2</sub> is physically and chemically stable and nontoxic therefore has a variety of applications such as self-cleaning surfaces, antimicrobial and environmental purification.

In this work TiO<sub>2</sub> thin films have been deposited on different metal substrates, using reactive Rf sputtering technique. The structural and chemical bonding characteristics were analyzed by X- ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). UV-Vis reflectance spectroscopy was employed to determine the band gap energy. The electrochemical properties of films on different metal substrates were obtained using the

electrochemical impedance spectroscopy, mott schottky and cyclic voltammetry. The results shown a strong dependence of the metal work function with the electrochemical properties of the films.

This work was supported by SIP-IPN under the multidisciplinary project 1697



[ SEM-288 ] Energy flux in a semiconductor sandwiched between two thermostats with different temperatures

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The energy flux in semiconductors depends not only on the temperature gradient but also on the gradient of electron and hole concentration, and also on the electric currents of electrons and holes [1]. Nevertheless, the expression for the energy flux can be presented as a function of only the gradient of the linear part of the temperature distribution in quasi-neutral approximation for any stationary process if the the semiconductor does not absorb nor irradiate light [2]. It is worth to mention that the temperature distribution in semiconductors is not a linear function of the coordinate in general case even in a linear approximation with respect to perturbation [1]. This temperature distribution is the superposition of the linear and exponential functions of the coordinate in a linear approximation with perturbation for any stationary process in a quasi-neutral case [1],  $T=C_1+C_2x+C_3 \exp(x)+C_4 \exp(-x)$ , where  $C_1, C_2, C_3, C_4$  unknown constants. Hence, to determine the energy flux in a semiconductor we need to find the constant  $C_2$ . Due to the temperature depends on four unknown constants, then we need to use four boundary conditions to determine the value of  $C_2$ : the conditions of the temperature continuity on contacts of the semiconductor sample with the thermostats and the conditions that the holes electrical currents are proportional to the surface recombination velocities [3]. We can solve this problem analytically in a linear approximation with respect to perturbation and obtain the expression for the energy flux in a semiconductor. This problem is solved and the general expression for the energy flux in obtained. The result shows that the energy flux in a semiconductor depends not only on the thickness of the semiconductor sample, thermal conductivity, and the temperature differences on the contacts, but also on the surface recombination velocity, the diffusion length, and the bandgap.

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**[ SEM-289 ] Numerical modelling of transport phenomena in optically excited GaN/AlN/Si heterostructures: Electrical properties**

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In the present work, a study of the electric displacement field in optically stimulated GaN/AlN/Si heterostructures (grown by molecular beam epitaxy technique) is presented by solving the photogenerated charge carrier diffusion equations and Maxwell's equations, considering both, constant illumination and periodically modulated illumination. The solutions for the dynamical equations are given by employing the Finite Element Analysis (FEM), and analytical methods. From the analytical and numerical studies, the open-circuit voltage and the short-circuit current of the GaN/AlN/Si heterostructures were calculated as function of the wavelength, and the results compared with those reported in literature, discussing the observed differences.



[ SEM-293 ] Growth and Characterization of Tungsten Disulfide (WS<sub>2</sub>) Monolayers

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Two-dimensional (2D) transition metal di-chalcogenides (TMDs), especially Molybdenum and Tungsten monolayer TMDs have attracted significant interest for optoelectronics applications due to the fact they can cover a large spectral range from 1 to 2.5 eV.

In this work, we present a method to obtain single monolayer WS<sub>2</sub> crystals based on Atmospheric Pressure Chemical Vapor Deposition (APCVD) technique. The growth of WS<sub>2</sub> crystals is promoted using WO<sub>2</sub> and sulfur precursors that are placed inside a tube quartz, Ar is used as a carrier gas and the growth temperature is set at 750° C during several minutes. WS<sub>2</sub> crystals morphology and structure is studied using Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). The optical properties were studied by means of Raman and Photoluminescence. Raman spectra show two contributions related to E<sub>2g</sub> and A<sub>1g</sub> modes, the separation of these two peaks is approximately 62 cm<sup>-1</sup>, confirming the presence of a single monolayer [1]. On the other hand, photoluminescence spectrum has an intense main peak around 2.01 eV, which is attributed to the WS<sub>2</sub> monolayer direct bandgap [2].

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**[ SEM-333 ] Degradation Photocatalytic of phenol using oxides of ZnAl whit and whitout a  
Surfactant**

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Synthezised by coprecipitation's method materyals type hydrotalcites (layered double hydroxide) whit and without the addition of a surfactant (SDS), after were calcined to 400°C for obtain mixed oxides ZnAl whit and whitout SDS. Were favored the semiconductors property and the photocatalytic activity in the degradation of Phenol to 40ppm in the presence of UV light (254nm). Was confirmed the presence the Surfactant material through techniques as DRX, IR and XPS spectroscopies. IR presented bands than belonging to sulphates and sulphides groups, DRX showed to increase parameter of network "C" associated of the surfactant material with the possible intercalation into the interlaminar space, and by XPS was achieved the detection sulphates ions Zinc and Aluminum.



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**[ SEM-336 ] Effect of annealing temperature on co-sputtered p type ZnO:Ag,N thin films**

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ZnO p type thin films was prepared by dual acceptor co-doping with nitrogen and silver via DC reactive magnetron co-sputtering. As precursor material were used a Zn and an Ag metallic targets. Energy dispersive spectroscopy (EDX) confirmed the presence of Ag and N in ZnO:Ag,N lms. The electrical properties were explored by Hall Effect measurement in the Van Der Pauw configuration. As deposited ZnO:Ag,N films presented a high resistivity and low hole concentration. However, after annealing at 400°C for one hour in nitrogen atmosphere the electrical properties were improved significantly. After annealing, the best ZnO p type thin film presented a low resistivity of  $8.56 \times 10^{-3} \Omega \cdot \text{cm}$ , Hall mobility  $23 \text{ cm}^2/\text{V} \cdot \text{s}$  and high carrier concentration  $3.17 \times 10^{19} \text{ cm}^{-3}$ .



[ SEM-341 ] SnO<sub>2</sub> Synthesis and its photocatalytic activity compared with TiO<sub>2</sub>

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The photocatalysis has been studied for decades looking for the best photocatalyst. Several semiconductors such as ZnO, SnO<sub>2</sub>, ZnS and Fe<sub>2</sub>O<sub>3</sub> can be applied as photocatalyst but the TiO<sub>2</sub> has been the most commonly studied, even the TiO<sub>2</sub>-P25 is used as the reference. The oxide semiconductors like TiO<sub>2</sub> and SnO<sub>2</sub> are suitable due its high reactivity, non-toxicity, chemical stability and lower costs due its abundance. The photocatalysis effect is produced on the nanoparticles surface, for that reason is important to increase the surface area. The activity depends on size; structure morphology of the nanoparticles is necessary control these properties. The solvothermal method is a convenient way to obtain the quality and the size appropriate to enhance the photocatalysis activity. In this work we show the photocatalytic activity of SnO<sub>2</sub> nanoparticles compared with commercial TiO<sub>2</sub>-P25. The synthesis of SnO<sub>2</sub> was using SnCl<sub>2</sub> as source, ethanol as solvent and acetic acid as catalyst. The Solvothermal method produces internal high pressure being able to obtain highly quality nanoparticles. The nanoparticles was characterized by X-Ray diffraction, Raman spectroscopy and Transmission Electron Microscopy to know the size, structure and phases presents. The degradation of methylene blue was achieving utilizing a UV lamp with the keeping the relation 1 mg of photocatalyst/1 ml of MB (15PMM). The nanoparticles crystallizes in SnO<sub>2</sub> with tetragonal structure with size lower than 10 nm. The degradation of methylene blue by SnO<sub>2</sub> is given in 40 min while TiO<sub>2</sub>-P25 takes 50 min.

**Keywords:** Tin dioxide, photocatalysis, methylene blue degradation.

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[ SEM-344 ] Synthesis and structural, thermal and electrical characterization of  $\text{CuAlO}_2$

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Copper aluminate ( $\text{CuAlO}_2$ ) is a kind of p-type semiconductive material, belonging to the delafossite group of ternary oxides. They occupy an important place in various fields by virtue of the diversity of physical properties; some applications are photovoltaic cells, transparent conductor, UV-emitting devices, gas sensors, biosensors and high temperature thermoelectric material. In this study,  $\text{CuAlO}_2$  was prepared by the Pechini method using copper chloride (II) ( $\text{CuCl}_2$ ), aluminum chloride (III) ( $\text{AlCl}_3$ ) as precursors, and citric acid ( $\text{C}_6\text{H}_8\text{O}_7$ ) and ethylene glycol ( $\text{C}_2\text{H}_6\text{O}_2$ ) for the metallic polyester formation. The sample was characterized by X-ray diffraction, Raman spectroscopy, thermal conductivity, Seebeck effect and Van der Paw method in order to corroborate the crystal structure and evaluate the thermal and electrical properties. This work was supported by SIP multidisciplinary project No. 20161804/0294.



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**[ SEM-362 ] Properties of reduced graphene oxide films**

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Graphene is one of the most relevant materials nowadays because of its extraordinary 2D properties that make it suitable for a good number of applications. This material is currently the subject of extensive research both basic and applied. Graphene oxide is also an important material because it allows the preparation of graphene-like water-based solutions due to the functionalization of the graphene layers. In this work are reported the properties of reduced graphene oxide (r-GO). The employed reducing agent was hydrazine and films of r-GO were deposited on glass substrates. Here we report the optical and electrical properties of r-GO films as a function of the hydrazine treatments, that is, of the reducing process. These properties were analyzed using optical transmission in the UV-Vis region and Hall effect measurements. The structural modifications due to the reducing processes were studied by means of X-ray diffraction and micro Raman spectroscopy.



[ SEM-364 ] P type impurification (doping) of  $\beta$ -GaN grown by PAMBE

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GaN is an intrinsic n type semiconductor. Even  $\alpha$ -GaN is commonly used in modern electronics. There are very few reports about p impurification in both phases, It is reported that Mg and Be are the usual dopants but information about fluxes and temperatures is not well determined.  $\beta$ -GaN and  $\beta$ -In<sub>x</sub>Ga<sub>1-x</sub>N alloys possess interesting optoelectronic properties due to the possibility of a tunable emission in the electromagnetic visible spectrum and the integration of several optoelectronic devices like Pin's and solar cells. We present in this work the Mg incorporation into  $\beta$ -GaN and its graded p type impurification in several samples. We started from the  $\beta$ -GaN growth conditions used in a PAMBE system. The p type doping was achieved as a function of the Mg flux during the  $\beta$ -GaN growth. Hall measurements of the different p type concentrations are shown in this work.  $\beta$ -GaN presents a conductivity behavior from n to insulating and finally p type . The I-V behavior of a  $\beta$ -GaN:n/  $\beta$ -GaN:p heterostructure grown in our system is also shown.



[ SEM-365 ] Properties of ZnO layers for gas sensor application

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The gas sensor most used in actuality is based in semiconductor oxides, whose electrical conductivity is greatly changed due to the reaction between the semiconductor and gases in the atmosphere. ZnO is a semiconductor that has more technological interest as gas sensors active material, due to it is excellent chemical and thermal stability. Moreover, ZnO has a good characteristic like chemical sensitivity to different adsorbed gases, amenability to doping, non-toxicity, and low cost [1,2,3,4]. In this work, ZnO layers were grown by means of vapor-solid technique. The samples were made from ZnS commercial powder (99.999% purity) as precursor. The starting powder is compacted in tablet form with dimension of 8 mm diameter and 2mm thickness. Once done it, the tablet was exposed to different treatment temperatures (800, 900 and 1000°C) at a nitrogen atmosphere. The morphological, structural, optical and electrical properties of the samples have been investigated by atomic force microscopy (AFM), X-ray diffraction (XRD), photoluminescence (PL) and Hall effect, respectively. Finally, ZnO sensing properties have been measured by monitoring the electrical resistivity in the presence of CO.

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**[ SEM-375 ] Optical and Morpho-structural Properties of ZnO Nanoparticles Synthesized from Aqueous Solutions at Low Temperature by Air-assisted-USP Method**

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High-purity, ZnO nanoparticles were synthesized at Low Temperature (500 °C) by air assisted Ultrasonic Spray Pyrolysis (USP) method, using different Zn nitrate precursor solution concentrations (0.01 M and 0.05 M). Particle structural, morphological and luminescence characteristics were studied based on X-ray diffractometry (XRD), Fourier transform infrared spectroscopy (FT-IR), transmission electron microscopy (TEM/HRTEM), UV-Vis diffuse reflectance spectra (DRS) and photoluminescence measurements (PL). XRD patterns revealed a hexagonal ZnO wurtzite-type crystalline structure with preferred orientation of (101) plane. FT-IR spectra confirmed the adsorption of surfactant molecules on the surface of ZnO nanoparticles and presence of the Zn-O bonding. TEM showed particles in shape from spherical/ellipsoidal to hexagonal, that do not change significantly with the increasing of precursor solution concentration. The size of nanoparticles was observed in the range from 16 to 23 nm. Using the Kubelka-Munk treatment on the diffuse reflectance spectra, the direct band energy has been estimated at 3.15 eV. The PL spectra mainly consist of four emission bands: (i) a strong UV emission band, (ii) a weak blue band, (iii) a blue-green band and (iv) a green-yellow band, respectively. The results proved that USP method successfully produces ZnO nanoparticles using neither dispersing agents nor post-heating treatments at high temperature, which allows rapid, continuous, single-step preparation, demonstrating a high potential for industrial applications.



**[ SEM-385 ] Preparation and characterization of TiO<sub>2</sub> based photocathodes for potential applications in photodegradation and photoregenerative cathodes in MFCS**

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TiO<sub>2</sub> has been largely known as a highly efficient photocatalyst. Some of its applications are in photodegradation of dyes, photodesnitrication in aquaculture tanks and photogenerative cathodes in microbial fuels cells between other, however due to its wide band gap these applications are limited to the UV-range. Alternatives to enhance TiO<sub>2</sub> response in the visible region such as dye and semiconductor sensitization and graphene decoration to increase the charge separation in TiO<sub>2</sub> based photocatalysts have been devised. In the present work we present the preparation of supported TiO<sub>2</sub> films by different methods such as electrophoresis and Pechini-doctor blade deposition. Semiconductor sensitization was done with chemically deposited CdS and SILAR SnS. Natural dye sensitization was done with hibiscus extract and also as graphene impregnation was done. Photocatalysts were supported onto glass substrates, conductive ZnO:Al electrodes prepared by spray pyrolysis and Pechini-doctor blade, SnO<sub>2</sub>:F commercial substrates and stainless steel disks and mesh. Structural, optical and photoresponse characterization is presented and compared and applications of interest will be discussed. Financed by SIP multidisciplinary project 20161804/0294 and 0299.



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**[ SEM-389 ] Carbon quantum dots into graphene oxide matrix prepared by low vacuum pulsed laser deposition**

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Carbon quantum dots (C-QDs) have applications ranging optoelectronics, light emitting devices and biomedical sensors between other. On the other hand, graphene oxide (GO) is an insulator material derived from chemical oxidation of graphite that presents an amount of luminescence derived from the ordered sp<sup>2</sup> dominion within the graphene basal plane. Preliminary results have shown a strong effect of film thickness on the photoluminescence spectrum of graphite films deposited by low vacuum laser ablation onto GaAs substrates, attributed to the presence of C-QDs. In the present work C-QDs are prepared by low vacuum laser ablation of a graphite target, deposited onto GO films prepared from a target made of pressed GO powders. GO was synthesized by the modified Hummers method. The laser was a pulsed Nd-YAG at 1064 nm operating in a vacuum about 10<sup>-3</sup> Torr. The effect of the number of pulses on the GO properties as well as on the morphology and luminescence of the C-QDs/GO structure was assessed. Financed by SIP 20160299.



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**[ SEM-404 ] Study of fluorescent carbon nanoparticles derived from carbon black**

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Fluorescent carbon nanoparticles (CPs) have attracted considerable research interest due to their excellent photostability, favorable biocompatibility, low toxicity, and good water solubility. They have promising applications in nanoelectronics, microelectrical devices, electrochemistry, sensor, catalysis, ultracapacitors, bioimaging, and drug delivery. We report on the preparation and characterization of carbon nanoparticles obtained from carbon black by nitric acid oxidation and refluxed at 100 °C for 8 h. This solution has particles having different sizes which were purified and separated with high speed centrifuge. The samples were characterized by X-ray diffraction, Photoluminescence, Raman, Fourier transform infrared and UV-visible spectroscopy. The CPs fluoresce under a single wavelength UV excitation. This work was supported by SIP multidisciplinary project No. 20161804/0299.



[ SEM-442 ] Photoluminescent and electrical properties of novel Nd<sup>3+</sup> doped ZnV<sub>2</sub>O<sub>6</sub> and Zn<sub>2</sub>V<sub>2</sub>O<sub>7</sub>

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Nd<sup>3+</sup> doped ZnV<sub>2</sub>O<sub>6</sub> and Zn<sub>2</sub>V<sub>2</sub>O<sub>7</sub> samples were synthesized by using melt-quenching method. X-ray diffraction patterns indicate that both samples are polycrystalline. The crystallinity was also verified by Raman scattering, from which the different vibrational modes of ZnV<sub>2</sub>O<sub>6</sub> and Zn<sub>2</sub>V<sub>2</sub>O<sub>7</sub> were detected. Electron dispersive spectroscopy (EDS) analysis shows that the Nd<sup>3+</sup> incorporation into the ZnV<sub>2</sub>O<sub>6</sub> and Zn<sub>2</sub>V<sub>2</sub>O<sub>7</sub> hosts is around 0.9 ± 0.1 and 0.2 ± 0.1 at%, respectively. The micrographs obtained by Scanning Electron Microscopy, reveal that the Nd<sup>3+</sup> doped ZnV<sub>2</sub>O<sub>6</sub> sample is predominantly composed by micro-rods, whereas the Nd<sup>3+</sup> doped Zn<sub>2</sub>V<sub>2</sub>O<sub>7</sub> one is only composed by irregular blocks. The band gap energies (E<sub>g</sub>) were calculated from the diffuse reflectance spectra by the Kubelka-Munk equation; E<sub>g</sub> values resulted to be 2.24 and 2.86 eV for the Nd<sup>3+</sup> doped ZnV<sub>2</sub>O<sub>6</sub> and Zn<sub>2</sub>V<sub>2</sub>O<sub>7</sub> samples, respectively. By means of two points dark conductivity measurements, conductivity values in the 10<sup>-4</sup>-10<sup>-6</sup> and 10<sup>-6</sup>-10<sup>-8</sup>(Ω cm)<sup>-1</sup> range for the Nd<sup>3+</sup> doped ZnV<sub>2</sub>O<sub>6</sub> and Zn<sub>2</sub>V<sub>2</sub>O<sub>7</sub> samples were measured, respectively. The conductivity as a function of the temperature indicated a semiconductor behavior. The photoluminescence spectra upon Ar<sup>+</sup> laser excitation at 488 nm, exhibited the Nd<sup>3+</sup> characteristics emissions. For instance, the Nd<sup>3+</sup> doped ZnV<sub>2</sub>O<sub>6</sub> sample displayed the Nd<sup>3+</sup> 4F<sub>5/2</sub> → 4I<sub>9/2</sub> and 4F<sub>3/2</sub> → 4I<sub>9/2</sub> emissions; while the Nd<sup>3+</sup> doped Zn<sub>2</sub>V<sub>2</sub>O<sub>7</sub> one showed the Nd<sup>3+</sup> characteristic emissions associated with the 4G<sub>7/2</sub>, 4F<sub>9/2</sub>, 4F<sub>5/2</sub> and 4F<sub>3/2</sub> → 4I<sub>9/2</sub> transitions. The lifetimes were 80 and 130 μs for the Nd<sup>3+</sup> doped ZnV<sub>2</sub>O<sub>6</sub> and Zn<sub>2</sub>V<sub>2</sub>O<sub>7</sub> samples, respectively. All these results suggest a successful synthesis of Nd<sup>3+</sup> doped zinc vanadate compounds by the melt-quenching technique.



[ SEM-462 ] Morfologic study by afm of epitaxial layers grown since inas liquid phases on substrates isoperiodic GaAs and InGaP

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In a previous work [1] it has been shown that Liquid Phase Epitaxy (LPE) can be used to grow quantum dots in systems that lie far outside the thermodynamic equilibrium when the growth process is determined by mechanisms leading to the establishment of the thermodynamic equilibrium in the liquid-solid interface [1]. The disequilibrium is caused by two factors: the first one – because of the difference in chemical compositions in liquid and solid phases, and the second one – because of the lattice mismatch between the epitaxial layer and substrate. The aim of this work is the morphological study of epitaxial layers grown by LPE on substrates with the same lattice parameter but with different compositions GaAs and InGaP from a single InAs liquid phase with liquidus temperature of 350 ° C and supersaturated for 6 ° C . Contact times between the substrate and the liquid phase were 1 , 5 and 10 sec . The samples were characterized by atomic force microscopy (AFM ) . Each area with epitaxial layers contains nanoislands whose heights and diameters, in the range of 5 to several tens of nm, depend on the growth time and the kind of substrate. We have found that the morphology of the epitaxial layers grown on GaAs is rougher compared to the epitaxial InGaP layers. We explain this phenomenon not only by the processes establishing equilibrium between liquid and solid phases during growth but also because the epitaxial layers on GaAs are formed with compositions within the area of spinodal decomposition as calculated taking into account the misfit elastic energy. Theoretical estimates show that solid solutions of GaInAs mismatched to GaAs are not stable, when their compositions are near InAs, due to the generation of elastic energy [2].

[1] Journal of Physics: Conference Series 274 (2011) 012115

[2] Estimation of the instable composition areas and its dependence on the thickness of GaInAsSb layers. grown on different substrates. Enviado a VIII Congreso Internacional de Ingeniería Física.



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**[ SEM-472 ] A Raman spectroscopy study of graphene oxide modified by reducing and heat treatment processes**

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Raman spectroscopy is one of the most powerful techniques to study carbonaceous materials. The large Raman scattering cross section presented by the allotropic forms of carbon makes this spectroscopy quite sensitive to structural changes, impurities, functionalization, and other types of modifications in carbon nanotubes, fullerenes, graphite, vitreous carbon, graphene sheets, etc. In this work is presented a detailed Raman spectroscopic study of reduced graphene oxide that underwent different treatments. For each case, different laser excitations were employed and the spectra were analyzed in terms of the frequency and relative intensity of the G, D, and 2D bands. These results were complemented with grazing-angle X-ray diffraction measurements for all the analyzed samples.



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[ SEM-498 ] Optical and structural characterization of InP quantum dots.

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The colloidal InP quantum dots (QDs) have generated great interest as potential materials to boost the development of new photoluminescent materials with many possible applications in optoelectronics, medicine, and biology due to its optical and electrical properties, the unique properties that result from quantum confinement, mainly is a blue shift of band-gap energy when the nanoparticle diameters are below a particular value that depends on the type of semiconductor. In this work, we describe the synthesis and characterization of InP QDs, these particles are produced using a one-pot method without precursor injection. The experimental conditions were as follows: 0.2 mmol of indium myristate and tris (trimethylsilyl) phosphine were mixed in 10 ml of octadecene, heating rate of 20 °C/min to an isothermal temperature of 250 °C for 2 h. The absorption spectra of InP colloids was found to be 500 nm, substantially blue-shifted in comparison with the bulk materials as the concentration of the P(TMS)<sub>3</sub> increase, this wavelength is used to determine the band gap of the InP nanoparticles (1.6 - 2.9 eV). Photoluminescence spectra of QDs have a wide band emission in the visible spectrum where peaks around 2.1 eV associated with the excitonic transition from the InP. The size and shape of the QDs were investigated using high- resolution TEM, with values between 2 and 8 nm, with spherical shapes. With these results, we can say that the average particle size increases with the increase of the molar concentration of P(TMS)<sub>3</sub> in the synthesis of InP Qds.



[ SEM-534 ] Study of low dimensional epitaxial layer growth using LPE in GaSb-GaAs system

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The growth of epitaxial layers with low dimensionality is very attractive for applications in a new generation electronic and optoelectronic devices. Modifications in the Liquid Phase Epitaxy method (LPE) allowed to obtain QDs in heterostructures in InAsSbP/GaAs[1], InAs/GaAs[2],[3], InSb/InAs[4],[5], PbSe/GaSb[6], GaP/GaAs[7], InP/GaAs[8]. QD are normally grown by Molecular Beam Epitaxy (MBE) and Metalorganic Vapour Phase Epitaxy (MOVPE). This paper reports the LPE growth of low dimensional epitaxial layers in the GaSb/GaAs system. In the first series we grew from liquid phases of Ga saturated with a GaSb substrate at 270 C for about 60 minutes. The contact between liquid phase and the substrate went from 1 to 30 seconds. Growth temperature was 264 C. In second series, liquid phases were composed by Sb saturated with GaAs for around 60 minutes at 510 C. Also, in this series, Sb masses were modified in different growths as well as the contact time from 1 to 30 seconds. Growth temperature was always 500 C. All the obtained samples were analyzed by an Atomic Force Microscope (AFM) and we were able to observe the nanostructures. The best results were obtained in samples grown at 264 C for 2 sec and 5 sec also at 500 C for 30 sec and 5 sec with the densities 323, 131,121 and 93 QD/ $\mu\text{m}^2$  with an average height of 15,8,5,10 nm and finally 5,5,8,7 nm of basis respectively.

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[ SEM-544 ] Characterization of porous silicon decorated with SnO obtained by anodizing electrochemically using HF-CH<sub>3</sub>CH<sub>2</sub>OH

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The results of characterization of metal-oxides nanoparticles into porous silicon obtained by electrolyte, HF-ethanol-Tin oxide is presented in this work. The porous silicon samples with metal oxide nanocrystal is characterized by gravimetry, UV-vis spectroscopy and photoluminescence. Besides free standing porous silicon samples with the same characteristics of porosity and thickness of 25, 50 and 100 nm were obtained. The electrochemical etching was carried out on a p-type (100) crystalline silicon wafer with 0.01-0.02Ω-cm resistivity in HF-CH<sub>3</sub>CH<sub>2</sub>OH-SnO solution, ratio 2:2:1. FTIR results show the three characteristic peaks; stretching, rocking and bending, of the silicon oxide in both type of samples, likewise in the UV-vis results of samples made with different porosity and electrolyte are not major differences[1][2][3]. The porous decorated with SnO-crystalline silicon interface is more defined with the ethanol, this result is confirmed by the fact that self-standing porous silicon sample is detached from uniform and homogeneous manner [4]. It is concluded that ethanol is a more appropriate surfactant to obtaining this material and penetrates more easily in areas where the chemical reaction leading to the formation of pores occurs, therefore the porous homogeneity is better.

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**[ SEM-557 ] A study of the structural and electronic properties of SiO<sub>2</sub>/ZnO/SiO<sub>2</sub> heterostructure deposited by reactive RF sputtering**

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The roughness associated with the sputtering deposition process has been employed to explore the possibility to produce ZnO nanoparticles embedded within a silicon oxide matrix on soda-lime glass and p-silicon substrates. Silicon dioxide and metallic Zn films were deposited employing silicon and zinc targets. An oxygen rich working plasma was employed. Oxygen content of the working plasma was modulated through argon partial pressure. A sequential deposition of SiO<sub>2</sub>/Zn/SiO<sub>2</sub> film was employed; SiO<sub>2</sub> layer was produced at 400 °C while deposition temperature of Zn layer was changed between 100 and 500 °C. Results of the chemical, structural and electronic properties are presented. Results indicated the successful production of ZnO with properties depending on deposition temperature. X-ray diffraction characterization do not shown the presence of metallic zinc. Secondary ion mass spectroscopy shown an interdiffusion of zinc throughout the SiO<sub>2</sub> matrix. TEM micrographs indicated the presence of nanoparticles. XPS shown ZnO formation under specific growth parameters. Photoluminescence emission at room temperature for samples grown on silicon substrates was not observed. Electrical transport properties are discussed on terms of deposition parameters.



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**September 26<sup>th</sup>-30<sup>th</sup> , Mazatlan, Sinaloa, México**

**[ SEM-587 ] Fabrication of CIGS/CdS solar cell. CIGS and CdS growth optimization, and its application to CIGS/CdS solar cell elaboration and performance evaluation**

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Cu(In, Ga)Se<sub>2</sub> (CIGS) and CdS thin layers were grown on Soda-Lime glass and SnO<sub>2</sub>:F substrates, respectively. A 700 nm Mo layer was deposited before the CIGS deposition. All CIGS layers were grown by thermal co-evaporation technique and CdS thin films were deposited by using chemical bath deposition (CBD) technique. CIGS samples were structurally and optically studied; all samples revealed a good polycrystalline quality with a chalcopyrite alfa-phase and Raman study showed three signals located at 184, 212 and 226 cm<sup>-1</sup>, related with A<sub>1</sub>, B<sub>2</sub> and E vibrational mode, respectively; the stoichiometry can be accurately controlled using Knudsen cells, with Ga and Cu concentrations (Ga/Ga+In = 0.25 and 0.34) and (Cu/In+Ga = 0.83, 0.88 and 0.94). CdS thin films were deposited with thicknesses around 40 nm. XRD characterization shows an hexagonal structure, while optical transmission values are around 85-90 % with a band gap value of 2.5 eV. CIGS-CdS solar cells were fabricated, showing conversion efficiencies as high as 10.9 %.

This work was supported by the National Council for Science and Technology (CONACyT), grants 47587, the Institute for Science and Technology (ICyT-DF) from Mexico City, grant PICS08-54 and CeMIE-Sol-207450 / P26. D. Jiménez-Olarte acknowledges support provided by the Energy Secretary (SENER) and CONACyT, through the SENER-CONACYT-energy sustainability postdoctoral fellowship program. All funding agencies are from Mexico.



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**[ SEM-592 ] Imaging of biased microelectronic integrated circuits using a combined modulated photoreflectance and thermoacoustic microscope**

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Thermo-reflectance microscopy has been used the last decade as a suitable for the investigation of micro- and opto- electronic devices in operating cycle <sup>[1]</sup>. It allows the determination of both heat source distribution and heat propagation properties within specific regions of micrometer devices. The technique is also useful for detecting and imaging defects. Besides the temperature field, it is also sensitive to local electric field, <sup>[2]</sup> as well as to free-carrier density, which are in their turn disturbed by defects. The noncontact and nondestructive character of the technique is one of its main advantages. It enables aging tests, which are a necessary step in the development of electronic devices, as well as progressive and repetitive treatment such as the application of voltage pulses intended to simulate electrostatic discharge damaging. As a result device scaling in microelectronics, interconnects have to tolerate higher current densities with a greater susceptibility to electro- migration failure. Electro-migration is the transport of material resulting the transfer of momentum the current conducting electrons to the metallic ions. The geometry and the microstructure of the conducting connection play an important role in electro-migration and on void formation <sup>[3]</sup>. High rate of heat generation (Joule dissipation) is associated with the high current density in such interconnects. In addition to Joule dissipation, other heat sources in interconnects originate in thermoelectric effects. Peltier effect was detected at the current modulation frequency  $f$ , while Joule effect was measured by analyzing the signal at  $2f$ . The electric current distribution is obtained by using high modulation frequencies to avoid thermal broadening. In this manner, the signal distribution is directly connected to the heat source distribution, which is, in turn, proportional to the square of current density. By lowering the modulation frequency, the heat propagation in the structure is observed in the results.

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# **THIN FILMS (THF)**

**Chairmen: Sandra Rodil (IIM-UNAM)**  
**Giovanni Ramírez (Argonne National Laboratory, USA)**

**SEM-POSTER SESSION**



**[ THF-3 ] Pressure induced morphological and directional transformations on closed space vapor transport deposited SnS thin films**

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In this work SnS thin films were deposited by employing the Closed Space Vapor Transport (CSVST) technique under air atmosphere. Single-phase, p-type, SnS thin films were synthesized by varying the final pressure in the chamber and its effect on the properties of SnS were studied. The pressure impact on the directional preferred orientation of grains is presented for the first time. A characterization analysis of different pressure values for deposited films was performed by X-ray diffraction analysis, Raman spectroscopy, scanning electron, atomic force microscopy, optical measurements, and electric characterization techniques.

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**[ THF-199 ] The relationship between the geometry of the race track and the magnetic field in a magnetron cathode**

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In magnetron sputtering, the momentum exchange between gas ions from the magnetically confined plasma and the cathode target causes the emission of atoms towards the substrate. The spatial geometry of the magnetron plasma is known to depend on the gas pressure, discharge voltage, current and magnetic field strength. The erosion racetrack formed in the target surface is determined by the spatial and directional distribution of the ions that are incident on the target, and these depend on a combination of the strength and configuration of the magnetic field. In this study we have measured the spatial variation of the magnetic field of one 2" diameter and two 4" diameter magnetron cathodes, each of different maximum magnetic field strengths, and we have compared that data with the spatial distribution of the erosion racetrack in the corresponding targets. Each magnetron had been used to deposit different materials, but similar discharge voltages and argon gas pressures had been used. The results showed that the inner and outer edges of the racetrack correspond to given value magnetic field vector. We report how the shape of the racetrack profile corresponds to the configuration of the magnetic field.



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**[ THF-206 ] Thin film design for complex micro-systems**

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Contactless energy transfer (CET) methods offer great flexibility in the design of complex micro-systems. In particular these techniques avoid electrical cables within the space limited working area of the structure. Wavelength dependent remote power supply for shape memory alloys (SMA) can demonstrate the selective addressing of a high number of micro-actuators placed in a small space. This can be realized with the help of optical thin film filters deposited by plasma techniques onto SMA based micro-actuators. The filters control the heating of laser irradiations and thereby the response of the SMA. Choice for the filter designs and materials will be discussed. Thermomechanical cycles have been performed to investigate the stability of these optical filters. Depending on the filter type there is a trade-off between wavelength selectivity and the stability. Beyond the optical filter application we will show that films deposited on SMA can provide appealing mechanical properties by generating a two ways memory effect that eliminates the load effect of a SMA element. This allows the concept of efficient wireless bistable micro-actuators.

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[ THF-207 ] Bismuth based oxide semiconductors for water treatment

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In previous works, we have shown that delta phase  $\text{Bi}_2\text{O}_3$  is a promising material for visible light photocatalysis. However, analyses of the total organic carbon demonstrate that the dye solutions are not completely mineralized. Bismuth oxide, bismuth tungsten oxide, bismuth niobium oxide, and bismuth copper oxide thin films were deposited by magnetron sputtering technique. The results indicated that it was possible to obtain  $\text{Bi}_2\text{O}_3$  films in pure cubic delta phase. Additionally we obtained bismuth based ternary composites ( $\text{Bi}_2\text{WO}_6$ ,  $\text{Bi}_5\text{Nb}_3\text{O}_{15}$ ,  $\text{Bi}_2\text{CuO}_4$ ). X-ray diffraction, scanning electron microscopy, optical transmission and spectroscopic ellipsometry were used to characterize the films. The photocatalytic activity for each one of the bismuth based films was evaluated testing the discoloration of indigo carmine dye ( $\text{C}_{16}\text{H}_8\text{N}_2\text{Na}_2\text{O}_8\text{S}_2$ ) solution (5 ppm) under UV and white light, using different values of pH (3.5, 7 y 11). The dye discoloration and the kinetic of the reaction were estimated measuring the variation of the dye absorption band as a function of the irradiation time. After calculating and comparing the reaction kinetic constants, it was concluded that using UV light and under acidic conditions, delta phase  $\text{Bi}_2\text{O}_3$  films had the best performance to decolorize the indigo carmine solution. These results suggest that bismuth based ternary composites don't present an improvement in the photocatalytic activity in comparison with delta phase  $\text{Bi}_2\text{O}_3$  films.

Acknowledgement: The research leading to these results has received funding from the European Community Seven Framework Programme (FP7-NMP-2010-EU-MEXICO) and CONACYT under grant agreements n° 263878 and 125141, respectively. Phocscleen 318977.



[ THF-285 ] Thin films of Ga<sub>2</sub>S<sub>3</sub> obtained by pulsed laser deposition

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Thin films of Ga<sub>2</sub>S<sub>3</sub> were successfully deposited on glass and silicon substrates using pulsed laser deposition (PLD) at room temperature under different pressures (0.1 mTorr, 1 mTorr, 10 mTorr, 50 mTorr and 100 mTorr) of Ar gas. A target with 99.99 % of Ga<sub>2</sub>S<sub>3</sub> was used as deposit material and Ar gas as deposit gas in PLDs general chamber. Argon pressure influence on optical, structural and morphological properties of thin films of gallium sulfide were investigated. The Thin films were characterized by Scanning Electron Microscop (SEM), Perfilometer, X-ray diffraction (XRD), Particle induced x-ray emission (PIXE) and Ultraviolet–visible spectroscopy (UV-Vis). SEM showed us the deposit rate needed to get 100 nm, and the microstructural morphology was obtained, in which grain distribution on the substrate for film formation is seen. Perfilometer helped us to comprobe that the thickness of each film was 100 nm. XRD showed us that the film obtained have an amorphous structure. PIXE was used to confirm that the stoichiometry between the target and the thin film deposited was the same. UV-Vis showed us the transmittance and absorbance and was also possible to calculate the bandgap to have the eV difference between all of the thin films.

Pulsed laser deposition technique was successful in obtaining thin films of gallium sulfide with good quality and good adhesion to the substrate.

**Keywords:** PLD, Gallium Sulfide, Thin Film

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[ THF-302 ] Deposition and Characterization of ZnS Thin Films by PLD at different temperatures

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Thin zinc sulfide (ZnS) films are successfully deposited on glass and silicon substrates using pulsed laser deposition (PLD) at room temperature under different pressures of argon gas (0.1, 1, 10, 50 and 100 mTorr) and 200 °C at 10 mTorr pressure. For depositions was used a ZnS target with a purity of 99.99%, argon gas was used in general chamber at PLD. Argon influence on optical, structural and morphological properties thin films of zinc sulphide were investigated. Thin films were characterized by SEM, AFM, XRD and UV-Vis. SEM showed us the thickness of 100 nm, and the microstructural morphology was obtained, in which grain distribution on the substrate for film formation is seen. AFM showed us roughness difference between thin films deposited at room temperature and using 200 °C temperature. XRD results indicate that the films have an amorphous structure with small crystalline at room temperature, to the deposition made at 200 °C has a higher crystallinity. UV-Vis showed us the transmittance, absorbance and was possible to calculate bandgap to have the eV difference between all of them. In this study, the film deposited at a pressure of 10 mTorr to 200 °C is optimal for better crystallinity and better microstructural system and indicates that the PLD technique provides high purity films.

Keywords: Thin film, zinc sulfide, pulsed laser deposition.

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[ THF-337 ] Study of the structure, composition and optical properties of Bi-Nb-O thin films prepared by co-sputtering

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The bismuth niobium oxides belonging to the  $\text{Bi}_2\text{O}_3 - \text{Nb}_2\text{O}_5$  pseudo-binary system show optical and electrical properties interesting for applications such as solid electrolytes, photocatalysts and high-k dielectrics. They are commonly produced by solid state reaction varying the proportion of the binary oxides in the mixtures. Fewer works have reported their synthesis as thin films; particularly when the sputtering technique has been used, the films were grown from single target having fixed composition. We proposed the synthesis of Bi-Nb-O phases by co-sputtering, starting from  $\text{Bi}_2\text{O}_3$  and Nb targets. The aim is to correlate the structure, composition and optical properties with the deposition conditions. The radio-frequency power applied to the  $\text{Bi}_2\text{O}_3$  target was fixed at 30 W, while the DC power of the Nb target was varied: 20, 30, 50, 70, 100 and 150 W. The films preparation was done under a reactive atmosphere of  $\text{Ar}:\text{O}_2$  and the substrates were silicon pieces, heated at 150°C before the deposition. The films structure was characterized by X-ray diffraction, and the morphology and composition were studied by scanning electronic microscopy and energy dispersive X-ray spectroscopy, respectively. The films resulted crystalline when the Nb target power was up to 50 W, above this value the films were amorphous. Additionally, the amorphous films were annealed at 600°C in air during 2 h, leading to structural changes showing Nb rich phases. Four crystalline structures have already being identified;  $\text{BiNbO}$  solid solution,  $\text{Bi}_3\text{NbO}_7$ ,  $\text{Bi}_5\text{Nb}_3\text{O}_{15}$ ,  $\text{BiNbO}_4$ . The optical properties were obtained by spectroscopic ellipsometry observing that the band gap ranges between 1.7 to 3.4 eV depending on the composition and structure.

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**[ THF-453 ] Spectroscopy Ellipsometry: beyond the thickness determination**

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Spectroscopic ellipsometry is an optical characterization tool to determine the thickness and optical properties of thin films. The technique is based on the measurement of the change in the polarization of the incident light as a consequence of its interaction with the reflecting surface, which can be a pure interface or a thin film. The change in polarization is represented by the change in the amplitude (Tan Psi) and phase (Delta) between perpendicular components of the incident light electric field. From these data and through the use of fitting procedures, a lot of information about the surface properties can be obtained, more than just the thickness.

Here, three examples of the use of ellipsometry will be presented; the change in the conducting properties of metal nitride nanocomposite thin films as Si was added during the deposition. The presence of an amorphous-substoichiometric NbO<sub>x</sub> phase within a film that according to the X-ray diffraction data was pure Nb<sub>2</sub>O<sub>5</sub>. Finally, the segregation of Ag into the surface when it was added to ZrO<sub>2</sub> thin films by a co-sputtering technique.



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**[ THF-501 ] Statistical analysis of the sputter parameters on the properties of ZnO thin films deposited by RF Sputtering**

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ZnO thin films were deposited on commercial glass substrates, at room temperature by RF magnetron sputtering. The effect of the sputtering variables; such as RF power, argon flow and deposition time on the structural, electrical and optical properties was studied and discussed using a full 3<sup>k</sup> experimental design. The analysis of the deposited films was studied by x-ray diffraction, 3D optical microscopy, four-point probe and UV-VIS spectroscopy. The X-ray diffraction revealed a preferential orientation along the 002 plane of the wurtzite-like crystalline structure. Depending of deposition parameters, the thickness of the films varied in the range of 23-163 nm and their resistivity varied from 10<sup>0</sup> to 10<sup>5</sup> Ω\*cm. Additionally, all films show good optical transmittance (higher to 70%) in the visible range. On the other hand, a regression linear simple was performed to predict the responses (average thickness and resistivity) in terms of the significant levels. Results suggest that the time, power-time and flow-time are predictors significant for the thickness model, while flow, flow<sup>2</sup>, power-flow and power-time are significant for the resistivity model.



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**[ THF-67 ] Blue and red Photoluminescence emission from nanocrystalline CdTe thin films grown by radio frequency sputtering.**

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Nanocrystalline CdTe thin films were grown by radio frequency sputtering on corning glass substrates. Films were characterized by X-ray diffraction (XRD), High Resolution Transmission Electron Microscopy (HR-TEM), and room temperature Photoluminescence (RT-PL). XRD results indicate samples grew in the CdTe stable cubic phase. The HR-TEM analysis corroborates the cubic nature of the films and shows the size and distribution of the CdTe nanoparticles. CdTe thin films exhibited strong blue and red RT-PL centered at 488 nm and 600 nm, respectively. These visible emissions far beyond the CdTe bandgap in bulk are explained in terms of quantum confinement of crystalline nanoparticles.



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**[ THF-91 ] Synthesis by SILAR Method of Lead Sulfide Thin Films and Evaluation as Absorber Layer for Solar Cells**

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Lead sulfide (PbS) is considered as a chalcogenide p-type semiconductor material, and it possess a main feature to absorb huge amounts of radiation inside the UV threshold. PbS has been excellent candidate for devices as photovoltaics in the research of solar cells. Based on this, the present work has employed the successive ionic layer adsorption and reaction (SILAR) method to achieve PbS thin films, which has ease of production over large areas as glass and plastic substrates and at a low temperature processing of 70°C, yielding excellent quality. During the PbS deposition, some variables in the synthesis were involved as can be molar concentration of cationic and anionic precursors, immersion times in precursors and rinsing solutions (5, 10 and 20 sec), pH, and number of cycles (20 to 120) as well as post-annealing. With these growing parameters for PbS, we investigated its high cubic structure by XRD, bandgap analysis by UV-vis, roughness and morphological quality by AFM and SEM of the absorber thin film as well as studies by stoichiometric composition by XPS and electrical behavior of the semiconductor film by Hall effect to evaluate the absorber characteristics for solar cells applications.

Keywords: Chalcogenides, semiconductor material, successive ionic layer adsorption and reaction (SILAR) method.



[ THF-93 ] Synthesis by SILAR Method of Cadmium Sulfide Thin Films and Evaluation as  
Window Layer for Solar Cells

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Cadmium sulfide (CdS) is a n-type metal chalcogenide of the group II-VI semiconductors with attractive features for optoelectronic devices as solar cells due its wide bandgap to be used as optical window. CdS has been broadly studied by different deposition methods and for several fields in science and technology. In the present work, CdS thin films have been obtained by the successive ionic layer adsorption and reaction (SILAR) method with a low bath temperature processing of 70°C being compatible from glass to plastic substrates, this method is simple and reproducible with low material consumption to cover large areas and yielding excellent quality. We study several factors in the chemical synthesis of CdS thin films by SILAR method as molar concentration, immersion times of the cationic and anionic precursors and rinsing times (5, 10 and 20 sec), pH, number of cycles (40 to 120) of immersion for the films deposition and post annealing. We did changes in the deposition parameters of the thin films by means of saving economical and energetic resources, and to optimize the hexagonal phase revealed by XRD. Bandgap, roughness and morphological characteristics were studied by UV-vis, AFM and SEM, in addition to the control of the stoichiometry and electrical characteristics by XPS and Hall effect, respectively, to evaluate the window layer for solar cells applications.

Keywords: Chalcogenides, semiconductor material, successive ionic layer adsorption and reaction (SILAR) method.



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**[ THF-148 ] Characterization of organic thin films elaborated with natural pigments of flowers  
and gelita bloom**

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In this paper the characterization of organic films prepared with natural pigments and gelita bloom is presented. The pigments were extracted from red and blue flowers. The organic thin films were prepared with different concentrations, and thickness 40 to 400 micrometers. Technique was used for the characterization of organic thin films: optical microscopy, FTIR spectroscopy, Raman spectroscopy and UV-NIR spectrometry, in which was observed the coloration of the film, the spectrum of the functional groups of the material, modes vibration frequency for the chemical and structural information, and the absorption spectrum of the material. A study of nonlinear optical properties because the natural pigments of fruits and flowers can be used in optoelectronic devices such as optical limiters or photodetectors/cameras protectors, which become very sensitive and fragile when subjected to maximum power.

Keywords: thin film organic, natural dye.



[ THF-196 ] Synthesis and characterization of In<sub>2</sub>S<sub>3</sub> microspheres grown on thin films  
elaborated by electrodeposition

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The indium sulphide (In<sub>2</sub>S<sub>3</sub>) is a metallic chalcogenide compound of type III-VI. This material has already been used as alternative buffer layer to cadmium sulphide in thin film solar cells, as it is known that cadmium is a very toxic element. There are also several reports about the use of In<sub>2</sub>S<sub>3</sub> as gas sensors. We present the advances in the elaboration and characterization of thin films of In<sub>2</sub>S<sub>3</sub> with hollow microspheres, synthesized by electrodeposition. The films were characterized by atomic force microscopy, scanning electron microscopy with electron dispersive spectroscopy, x-ray diffraction, Raman spectroscopy, and ultraviolet-visible spectroscopy. In electrical characterizations we carried out electrochemical impedance spectroscopy and we measured photoelectrochemical and photoelectric response. We elaborated films with hollow microspheres of bimodal distribution, being the bigger spheres of 5 µm in diameter. The average atomic relation S/In for the film and for the spheres was ~1.4. With x-ray diffraction we identified tetragonal and cubic structures and Raman spectroscopy revealed that the main phase was β-In<sub>2</sub>S<sub>3</sub>. The band gap calculated by optical characterization was ~2.4 eV. Characterization with Mott-Schottky plots revealed that we obtained an n-type material and it was confirmed by photoelectrochemical measurements. In addition, in photoelectric characterization we observed fast response and decay as light was turned off. The fast and stable response in electric characterizations suggest that this films could have application in solar cells and gas sensors.



[ THF-224 ] Optical Characterization of InAsSb layers on GaSb substrates by Liquid Phase Epitaxy

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The band-gap energy in semiconductor ternary alloys of the type InAs<sub>1-x</sub>Sb<sub>x</sub> can be tuned in the range 0.42-0.24 eV (2.95-5.25 microns) by adjusting the alloy stoichiometry between InAs and InSb. For applications in the detection of polycyclic aromatic hydrocarbons (PAH's), we need to develop the protocols to grow high quality InAs<sub>1-x</sub>Sb<sub>x</sub> epitaxial layers with band-gap energy values around 3.0-3.3 microns, the spectral region where the main absorption bands of the PAH's relies. Using the liquid phase epitaxy (LPE) growth technique, we have grown these InAs<sub>1-x</sub>Sb<sub>x</sub> layers on top of n-type (100). The crystalline structure and lattice mismatch between film and substrate were investigated by high-resolution X-ray diffraction (HRXRD). The surface roughness and the interface morphology of the epitaxial film-on-substrate were characterized by atomic force microscopy (AFM), scanning electron microscopy (SEM) and optical microscopy. These results show the high-purity InAs<sub>1-x</sub>Sb<sub>x</sub> epitaxial layers with mirror-like surface and rms ranges from 0.5 to 2 nm, and a sharp interface between substrate and ternary film. The optical properties of the layers were studied by low temperature photoluminescence (PL) spectroscopy. PL spectrum of the ternary film shows one radiative emission peak with narrow full width at half-maximum, which is an evidence of the good crystalline quality of the epilayer. It is worth to mention that the InAsSb films were grown on GaSb substrates for compositions of Sb with x=0.16 without introducing any intermediate composition buffer layer between the GaSb substrate and the film as reported in previous works.



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[ THF-228 ] Mathematical model that describes the behavior of stoichiometric BST solid solution

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In this work we present the behavior of stoichiometric solid solution of Barium Strontium titanate  $Ba_xSr_{1-x}TiO_3$  (BST) deposited on quartz by RF co-sputtering, described by a mathematical model to predict the optimum parameters for a film with stoichiometric controlled content (parameter “x”) when we use complementary powers on magnetrons.

BST is a ceramic material deposited as a thin film of nanometer order has a property called alternating resistive (unipolar or bipolar), when measured its electrical resistance.

This property allows BST to be considered as a promising material for non-volatile memories (1,2) 1. It is then relevant to investigate properties related to this phenomenon such as: a) potential barrier ( $E_{gap}$ ), b) surface resistivity and c) the influence of the stoichiometric content of Ba and Sr in the BST.

Samples were deposited on quartz substrates using two magnetrons with targets of  $BaTiO_3$  and  $SrTiO_3$ . The total power applied was of 120 W that were distributed between the two magnetrons as: 120-0 W, 105-15 W, 90-30 W, 75-45 W, 60-60 W, 45-75 W, 30-90 W, 15-105 W and 0-120 W, respectively. The deposition temperature was also varied: a) environment, b) 450°C, c) 550°C, d) 650°C e) 740°C.



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[ THF-251 ] Ripple formation on Ti implanted with Au ions: XPS characterization

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Ripples, dots and other periodic structures are produced on the surface of solids by ion implantation. Experimental parameters like ion species, sample temperature, fluence and incidence angle, play fundamental roles on the morphology and size of the formed structures. Well known models in the formation of surface ripples for elementary and binary materials point out possible influence of the formation of compounds as initial precursors for surface structures, while others take into account sputtering as the dominant process to generate these patterns. The aim of this work is the study of the chemical compounds on the titanium surface, after their implantation with Au ions. This work shows the results of X-ray Photoelectron Spectroscopy (XPS) analysis of Ti irradiated at room temperature, with 1.0 MeV Au ions. Titanium slices (99.6% of purity) polished with a mirror-finish were implanted in the IFUNAM Pelletron accelerator, with a fixed angle of 45°, for a total dose of  $6.4 \times 10^{16}$  ions  $\text{cm}^{-2}$ ; this is close to an *incubation fluence* for the formation of ripples. The XPS analysis was performed on a Scientific K-Alpha X-Ray Photoelectron Spectrometer, with Al K $\alpha$  monochromatic radiation ( $h\nu = 1486.6$  eV) and the Thermo Advantage software v5.95, for data acquisition. Chemical element profiles were obtained after 16 erosive stages (10 seconds each one), using a 0.5 keV argon ion gun. Intermetallic compounds, titanium and gold oxides (reported in the literature) were considered as possible species in the samples. Results show the presence and distribution of AuTi<sub>3</sub>, Au<sub>2</sub>Ti, Au<sub>2</sub>O<sub>3</sub> and some of the common native oxides of titanium: TiO<sub>2</sub>, Ti<sub>2</sub>O<sub>3</sub> and TiO.

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**[ THF-255 ] I vs V characteristics in InGaAsSb/GaSb junctions grown by Liquid Phase Epitaxy**

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pGaInAsSb/nGaSb junction with breakdown voltages as high as 38 V and abrupt breakdown characteristic have been fabricated by Liquid Phase Epitaxy. To obtain these characteristics the structures have been submitted to annealing processes just after epitaxial growth. The diffusion of dopant from the GaSb substrate towards the epitaxial layer separates the electrical junction from the epitaxial interface and produces junctions with better inverse polarization behavior. We describe here their characterization by High Resolution X-Ray Diffraction (HRXD) and Photoluminescence as well as the measured I-V properties. A microphotography of an epitaxial structure after baking is included and show clearly that the metallurgical and electrical interfaces are spatially separated. Photoluminescence spectra characterization of a typical layer will be presented and it show a clearly emission at room temperature with a bandgap around 0.57 eV. High Resolution X-Ray Diffraction rocking curves of some structures are included too and show very good reticular match to the GaSb substrate. Finally the epitaxial structures were processed by standard photolithographic technique to fabricate diodes with mesa structures. As ohmic contact Au-Zn(5%) alloyed at 350 °C was used for P type regions and Au-Ge (5%) alloyed at 350 °C for the N type regions. Finally I-V characteristics were obtained for several pGaInAsSb/nGaSb diodes.



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**[ THF-264 ] Structural and compositional studies of BiFeO<sub>3</sub> films grown by Spray Pyrolysis**

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The bismuth ferrite BiFeO<sub>3</sub> (BFO) films on glass and silicon substrates was grown by ultrasonic spray pyrolysis. The precursor consisted of bismuth and iron nitrate, dissolved in acid acetic and 2-methoxy ethanol. The temperature of growth was in the range 300 - 500 °C with posterior annealing at 550 °C. The films obtained are uniform and showed good adherence to substrate. We analyzed the elemental composition, surface morphology and crystal structure of the films as functions of concentration of precursors, type of substrate and annealing temperatures. Results by XRD indicated that BFO is the majority phase in the films with a rhombohedrally distorted structure with R3m symmetry.



[ THF-272 ] Design of calcium phosphate coating for biomedical applications using a base dual layer of TiN/TiO<sub>2</sub> to improve the substrate adherence

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The calcium phosphate coatings (CP) are widely used in the field of the orthopedic medicine and the manufacture of dental implants. These coatings have a similar composition to inorganic bone phase. These properties allow the material to react chemically with surroundings and to form bone-alike mineral layers. This way, the use of CP promotes the adhesion of the extracellular matrix forming strong links in the interface of the implant and the host tissues. Nevertheless, several methods specialized in CP manufacture have shown some limitations according to the low adherence, microcracks, high temperature phase changes and heterogeneous thickness, which have negative effects on the final material performance.

In this research, CP coatings composed on dual layer TiN/TiO<sub>2</sub> coatings, through the reactive magnetron sputtering on alloy Ti<sub>6</sub>Al<sub>4</sub>V substrates was manufactured. The manufacture of the bilayer based on TiN and TiO<sub>2</sub> was deposited using a Ti target (99% of purity) sputtering with a direct current source (DC) to 1.2kW in argon/nitrogen and argon/oxygen atmospheres, respectively. For the CP coatings deposition a hydroxyapatite (Ca<sub>10</sub>(PO<sub>4</sub>)<sub>6</sub>(OH)<sub>2</sub>) target sputtering with a radio frequency (RF) source of 13.56 MHz to 650W in controlled argon atmosphere was used. To improve the crystallinity of the calcium phosphate coating, a thermal treatment to 650°C was carried out for 3 hours. The compositional and microstructural analysis of synthesized coatings were carried out by FTIR, microraman, XRD and SEM/EDS techniques. The mechanical properties behavior of substrates were characterized by nanoindentation and scratch test. The corrosion properties of the specimens were examined by a potentiodynamic polarization test in simulated body fluid (SBF) solution at 25°C. The adherence of the CP coating on substrate increased a 50% through the use of the dual layer TiN/TiO<sub>2</sub>. The deposition of the developed TiN/TiO<sub>2</sub>/CP coating system allowed an improvement of the corrosion resistance of Ti<sub>6</sub>Al<sub>4</sub>V alloy. Consequently, the TiN/TiO<sub>2</sub> dual layer becomes an alternative for substantial reduction of failures by detachment between the CP coatings and the metallic substrates.



[ THF-287 ] Optical and Structural Characterization of n-ZnO/p-ZnO:Ag, N structure.

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Transparent n type ZnO/p type ZnO:Ag, N thin films were deposited on Si(100) substrates by DC reactive magnetron sputtering at room temperature under different nitrogen concentration in the plasma and reactive atmosphere. As precursor, a Zn target with a purity of 99.99% was used and a Ag target was used in the p-type films. Oxygen is introduced to form the ZnO, with O<sub>2</sub> gas with a purity of 99.99%. The effect of the incorporation of nitrogen and silver on the structural, electrical and optical properties was amply studied, as the changes in the composition through the n-type films and p-type films as the effect on the interface system p-type/n-type. Energy Dispersive Spectroscopy (EDXRF) confirms the presence of Zn, Ag, O, and N in the deposited film structure. XRD show the typical hexagonal structure, with the effect of the oxygen and silver on the ZnO:Ag,N component. UV-Vis and IR spectroscopy showed the behavior associated to the ZnO for IR vibrational modes and band gap, with the effect of the impurities.



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[ THF-294 ] Variation microwave irradiation time in the synthesis of films ZnO:Mn, obtained by  
MWCBD

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By Microwave Chemical Bath Deposition (MWCBD), thin films of ZnO:Mn were obtained from a solution made of zinc acetate (0.1 M) and manganese acetate (0.01M) at pH=8.0. During synthesis of the thin films, the microwave irradiation time was varied at 1, 2 and 3 minutes and the influence of this variation (temperature), on the structural, optical, morphological, and compositional properties of synthesized films was analyzed. The X-Ray Diffraction results show, the diffraction peak positions match the database 01-079-0206 hexagonal wurtzite ZnO; also it observed that with increasing temperature, Mn is incorporated in greater amounts. Photoluminescence spectra showed higher emission intensity in the UV region than in the visible region, indicating that there are a few defects in the synthesized films. Deconvolution of spectra PL, showed that there is a peak emission at 390 nm and another peak at 404 nm, associated with the presence of nanoparticles and the substitution of Zn ions by Mn ions respectively, indicating the addition of Mn to the ZnO crystal lattice. These emissions are consistent with the shifts observed in XRD and results obtained by other techniques. With the compositional analysis by EDS, the above results are corroborated, as with increasing microwave irradiation time there is a greater incorporation of Mn ion. From the above results, it was found that the optimal time for the addition of Mn is 3 minutes.



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**[ THF-311 ] Mechanical properties of aluminum oxide films grown on 416 stainless steel**

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The 416 stainless steel has structural applications and in the metalworking industry. While the oxidation resistance is an important property of this steel under conditions of use in highly oxidizing and corrosive environments for long times this material deteriorates. It is therefore necessary to protect it. Among the treatments that are being used to reduce the deterioration of the metal surface protection with ceramic coatings. In this paper results on the mechanical properties of coatings formed by aluminum oxide films we are presented. The films are grown on the surface of steel sheet of 0.3mm thickness, shaped for tensile tests of small dimensions. The films were deposited using the ultrasonic spray pyrolysis technique, obtaining source materials from solutions of aluminum nitrate dissolved in deionized water (Al-N) and aluminum acetylacetonate dissolved with dimethylformamide (Acet-Al) both deposited for 5 min and at 550 ° C. Films increase some mechanical properties; Vickers microhardness of testing sample change of 146.6 to 257.5 and 262.4 from Al-Nit and Al-Acet respectively. Differences marked are also obtained for the Young's modulus values in each case of the tensile test for low deformation rate and maximum stress. Fracture morphology in the films is analyzed in the elastic region during tensile test.



[ THF-315 ] The effect of the substrates (Si and quartz) on the properties of fluorine-doped zinc oxide prepared by sol-gel spin-coating

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Fluorine-doped zinc oxide (FZO) is a cost-effective material to replace indium-doped tin oxide (ITO) for thin film applications because of its high transmittance in the visible region and low electrical resistivity [1]. Crystalline ZnO thin films have been attempted on a variety of substrates such as c-plane sapphire, showing that the substrates have effect on the structural, morphological and electrical properties of the films [2]. Despite of their technological potential, FZO films have been barely studied due to the difficulties of demonstrating the effective fluorine doping [3]. In this study, we reported the preparation of ZnO and FZO films by sol-gel spin-coating method, we investigated the comande treatment effect of the substrate surface on the structural and microstructural properties of films. FZO films were prepared from zinc acetate dehydrate ( $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ ) and ammonium fluoride ( $\text{NH}_4\text{F}$ ) as source materials, using ethanol and isopropanol solvents and monoethanolamine ( $\text{NH}_2\text{C}_2\text{H}_4\text{OH}$ ) as stabilizer agent. The influence of fluorine doping on the electrical, structural, morphological and optical film properties was investigated. Fluorine doping concentration was controlled from 5 to 15 at%. The precursor sol was spin coated onto Si and amorphous quartz substrates at 300 rpm for 5 s and they 3000 rpm for 30 s. Subsequently, the coated substrates were pre-heated at 200 °C for 10 min and the resulting films were annealed at 600 °C in air for 2 h. We demonstrated the effective doping of ZnO by Photoluminescence, X-ray diffraction (XRD), transmittance electron microscopy (TEM) And scanning electron microscopy (SEM). SEM and XRD results revealed wurtzite-type uniform films with smooth surface morphology. No additional phases involving fluorine compounds were observed even at the high doping level (15 at% F). The fluorine doping affected the structural, optical and electronics properties of ZnO films.



[ THF-328 ] Effect of nitrogen in the properties of IZO thin films

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Transparent Indium Zinc Oxynitride thin films were deposited on Si(100) substrates by RF reactive magnetron sputtering at different substrate temperature from 25°C to 300°C. All the films were deposited in a reactive atmosphere of 5 sccm of N<sub>2</sub> and 5 sccm of Ar. Using an IZO target as precursor with a purity of 99.99%. EDS results show that the indium and zinc percentage not change systematically, On the other hand the nitrogen content change inversely in proportion with oxygen atomic percentage. X-Ray diffraction technique was used for analyzing structures of the films, The IZO:N thin films prepared were amorphous for 25°C, 100°C, and 200°C changing to polycrystalline for 300°C. The electrical resistivity, the mobility and the carrier concentrations were determined from Hall Effect measurements using the Van der Pauw configuration. The resistivity of IZO:N films decreased as the deposition temperature increased. The lowest resistivity was obtained for the film grown to 200°C and the values are  $1.02 \times 10^{-3} \Omega \cdot \text{cm}$  with a mobility of  $15.54 \text{ cm}^2/\text{V} \cdot \text{s}$ , and carrier concentration of  $2.99 \times 10^{20} \text{ cm}^{-3}$ . Uv-Vis spectroscopy was performed to determinate the absorption and transmission. All the films presented a high transparency upon 500 nm and the near infrared region. The refractive index and the extinction coefficient have been obtained from spectral ellipsometry analyses using the Classical and Adachi models, both models agree qualitatively and quantitatively, in addition with the optical parameters, the plasma frequency, the infinite dielectric function and the effective mass were obtained from the Classical dispersion model.



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**[ THF-329 ] Structural Characterization of TiN and CN coatings synthesized on glasses and silicon substrates by DC pulse magnetron sputtering**

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TiN and CN coatings were synthesized using Ti and C as target on glass and silicon substrates by DC pulsed magnetron sputtering changing the concentration of nitrogen (8-14 %) and power (200-400 W). These films were characterized by optical profilometry, X-ray diffraction, scanning electron microscopy, atomic force microscopy and Raman spectroscopy. The results showed crystalline TiN coatings like NaCl with lattice parameters of 0.424 nm and thicknesses in a range of 107 to 1033 nm. The thickness of the coatings and the lattice parameter increases with the content of nitrogen and the power. In addition, the scanning electron microscopy showed periodic arrangements in the structure of the coating that, together with the results of the X-rays diffraction confirms the obtained crystalline coating. For CN coatings, the obtained thicknesses were in a range of 1.9 to 44.86 nm. Results of atomic force microscopy and Raman spectroscopy for both coatings were obtained.



[ THF-335 ] Synthesis and structural characterization of TiAlN hard coatings deposited by magnetron sputtering

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It has been shown that adding aluminum (Al) in titanium nitride (TiN) coatings produces structural changes depending of the process and the synthesis parameters provide better characteristics to the conventional TiN coatings. This work present a study of changes occurred by incorporation of Al in these coatings which were deposited by DC pulsed magnetron sputtering on glasses and silicon substrates at temperature of the sputtering chamber. For the growth of coatings some deposition parameters were varied, such as; work pressure, power (100-200 W), the nitrogen flow into the chamber (6-10%) and the percentage of aluminum (~25 and ~50%) used in the target. The results of optical profilometry showed an average thickness of 204 and 400 nm obtained for TiAlN coatings synthesized with ~25% and ~50% of Al in the target respectively. The X-ray diffraction (XRD) test showed the presence of a crystalline phase, irrespective of the working power and the flow of nitrogen, in coatings synthesized with ~25% of Al in the target, which is confirmed by the images of the scanning electron microscopy (SEM) in which it showed a periodic arrangement. On the other hand, the phase crystalline is only present when the working power is the highest (200 W) in the case of coatings synthesized with ~50% of Al in the target. Additionally atomic force microscopy (AFM) and Raman spectroscopy tests were also realized.



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**[ THF-378 ] Structural and Functional Properties of ZnO/Si heterojunction structures fabricated by USP technique from non-aqueous solutions**

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In this work, we deal with the processing and characterization of transparent conducting ZnO thin films on p-type Silicon substrates (100) using a home-made air-assisted-USP system. The thin films from different Zn acetate precursor solution concentrations (0.1, 0.2, 0.3 and 0.4 M) were deposited at several temperatures (400, 450 and 500 °C) with thickness from ~100 to ~500 nm. The effects of precursor solution concentration, deposition time and temperature on the structural, morphological, optical, and electrical properties of ZnO films were studied by X-ray Diffraction (XRD), Atomic Force Microscopy (AFM), UV-Vis-NIR spectroscopy, and Hall Effect techniques, respectively. It has been shown that on the ZnO film surface, the preferred orientation, the average crystallite size, the electrical resistivity and the RMS surface roughness depend on the substrate temperature. The grown films have showed a good adhesion and an excellent optical transmission of about 80-95 % within the visible range (400-800 nm) and a direct band gap from 3.35 to 3.23 eV with the increase of the substrate temperature and the deposition time. All the PL spectra have exhibited a typical green-yellow emission band. Additionally photovoltaic (PV) activities of n-ZnO/p-Si heterostructures fabricated are investigated.



[ THF-382 ] Characterization of polycrystalline silicon thin films obtained by rf-sputtering deposition and crystallization of amorphous silicon

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In this work we present results regarding structural and electrical characterization of thin films polycrystalline Si (pc-Si) n-type and p-, the deposition of amorphous Si (a-Si) obtained by RF sputtering, and subsequent crystallization by rapid thermal annealing (RTA). To study the plausibility of these pc-Si films to conform single-junction pc-Si solar cells, or even hetero-junction solar cells based on crystalline Si (c-Si) and pc-Si, we deposited single p-type and n- a-Si thin films on both glass and, n-type and p- c-Si substrates, respectively. After deposition, the samples were subjected to RTA processes at temperatures of 900, 950 and 1000 °C to achieve crystallization. The a-Si films deposited onto glass were used to analyze the evolution of crystallization upon RTA annealing, through UV-vis reflectance, Raman spectroscopy, optical microscopy and X-ray diffraction measurements. Grain sizes with average sizes larger than 50 µm were observed. In turn, pc-Si samples fabricated onto c-Si substrates (i.e. c-Si/pc-Si hetero-junctions) were used to analyze the electrical characteristics of the obtained pc-Si samples by measuring their I-V curves. The observed structural and electrical characteristics evidenced that the fabricated pc-Si films can be implemented in solar cells.

Keywords: Thin film; Amorphous silicon; Polycrystalline silicon; RF sputtering; Rapid thermal Annealing; Solar cells.



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[ THF-386 ] Optical and structural analysis of p-type ZnO:Ag,N thin films

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P-type ZnO:Ag,N thin films were deposited by dual acceptor co-doping with nitrogen and silver by DC reactive magnetron co-sputtering. As precursor material were used a Zn and an Ag metallic targets with a purity of 99.999%. The films were annealed at 673 K and 723 K for one hour in nitrogen atmosphere. The electrical properties were explored by Hall Effect measurement, and the optical transmission and absorption spectra were obtained by Uv-Vis spectroscopy. The films present p-type conductivity with a low resistivity, and very high hole concentration ( $10^{19} \text{ cm}^{-3}$ ). Raman and IR spectroscopy confirmed the incorporation of Ag and N into the ZnO structure and the possible formation of  $\text{AgZn-N}_\text{O}$  pairs and/or  $\text{N}_\text{O-AgZn-N}_\text{O}$  triangles.



**[ THF-400 ] Porous silicon based UV Fabry-Perot filters: optimization of oxidation temperature.**

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This work presents an experimental study of the evolution of the spectral reflectance of Fabry-Perot Filter (FPF) produced by porous silicon multilayers (PSM), were formed by alternating high and low refraction index of porous silicon (PS) with an active layer between two Bragg reflectors, manufactured by electrochemical anodization of p+ type crystalline silicon substrates in aqueous hydrofluoric acid solutions and ethanol.

FPF were subjected to various processes of thermal oxidation, where a shift of the wavelength at high energy were observed, the oxidation time were increased from 10 minutes to 1 hour. Thermal oxidation process creating an oxidized porous silicon that induce a shift of the response of FPF from 500 nm to 340 nm in the peak minimum of the reflectance spectrum near ultraviolet (UV), a decrease of Full Width at Half Maximum (FWHM) is also observed. The shift is explained as due to the formation of silicon dioxide, which has a lower refractive index than that of silicon but slightly higher than the air. The oxidation causes changes in the optical characteristics of FPF, decrease the refractive index and the optical path, while keep the physical thickness. Characterization of FPF was performed by UV-Vis-NIR spectroscopy before and after the oxidation process and by Scanning Electron Microscope (SEM).



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[ THF-402 ] Optical, structural and electrical characterization of sol-gel spin coated M: ZnO (M= Al, Al-N y Ag-N) thin films

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In this work, we report the optical, structural and electrical characterization of M doped ZnO thin films (M= Al, Al-N and Ag-N) deposited by sol gel spin coating method. As-deposited thin films are polycrystalline and show the wurzite type structure, with an average crystallite size of ~20 nm determined by Scherrer formula. By mean of scanning electron microscopy, we observed the presence of wrinkles in M doped ZnO, and their formation is related to deposition conditions and precursors used in the synthesis. Moreover, M doped ZnO thin films exhibit a high transparence in visible region and sharp absorption at band gap energy with an optical band gaps of 3.27 eV, 3.29 eV, 3.26 eV and 3. 25 eV for undoped ZnO, Al: ZnO, (Ag, N): ZnO and (Al, N): ZnO thin films respectively. Moreover, chemical composition of M doped ZnO films were determined using energy dispersive spectroscopy. Additionally, we monitored the incorporation of Ag<sup>+</sup> ions in (Ag, N): ZnO thin films using UV-VIS spectroscopy. By mean of Hall effect measurements, we determine a “n” type conductivity for undoped and Al doped ZnO thin films. Also, “p” type conductivity was determined for (Al, N): ZnO and (Ag, N): ZnO thin film. Activation energies were calculated by mean of impedance spectroscopy data for Al: ZnO and (Al, N): ZnO.



**[ THF-420 ] Influence of precursor ball milling in enhancing the structural, morphological, optical and electrical properties of AIZO thin films**

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Aluminium and indium co-doped zinc oxide thin films (AIZO) were prepared using ultrasonic spray pyrolysis (USP) technique. The precursors of Al, In and Zn were aluminium acetyl acetate, indium acetate, and zinc acetate dihydrate respectively. Prior to the preparation of starting solution, zinc precursor was milled for an hour in a Pulverisette 7 (Fritsch) planetary ball milling equipment, using the following conditions: volume of the vessel-250 ml, ball to powder ratio-5:1 and angular speed-300 rpm. After milling, the Zn precursor (0.2M) was dissolved in a mix of acetic acid, water and methanol. Then, 1.5 at% of Al and 1.5 at% of In were added to the zinc precursor solution and depositions were carried out in USP. The physical properties such as structural, morphological, optical and electrical properties were investigated with respect to variations in the deposition times. For comparison purpose, one AIZO thin film was grown on glass substrate using unmilled zinc precursor.

The structural characteristics obtained from X-ray diffraction patterns revealed that AIZO films were grown with (002) plane preferential orientation. The morphological investigations from Scanning Electron Microscopy showed different nanostructures such as hexagons and compact elongated grains. The optical transmittance in the 300-1000nm region confirmed that AIZO films were transparent and exhibits transmittance >80%. AIZO films showed an electrical resistivity varying in the range of 2.35 –  $4.59 \times 10^{-3}$  Ohm-cm. Finally, when we compared these results with AIZO films deposited using unmilled zinc precursor; we found that ball milling the precursor has a beneficial effect in enhancing the physical properties.

In addition, AIZO thin films fabricated using ultrasonic spray pyrolysis are highly suitable for transparent conductive oxide (TCO) applications.



[ THF-458 ] Annealing Effect on the structural and morphological properties of  
Pr<sub>0.7</sub>Ca<sub>0.3</sub>MnO<sub>3</sub> Thin Films growth on substrates of SrTiO<sub>3</sub> (100)

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Manganese oxide with perovskite structure  $R_{1-x}A_xMnO_3$  (where R and A are rare or alkaline earths metallic elements) has two basal states possible: ferromagnetic metal and antiferromagnetic insulator, accompanied by orbital and / or load systems. This material is known as manganite, where  $Pr_{0.7}Ca_{0.3}MnO_3$  phase is an antiferromagnetic insulator with a loading system at zero magnetic fields.  $Pr_{0.7}Ca_{0.3}MnO_3$  films were grown in substrates  $SrTiO_3$  (100) by DC sputtering technique with 0.5, 1, 2 and 3 h deposition time. The films grown were chemical, structural, morphological, magnetic and electric characterized by Energy-dispersive X-ray spectroscopy (EDS), X-Ray Diffraction (XRD), Atomic Force Microscopy (AFM), hysteresis isotherms and I-V curves, respectively. AFM results were statistical analyzed with surface roughness parameters in AFM images as saturation roughness, lateral correlation length and the roughness coefficient. To improve surface characteristics and crystallinity (which favors the appearance of antiferromagnetic conductive phases) the samples were subjected to annealing cycles of 2h, 4h and 6h, providing a better surface with a roughness reduction in dependence of length increment. This study determined suitable conditions for growth of thin  $Pr_{0.7}Ca_{0.3}MnO_3$  films by DC sputtering system.



[ THF-459 ] Study of electrical properties on HfO<sub>2</sub> thin films growth by RF sputtering

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The hafnium oxide is a material with high dielectric constant ( $\epsilon \approx 22$ ), and a band gap nearly 5.7 eV. Furthermore, it can be deposited on silicon, permitting use in microelectronics applications and storage information (ReRAM), as possible applications for systems based on the study of resistive switching. We fabricated HfO<sub>2</sub> thin films with different thickness on Pt/TiO<sub>2</sub>/SiO<sub>2</sub>/Si, using the magnetron RF sputtering deposition technique in an oxygen atmosphere with 10<sup>-1</sup> mbar pressure and temperature substrate of 550°C. The thin films was characterized through X ray diffraction (XRD), atomic force microscopy (AFM) and voltages current curves (I-V) by the two points method with the Keithley 2450 SourceMeter. We identify the characteristic peaks of platinum and HfO<sub>2</sub> thin film for all thickness, without impurity even additional phases. A statistical analysis was performed by obtain the average roughness, correlation length, roughness coefficient and the dependence with HfO<sub>2</sub> thickness. I-V curves allow us to identify the mechanism of electrical conduction in the samples and how they relate with the roughness on the surface of the film. This work was support by the project: “Resistive switching in oxides with metal-insulator transitions for applications in random access memories. CI: 7999” UNIVALLE and Centro de Excelencia en Nuevos Materiales –CENM.



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**[ THF-460 ] Synthesis and Characterization of AZO thin films grown by balanced DC-sputtering**

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Transparent conductive oxides (TCO) combine high optical transparency with low resistivity and have been used extensively for optoelectronic devices, panel displays, solar cells, etc. Zinc based TCO materials have good optical and electrical properties comparable to the ITO. To date, ITO is the most common material used. However, ITO present some drawbacks due to the material properties including lack of chemical and thermal stability, lack of flexibility, fragility or even toxicity combined with an expensive cost. ZnO is attracting significant attention in this regard; is a natural semiconductor material with a band gap of 3.3eV and the excitón binding energy of 60 meV; and is considered as a promising candidate for next generation in optoelectronic materials. The band gap of ZnO can be tuned by different elements such as Mg, Al, Ti and Ga doping. Aluminum doped zinc oxide have attracted a lot attention because is cheap, environmental friendly, more abundant and highly stable. AZO presents n-type behavior with best optical and electronic properties than ZnO pure because Al doping increase in the carrier concentration and mobility. AZO can be prepared by different techniques as Pulsed laser deposition (PLD), chemical vapour deposition (CVD), sol-gel and magnetron sputtering methods among others. Although characterization, optical and electrical properties of the AZO have been studied. Structural and morphological proprieties of these materials have been also evaluated.

In this research, we investigated the structural, electrical and optical properties of AZO, consisting of aluminum-doped zinc oxide becomes increasingly popular as a transparent conducting oxides (TCO) replacement for tin-doped indium oxide (ITO). However, ITO is limited to use due to its high price and toxicity, so, alternate materials are required. Actually, ZnO has attracted much attention because of desirable properties such as high transmittance, non-toxicity and lower cost. There are several reports on the doped ZnO with different elements such as Al, Ti, Mg, Ga, etc and multilayer arrangements are fabricated such AZO/Metal/AZO with different metallic elements such as Au, Cu, Ag, Ni, etc.



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**[ THF-463 ] EXAFS Characterization of TiN/CrN/TiN and CrN/TiN/CrN Thin Films Hard Coatings**

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TiN/CrN/TiN and CrN/TiN/CrN hard coatings were grown by using the sputtering technique with balanced magnetron. Experiments were carried out in an INTERCOVAMEX V3 sputtering chamber equipped with three magnetrons, RF and DC power supplies. In order to determine their structural parameters, samples were characterized by HRTEM and XAS. EXAFS measurements were carried out in the SSRL synchrotron radiation source in transmission mode. TEM images shown the well defined interface among these nitride compounds. Lattice parameters were also compared with those obtained by XAS after the FEFF adjustment. In this work the chemical phase transferability was also validated. The obtained results confirm the good quality multilayers samples of nitrides formed in the sputtering process under controlled conditions.



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[ THF-470 ] Rietveld analysis of lattice parameters zinc oxide films grown by PLD

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Zinc Oxide (ZnO) is a unique material that exhibits different properties such as wide bandgap (3.37 eV), high chemical stability, piezoelectricidad, and Pyroelectricity. Another important aspect of the material is that it is inexpensive and nontoxic. These properties make it attractive to study and use photo-electronic materials or buffer layer solar cells, among others. ZnO thin films were grown by technique of "Pulse Laser Deposition" (PLD), this technique has the advantage of preserving the stoichiometry of the material [1,2,3].

The films were grown on a commercial glass, at four different pressures of oxygen (Po) and substrate temperature 573.15 K fixed. Followed, diffractograms were obtained which were refined by the Rietveld method and the results were compared. A preferential orientation plane (002) was observed. Rietveld refinement, no changes were observed in the lattice parameters for different pressures in the range 10-25 mTorr. However, coordinate value Z of Wyckoff position 4b was changed. The variation in the occupation of zinc and oxygen which indicated the conductivity is known also observed It has the material (Table 1).

**Table 1. Lattice parameter and fractional coordinates of ZnO films.**

Po (mTorr)	Lattice parameters		Fractional coordinates		
	a (Å)	c (Å)	Atoms	z	Occ
10	3.253483	5.2216351	Zn	0.00403	0.9358
			O	0.50364	1
15	3.2534162	5.213256	Zn	0.01277	0.9393
			O	0.51039	1
20	3.2501127	5.2121241	Zn	0.00365	0.9997
			O	0.50449	0.308
25	3.2530227	5.211691	Zn	0.04530	0.9087
			O	0.54512	0.8151



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**[ THF-490 ] Structural characterization of IZO films deposited by RF-Sputtering under nitrogen ambient.**

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Indium Zinc Oxide (IZO) thin films were deposited by RF-Sputtering at reactive ambient of nitrogen, at different substrate temperature (25°C -300 °C) to form Indium Zinc Oxynitrides. All these films were deposited at 15 sccm N<sub>2</sub>/5 sccm Ar. A precursor target IZO (90 % In<sub>2</sub>O<sub>3</sub>, 10% ZnO) was used. EDX confirmed the presence of Zn, In, O and N, and the percentages of each components. It is shown that nitrogen is highly incorporated in the films, replacing oxygen; percentages of Zn contents are low. XRD showed that predominantly the structure is amorphous, with some components related to short range and associated to hexagonal ZnO (100) at low temperature (25 °C) to cubic bixbyite In<sub>2</sub>O<sub>3</sub> at relatively high temperature (300 °C). Deconvolution analysis were realized to check how the structure was changing in the predominant signal and to correlate with temperature deposition process.



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**[ THF-495 ] ZnO thin films deposited by Sol-Gel from precursor solutions containing different concentrations of graphene.**

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ZnO is wide band gap semiconductor (3.3 eV) that has interesting optoelectronic properties. When doped with different materials its physical properties such as light absorption or electrical conductivity can be modified. It has been proved that dip coating sol-gel deposition technique can produce high quality ZnO thin films reducing fabrication costs as compared with more sophisticated techniques. On the other hand it is well known that graphene has unique properties such as Hall effect, high electrical conductivity, thermal conductivity, among others.

In the present work the incorporation of graphene into zinc oxide thin films deposited by dip coating sol gel is studied. Prior the deposition of the films, graphene synthesized by the modified Hummer method were added in different amounts into the sol- gel precursor solution. The films were then deposited by the dip coating technique with five immersions for each sample. The effect of annealing temperature (100-400 °C) on the properties of the ZnO-Graphene thin films was analyzed. The samples were structurally characterized by X-Ray diffraction. Optical properties of the films were determined by UV-Vis spectroscopy. Scanning electron microscopy was used to evaluate surface morphology of the films. The chemical composition was obtained by energy dispersive x-ray spectroscopy. Results are discussed as a function of annealing temperature.



[ THF-513 ] Microstructural and mechanical characterization of MoS<sub>2</sub>-CN<sub>x</sub> coatings

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Monolayers of MoS<sub>2</sub> and CN<sub>x</sub> have been identified to be good solid lubricants nevertheless it is widely known that multilayer coatings have superior properties than single layers. In this work bilayer and multilayer MoS<sub>2</sub>-CN<sub>x</sub> coatings were developed; the MoS<sub>2</sub> thin films were deposited using R.F. sputtering in a neutral atmosphere (Ar), and CN<sub>x</sub> layers were synthesized by using reactive DC sputtering and a high purity graphite target in a N<sub>2</sub> atmosphere. Both coatings have been deposited at 400°C onto Si wafer and stainless steel substrates, these were analyzed by scanning electron microscopy with electron backscatter diffraction (SEM-EBSD), wavelength dispersive spectroscopy (WDS), and X-ray diffraction (XRD) to characterize the morphology, composition, crystallographic orientation and phase identification. The microstructure analysis of the coatings was correlated with mechanical properties (elastic modulus and hardness) using nanoindentation tests.



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**[ THF-526 ] A comparison of the properties titanium nitride films produced by dc and pulsed dc magnetron sputtering**

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Transition metal nitride films deposited by physical vapor techniques, such as reactive magnetron-sputtering (RMS), are well established materials for modifying mechanical properties on the surface. Despite the wide use of TiN, it is still of special interest to improve its performance. This could be achieved through the control of the processing conditions and by the reduction of impurities such as oxygen. In this study, TiN films were deposited by dc magnetron sputtering (DCMS) and pulsed magnetron sputtering (PMS) employing a deposition power of 50 W and 250 W, respectively. The working pressure was  $\sim 5 \times 10^{-3}$  Torr and the base pressure  $\sim 5 \times 10^{-7}$  Torr. The processing conditions (substrate temperature, Ar and N flow rates, substrate bias, and discharge current) were optimized to obtain high quality TiN films. X-ray diffraction and scanning electron microscopy were used to study the microstructure. The composition was evaluated using XPS-Sputter. Mechanical properties such as hardness and adherence were evaluated using nanoindentation and pin on disc tests. The thickness was characterized through profilometry. The corrosion resistance was studied electrochemically by potentiodynamic polarization and impedance spectroscopy tests with a 3% NaCl solution, varying the test time until 168 hours.

TiN films obtained by DCMS, with 39 % atomic Ti and 36 % atomic N, showed 9 % more oxygen content as compared to TiN films obtained by PMS. This is probably due to the greater energy of atoms in PMS mode and deposition power. TiN films grown by PMS showed a stoichiometric composition, i.e., 44 % Ti and 44 % N. The potentiodynamic polarization results show better corrosion resistance of TiN films grown by PMS.



[ THF-536 ] Effect sensor and actuator piezoelectric of ZnO thin film study

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Piezoelectric materials are very important because they have been integrated into microsensors or microactuators MEMS devices. Some of these piezoelectric applications include acoustic emission, microsensors, vibration monitors, biosensors molecular recognition precision positioners, micro-pumps, motors linear steps among others. Thin films of zinc oxide (ZnO) on silicon substrates obtained under certain conditions, have the piezoelectric effect; ie, delivered voltage when deformed mechanically and reverse deform or vibrate when a altern voltage is applied. These ZnO films have been obtained by piezoelectric various mediums, such as cathodic pulberización, CVD and its variants, or by chemical means. In this paper, a simple and inexpensive way, has been used a system of ultrasonic pyrolysis spray to deposit thin pelicuas ZnO on silicon substrate and the piezoelectric effect sensor is studied (up 5mVpp) under mechanical impulse and its actuator effect applying 10 Vpp AC voltage in movies espesoes between 50 to 200 mm thick.

Keywords: ZnO, piezoelectric, sensor, actuator.



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**[ THF-553 ] Fabrication and characterization of zinc oxide double layer anti-reflective coating**

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ZnO double layer anti-reflection coatings were fabricated by spray pirolisis method, the structure consisted of a thin film of ZnO synthesized using an aqueous solution of zinc nitrate with concentration of 20 wt% recovery by a layer of ZnO nanoparticles. The zinc oxide (ZnO) nanoparticles were synthesized using an aqueous solution of zinc acetate at various concentrations from 5 to 30 wt%. The decomposition of precursor solutions was carried out at 400, 450 and 500°C under different atomizing pressures. The crystal structure and morphology of synthesized nanoparticles were characterized by X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM), which indicated that ZnO nanoparticles were of hexagonal wurtzite structure. The XRD and SEM analyses of prepared ZnO films with concentrations of 5-20 wt% showed that the crystallite size diameter of particles were in the range of 10-35 nm. The transmittance was increased from 80% to 85-92% in the visible region indicating and effective reduction of frontal reflection.



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# **TRIBOLOGY (TRB)**

**Chairman: Joaquín Oseguera Peña (ITESM)**

**[ TRB-1 ] Study of Two-Body and Three-Body Abrasive Wear of an Elastomeric Dynamic Seal Using a Micro-Abrasion Tester**

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Dynamic seals are widely used in machinery in order to retain fluid and to exclude external contaminants. One of the most recurrent failure of seals is caused by abrasive wear under prolonged sliding contact. It is produced either by partial dry running (two-body abrasion) and/or by interacting with abrasive hard fine particles which are immersed in the retained fluids generating three-body abrasive wear. This work aims to reproduce separately both types of abrasion using a micro-scale abrasion tester. For this, small samples were extracted from an Acrylonitrilebutadiene rubber (NBR) lip of an actual dynamic seal. Firstly, they were tested under dry conditions to generate two-body abrasive wear. Then, a wet/muddy environment was used to reproduce three-body abrasion. The load was selected in order to reach the actual mean contact pressure of seals against rotary shafts. Hence, a stress relaxation test of the NBR samples was carried out to find the contact pressure behavior since it corresponds to a viscoelastic behavior. Also, it was considered to the testing development. The wear scar morphologies and size changes were analyzed in detail by SEM analysis and Optical Profilometry. Finally, the experimental test was suitable to reproduce two-body and three-body abrasion of the NBR elastomer since the particular wear mechanisms and regular wear craters were generated.



[ TRB-314 ] Tribological behavior of FeB/TiN coatings on AISI-H13 formed by paste-boriding process and PDV respectively.

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In the present work obtained the mechanical and tribological properties of TiN coatings on AISI H13 steel, previously borided. It was to analyzed the layer (Fe<sub>2</sub>B) obtained for the borided process. The deposition of the thin films of TiN was carried out by unbalanced reactive magnetron sputtering of Ti whit target in a Ar+N atmosphere and using a DC power source. The microstructures of all the coatings were characterized by Optic Microscopy (OM), analyzed with Energy Dispersive X-ray Spectrometry (EDS), Scanning Electron Microscopy (SEM) and Pin on Disc. These experiments were performed to investigate the influence of sliding speeds on Tribological behaviours of the thin film with good density and adhesion on a hard layer of boride.

**Keywords:** PVD TiN coating, boriding, Friction, Wear.



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**[ TRB-339 ] Structural and mechanical properties for Nb<sub>2</sub>O<sub>5</sub> coatings as a function of Si additions**

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The Nb<sub>2</sub>O<sub>5</sub> has many polymorphs and each one has interesting properties, which has been explored for biomedical, photocatalytic and optical applications, but it is not generally used for mechanical applications due to the low hardness (8 GPa). The aim of this work is to add Silicon (Si) into the Nb<sub>2</sub>O<sub>5</sub> structure to increase the hardness through the formation of a nanostructured composite coating, similar to the nanocomposite coatings based on metal nitrides and amorphous silicon. In this work, we report the structure, mechanical properties and the friction coefficient in 3 different temperatures (298, 573 and 873K). The coatings were deposited on silicon and D2 steel substrates using a confocal-dual magnetron sputtering system. In order to vary the Si content, the power applied to the Si target (99.999%) was changed from 0 to 200W (radio frequency); meanwhile the power applied to the Nb target (99.95%) remained fixed at 400W (direct current). A reactive atmosphere of Argon/Oxygen (gas flow ratio 24/6) was used and the deposition pressure was  $6 \times 10^{-2}$  Pa. The coatings were deposited at 773K to obtain a crystallization of the coatings. The mechanical properties were obtained by nanoindentation and the friction coefficient using a pin-on-disk tribometer. The structure of the coating was characterized by X-ray diffraction; the results showed the T-Nb<sub>2</sub>O<sub>5</sub> phase in all coatings, without variations as the Si content was increased. The Si content was measured by energy dispersion X-ray spectroscopy, but only for deposition powers above 75W, varying from 1.8 to 5.8 at%. Interestingly, the hardness showed a maximum of 16 GPa for the samples deposited at 75 W in the Si target.

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[ TRB-477 ] Tribology study of stainless steel (AISI 410 and 304), titanium and titanium alloy (TiAlV) at Room Temperature (RT), 150, 300 and 450 °C.

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One of the most aggressive environments for the tribological operations is where the surfaces in contact are submitted to high temperature. This increases the wear, plastic deformation and surface oxidation. These issues reduced the parts life time and increase the spent energy in each operation, and although special materials like stainless steel and titanium alloys have been used in order to reduce the temperature effects, these have not been enough to prevent or increase the surfaces life time.

For that, this work was dedicated to study the surfaces changes produces during a sliding work operation at four temperatures on fourth different commercial materials that are used frequently for this applications. This was carried out using a Pin on Ball test configuration, using disk of stainless steel AISI 410, AISI 304, Titanium and TiAlV with Alumina ball like counterbody. The Friction Force (F.F.) was registered during the tests. It showed a decrement in its value with the temperature increment on the stainless steel and titanium surfaces while on the titanium alloy the F.F. value was almost similar for all temperatures. The wear track produces on the surfaces was characterized by optical profilometry and SEM. These presented a not homogenous wear and high plastic deformation, principally at 300 and 450 °C. The chemical changes produce on the surfaces by the tests and the wear tracks were studied using RAMAN and EDS.



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**[ TRB-546 ] A comparison of the tribological performance of an H-DLC coating deposited on  
AISI 52100 and API X65 steels**

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Carbon-based coatings are of wide interest due to their application in machine elements subjected to continuous contact where fluid lubricant films are not permitted. This paper describes the tribological performance under dry conditions of duplex layered H-DLC coating sequentially deposited by microwave excited plasma enhanced chemical vapour deposition on AISI 52100 and API X65 steels. The architecture of the coating comprised Cr, WC, and DLC (a-C:H) with a total thickness of 2.8  $\mu\text{m}$  and compressive residual stress very close to 1 GPa. Surface hardness was approximately 22 GPa and its reduced elastic modulus around 180 GPa for the H-DLC coating deposited on AISI 52100. Scratch tests indicated a well adhered coating achieving a critical load of 80 N. Whilst for the carbon steel, the critical load was around 45 N. The effect of normal load on the friction and wear behaviours were investigated with steel pins and ceramic balls sliding against the coatings under dry conditions at room temperature. The results showed that coefficient of friction of the coating decreased from 0.21 to 0.13 values with the increase in the applied loads (10 - 50 N). Poorer results for the API X65 coated surface were found though. Through Raman spectroscopy and electron microscopy it was confirmed the carbon-carbon contact, due to the tribolayer formation on the wear scars of the coating and pin.



**[ TRB-76 ] Tribological behavior of a high carbon martensitic stainless steel hardened by means of a national boriding mixture**

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This work associates the tribological behavior of an AISI 440 C untreated and treated by the boronizing powder pack method. The treatment was carried out using a national boriding mixture made with 70% of SiC, 20% of B<sub>4</sub>C and 10% of KBF<sub>4</sub>. The total layer (FeB/Fe<sub>2</sub>B) formed at the surface of (25.4 mm diameter and 5 mm thick disks) of an AISI 440 C stainless steel was about of 22.42 μm. Sliding wear tests were carried out by the pin-on-disk method. The sliding distance and the sliding speed remained constant at 1000 m and 0.1 m/s, respectively, with applied loads of 3, 5 and 7 N; a 5 mm diameter WC ball was used as counter-part. The wear scar diameter and the worn surfaces of the untreated and treated steels under dry sliding conditions were characterized by SEM and MO to understand the wear mechanisms. The coefficient of friction (CoF) was evaluated for the tribo-pair borided layer vs WC ball, as well for the untreated stainless steel vs WC ball. The CoF values for the tribo-pair borided layer vs WC ball were very similar than the values obtained for the other one.

Keywords: Pin-on-disk, Martensitic stainless steel, Boronizing, Coefficient of friction.



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**[ TRB-79 ] Tribological behavior of a martensitic stainless steel 420 ESR hardened by means of a thermochemical treatment using a national boriding mixture.**

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In this study the tribological behavior of an AISI 440 C untreated and treated by the boronizing powder pack method has been evaluated. The treatment was carried out using a national boriding mixture made with 70% of SiC, 20% of B<sub>4</sub>C and 10% of KBF<sub>4</sub>. The total layer (FeB/Fe<sub>2</sub>B) formed at the surface of (25.4 mm diameter and 5 mm thick disks) of an AISI 420 ESR stainless steel was about of 19 µm. Sliding wear tests were carried out by the pin-on-disk method. The sliding distance and the sliding speed remained constant at 1000 m and 0.1 m/s, respectively, with applied loads of 3, 5 and 7 N; a 5 mm diameter WC ball was used as counter-part. The wear scar diameter and the worn surfaces of untreated and treated steels under dry sliding conditions were characterized by SEM and MO to understand the wear mechanisms. The coefficient of friction (CoF) was evaluated for the tribo-pair borided layer vs WC ball, as well for the untreated stainless steel vs WC ball. The CoF values for the tribo-pair untreated stainless steel vs WC were slightly lower than the values obtained for the other one.

**Keywords:** Pin-on-disk, Martensitic stainless steel, Boronizing, Coefficient of friction.



**[ TRB-162 ] Effect of the chemical composition of alloys of a filler material deposited by the technique of shielded metal arc welding on the microstructure of a hardfacing and its influence in the abrasive wear resistance**

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After being deposited by the technique of shielded metal arc welding (SMAW) on a A36 steel, the final microstructure that acquires a hardfacing depends directly on the chemical composition of the alloys of a filler material. The hardfacing microstructure was characterized using optical microscopy and analysis energy dispersive spectroscopic (EDS). Different coatings were tested for abrasive wear under ASTM G65 requirements standard for comparisons. In order to characterize the wear mechanisms in coatings the Scanning Electron Microscopy (SEM) was used. The results show that high Mn coatings obtain an excellent wear resistance at low hardness. Coatings with different phases in its microstructure show variations in their hardness, however they result with a low wear resistance and little variations in mass loss. The formation of eutectic carbides in interdendritic areas with rich Cr alloys increase the hardness, although it improves wear resistance did not show uniformity in the measurement of hardness and mass loss. The carbides of type MC and  $M_7C_3$  give a high wear resistance. However the carbides MC break off from the ferritic matrix and coarser carbides  $M_2C$  and  $M_{23}C_6$  crack under high strain, being this the main form of mass loss.



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**TRB-202 ] Comparison of the tribological behavior of a tool steel: coated with AlCrN versus conventional quenching & tempering treatment, under dry sliding conditions.**

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This study compares the tribological behavior of an AISI D2 steel that has been treated by two techniques: PVD by the technique Cathodic Arc and conventional quenching and tempering treatment. Sliding wear tests were carried out by the pin-on disk method. A 5 mm diameter WC ball and 38.1 mm diameter and 5 mm thick disks were used as a tribo-pair. The worn surfaces on the disks and the ball were evaluated by SEM and MO, respectively, to understand the wear mechanisms. The coefficient of friction (CoF) for the tribo-pair AlCrN Coating and WC ball were lower than the values obtained for the other one. A similar behavior was found for the wear rate. The tribo-pair AlCrN coating and WC ball showed the best tribological performance under dry sliding conditions in comparison with the other tribo-pair.

Keywords: Pin-on-disk, tool steel, Cathodic Arc, Tempering and quenching, Coefficient of friction, Wear rate.



**[ TRB-392 ] Growth and characterization of nanocrystalline ZrN, ZrN:Nb and ZrN:Cr hard coatings**

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In this work are reported on the physical and tribological properties of reactively sputtered ZrN, ZrN:Nb and ZrN:Cr, deposited on steel sheets and crystalline (100) silicon wafers as substrates. These films were grown using a fixed power to the Zr target (80 W), but with a variable power to the dopant target (Nb or Cr). The chemical composition was obtained from EDX measurements. X-ray diffraction revealed that a two-phase nanocomposite material was formed, for the both doped cases. The nanocomposite consisted of nanocrystals of (Me, Zr)N, embedded in an amorphous matrix. The optical constants were measured using spectral ellipsometry and were simulated using a Drude-Lorentz model. The hardness and elastic modulus values were measured by nanoindentation and were correlated to the microstructure of the films.



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**[ TRB-448 ] Fabrication and wear properties of co-deposited Ni-Cr and Ni-Cr-B nanocomposites coatings**

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Ni-20wt%Cr and Ni-20wt%Cr-10wt%B nanocomposites coatings with an average thickness of 15µm were co-deposited by electrodeposition method from a nickel sulfate solution containing nanoparticles of Ni-Cr and Ni-Cr-B with an average particle size of 45 and 50 nm respectively. These alloys were synthesized by Mechanical Alloying process during 20h of milling and characterized by XRD, Scanning Electron Microscopy (SEM) and Particle Size Laser Measurement (PSLM). Physical properties of the Ni-Cr and Ni-Cr-B nanocomposites coatings and pure Ni film were assessed by SEM and wear test. The results showed that the wear behavior of Ni-Cr-B nanocomposites is slightly higher than Ni-Cr coating; however, their wear resistance are much better than the pure Ni coating. Similarly, the corrosion resistance of the Ni-Cr and Ni-Cr-B nanocomposites coatings are better than the electrodeposited Ni film.



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Cárdenas Garcia M. *BIO-431, BIO-433*  
Ceballos Mendivil Laura Guadalupe *AMC-409, RWE-466, AMC-562*  
Ceballos Sánchez Oscar *THF-526*  
Celaya Christian A. *ACS-511*  
Cervantes José Luis *ALD-509*  
Cervantes-Contreras Mario *SEM-557*  
Cervantes-Juárez E. *SEM-442, PLV-356*  
Chalé Lara Fabio Felipe *SEM-396, SEM-404, RWE-383, SEM-385*  
Chan y Díaz Enrique Josué *NSN-471*  
Charvet Stéphane *THF-206*  
Chavez Portillo Melissa *SEM-174*  
Chazaro Luis Felipe *NSN-446*  
Chávez Urbiola Iker Rodrigo *RWE-360*  
Chávez Chávez Arturo *NSN-408, NSN-478, NSN-481*  
Chávez Hernández Karina Viridiana *NSN-517*  
Chávez Ramírez Fernando *SEM-506, NSN-507*  
Chávez Urbiola Iker Rodrigo *RWE-30, AMSCR-24*  
Chávez-Galán J. *THF-378, SEM-375*  
Cheng Kai *LPM-222*  
Chico Vázquez Martha *CHM-541*  
Chinchillas Chinchillas Manuel *NSN-522*  
Chino Ulloa Alexis *CHM-292, CHM-290*  
Chipatecua-Godoy Yuri Lizbeth *THF-526, CHM-550, MEM-551*  
Cifuentes Ángel *PTP-450*  
Clemente Guadalupe Alvarado Beltrán *SEM-341*  
Cocchetti F. *LPM-578*  
Cocoletzi G H. *ACS-573*  
Colunga Saucedo Monica *NSN-512*  
Comparán Padilla Víctor Eduardo *ACS-324*  
Compeán Jasso Martha Eugenia *NSN-486*  
Compeán Jasso Victor Hugo *THF-255*  
Contreras Turrubiarres Maria Magdalena Montsserrat *ALD-363, ALD-64, ALD-348*  
Contreras Gerardo *RWE-469*  
Contreras Oscar E. *NSN-239*  
Contreras Bárbara José Roberto *AMSCR-561*  
Contreras Puente G. Contreras Puente Gerardo Silverio *RWE-173, NSN-151, RWE-524, RWE-523, RWE-193, RWE-194, RWE-418, AMC-125, NSN-528, PLV-270, RWE-100, RWE-96, SEM-146, SEM-587, PLV-518*  
Contreras-Navarrete José de Jesús *NSN-483, AMSCR-487*  
Coria Tellez Ana V. *NSN-435*  
Corona García Carlos Antonio *NSN-410*



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Corona Rivera Miguel Ángel *THF-228*  
Coronel-Hernández J. *AMC-125*  
Corral Higuera Ramón *NSN-358, NSN-522*  
Correa Pacheco Zormy Nacary *PTP-317*  
Cortazar-Martinez Orlando *CHM-550, MEM-551*  
Cortés Suárez Jorge Victor *CHM-313*  
Cortés-López Silvia *NSN-181*  
Cortes Mestizo Irving Eduardo *NSN-57, 1NSN-577, MEM-505, NSN-512, NSN-569, NSN-2*  
Cortez-Valadez Manuel *SEM-177, NSN-49, NSN-77*  
Corzo-Ruiz Susan Cristina *PTP-520*  
Cota Leal Marcos Alan *RWE-388*  
Cota-Martínez Isis María *AMC-537*  
Courel M. *RWE-580*  
Courel Piedrahita Maykel *THF-3*  
Crisóstomo Reyes Margarita Clarisaila *ACS-27*  
Crisoforo Morales *SEM-544*  
Cruz Daniel *AMC-457*  
Cruz Julio *AMC-456, THF-199, PLV-503*  
Cruz M. P. *CHM-423*  
Cruz Valeriano Edgar *BIO-545*  
Cruz Delgado Victor J. *LPM-510*  
Cruz Gandarilla Francisco *THF-3*  
Cruz Gonzalez N. *SEM-274*  
Cruz Hernández Esteban *SEM-462, ACS-22, NSN-416, NSN-542, NSN-464, NSN-571*  
Cruz Irisson Miguel *ACS-27, SEM-26, ACS-28*  
Cruz Jáuregui Ma. de la Paz *AMC-238, AMC-237*  
Cruz Orea Alfredo *PTP-319, PTP-473, PTP-317, PTP-520, PTP-491*  
Cruz Valeriano Edgar *THF-513, THF-526, AMC-238, AMC-237*  
Cruz-Delgado Víctor J. *BIO-219, LPM-253, BIO-201.*  
Cruz-Irisson Miguel *NSN-441*  
Cruz-Valeriano Edgar *MEM-551*  
Cubillas Ernesto *AMSCR-449*  
Cuerno Rodolfo *NSN-213*  
Cuevas José Luis *NSN-441*  
Cuevas García Rogelio *AMSCR-561*  
Curiel Mario *ALD-377, ALD-376, ALD-374*  
David A. King *ACS-134*  
Díaz Daniela *MEM-372*  
Díaz Tomás *NSN-369, SEM-143, SEM-40*  
Díaz Becerril Tomás Francisco *THF-400, SEM-249, THF-294, SEM-558*  
Díaz Cano Aarón Israel *NSN-68*  
Díaz Reyes Joel *NSN-570*  
Díaz Saldaña Alberto Isaac *PLV-479*  
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Díaz-Guerrero Dan Sidney *NSN-220*  
Díaz-Torres Luis Armando *AMSCR-555*  
De Anda Jessica *MEM-322, MEM-366*  
De Anda Salazar Francisco Javier *SEM-462, SEM-534, THF-255*  
De Demoure Francisco *PLV-267*  
De Jesús Cirilo Mirelly *BIO-90*  
De La Cruz Wencel *THF-526, CHM-254*  
De la Cruz-Vicencio M. G. *NSN-528*  
De La Luz Tlapaya Veronica *RWE-548*  
De la Peña-Seaman O. *NSN-208*  
De la Presa Patricia *NSN-540*  
De La Torre-Sáenz Karina Patricia *AMC-537*  
De la Vega Luis Ricardo *NSN-213*  
De La Vega Ballesteros Luis Ricardo *THF-251*  
De León Olarte Héctor Adrián *TRB-79*  
De Lucio Óscar *PLV-503*  
De Luna Bugallo Andrés *NSN-307, NSN-258, NSN-293, SEM-502, NSN-179, MEM-551*  
De Melo-Pereira Osvaldo *PLV-518*  
De Moure Flores Francisco Javier *RWE-194, RWE-173, NSN-151, RWE-193, PLV-499, RWE-492, SEM-146, AMC-125, PLV-270, RWE-96, PLV-518, RWE-100*  
De Santiago Diego *AMSCR-244*  
De Santiago Francisco *NSN-441*  
Del Ángel Cruz Sarai *TRB-76, TRB-79*  
Delgado Hernandez Alberto *BIO-515*  
Delgado-Nieblas Francisco *NSN-268*  
Denis Alcocer Eduardo *NSN-471*  
Depablos-Rivera Osmar *THF-337, THF-207, THF-337*  
Diaz Rodriguez Tania G. *ACS-326*  
Diaz Torres Elizabeth *PTP-317*  
Diaz-Torres Luis Armando *NSN-209*  
Diaz-Valdéz E. *AMC-125*  
Diego Torres Ricardo *TRB-202*  
Diliegros Godines Carolina Janani *CHM-241, PLV-412, CHM-352, CHM-223*  
Diosdado de la Peña José Ángel *RWE-286, RWE-568*  
Doñu Ruiz Marco Antonio *CHM-313*  
Domínguez David *CHM-25, CHM-25, ALD-371, ALD-377, ALD-376, ALD-374*  
Domínguez Pacheco Flavio Arturo *PTP-319*  
Domínguez Rodríguez Ricardo *TRB-162*  
Domínguez-Herrera José Ernesto *CHM-559*  
Domínguez A. *AMSCR-210*  
Domínguez D. *ALD-390, ALD-141, ALD-214*  
Dominguez David *ALD-438*  
Domínguez Miguel *NSN-205*  
Domínguez Miguel Ángel *THF-536*



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Domínguez Pacheco Arturo *PTP-31, PTP-491*  
Domratheva-Lvova Lada *AMSCR-487, NSN-483*  
Donatini Fabrice *NSN-179*  
Doré Emmanuel *THF-206*  
Dost A. V. *NSN-208*  
Douda Janna *NSN-68*  
Duarte Moller Jose Alberto *THF-463, THF-460, AMSCR-461*  
Duran Ledezma Angel Adalberto *CHM-180*  
Durán Alejandro *ALD-371*  
Dutt Ateet *RWE-62, RWE-50*  
Efimov A. Yu. *NSN-229*  
Eisenschmidt Christian *NSN-588*  
Elias Espinosa Milton Carlos *TRB-314*  
Elizalde E. A. *AMSCR-210*  
Elizalde Galindo José Trinidad *NSN-411, AMC-539*  
Elizalde Peña Eduardo Arturo *AMSCR-243, AMSCR-244, BIO-273, AMSCR-245, NSN-263*  
Elizalde-Sandoval Ricardo *MEM-54*  
Enríquez Carrejo José Luis *NSN-411*  
Enríquez Flores Christian Ivan *AMC-238, CHM-379*  
Enrichi F. *LPM-578*  
Enriquez Flores C.I. *AMC-237*  
Enriquez Izazaga Yaritza *RWE-100*  
Enriquez Carrejo Jose Luis *ALD-203, ALD-348, ALD-417* Erdemir Ali *TRB-339*  
Escalante Germán *SEM-365*  
Escalante K. *AMSCR-262*  
Escalona García M.A. *SEM-275*  
Escamilla-Herrera Lenin-Francisco *PTP-350*  
Escobar Carrasquilla Juan David *RWE-62*  
Escobar-Alarcón L. *AMSCR-243*  
Escobedo Bretado Miguel Ángel *AMC-191*  
Escobedo Morales Alejandro *NSN-440*  
Escobedo-Alcaraz Roberto *SEM-557*  
Esneider Alcalá Miguel Angel *CHM-496*  
Esparza Ponce Hilda Esperanza *THF-463*  
Esparza-González Sandra Cecilia *BIO-368*  
Esparza-Ponce Hilda Esperanza *CHM-559*  
Espino Valencia Jaime *SCD-120*  
Espinosa Guillermo *BIO-90*  
Espinosa Jose Miguel Angel *AMSCR-449*  
Espinosa Faller Francisco Javier *SEM-385*  
Espinosa Vega Leticia Ithsmel *NSN-2*  
Espinosa-Arbeláez Diego *CHM-254*  
Espinosa-Vega Leticia-Ithmel *NSN-530, NSN-577, CHM-576*  
Espinoza Cristóbal León Francisco *BIO-234*



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Espinoza Figueroa José Ángel *NSN-2, NSN-569, NSN-512, NSN-542*  
Espinoza-Figueroa J. A. *RWE-469, NSN-577, NSN-571*  
Esquivel Escalante Karen *AMSCR-245, BIO-273, AMSCR-243, AMSCR-244, AMSCR-210, NSN-263*  
Esquivel-Marin J.J. *SEM-242*  
Estrada Claudio A. *AMC-562*  
Estrada Gasca Claudio Alejandro *RWE-466*  
Estrada Moreno Carolina *SEM-344, SEM-404*  
Eugenio López Eric *NSN-2, NSN-577, NSN-571, NSN-569*  
F. Puch Ceballos *AMSCR-269*  
Falcony Guajardo Ciro *THF-287, LPM-56, LPM-257, PLV-479, THF-490, LPM-218, THF-402, LPM-259, LPM-582, LPM-581, LPM-298, THF-328, PLV-398, THF-553, LPM-584, LPM-564, LPM-585, NSN-465*  
Farías Sánchez Mario *ALD-87*  
Farías Bárbara *AMC-539*  
Farías M.H. *AMSCR-575*  
Farías Mario *ALD-376, ALD-374, ALD-371, ALD-377, ALD-439, ALD-438*  
Farías Rurik *AMC-539, AMC-538, AMC-537*  
Farfan-Cabrera Leonardo Israel *TRB-1*  
Farias Bárbara *AMC-538*  
Farias Mancilla Jose Rurik *MEM-556*  
Farias Sanchez Mario Humberto *ALD-88*  
Favergeon Jérôme *THF-206*  
Felix Quintero Héctor Aníbal *AMSCR-204*  
Fernandez Muñoz J.L. *SEM-274, SEM-275*  
Fernández Muñoz José Luis *THF-228*  
Ferrari M. *LPM-578*  
Fierro-Ruiz Cesar David *AMC-538, AMC-539, AMC-537, MEM-556*  
Figueroa López Ulises *CHM-290, TRB-76, CHM-292, TRB-79, TRB-202*  
Figueroa Vargas Ignacio Alejandro *AMSCR-468*  
Flores García Eneftali *THF-501*  
Flores Gracia José Francisco J. *NSN-205*  
Flores J. Cristina *LPM-271*  
Flores Jiménez María Cristina *AMSCR-204*  
Flores Martínez Martín *NSN-124, NSN-123, NSN-231, THF-196*  
Flores Méndez Javier *SEM-558*  
Flores Reyes Teresa *SEM-389*  
Flores S. M. *NSN-293*  
Flores Salazar Mario *NSN-258, NSN-307*  
Flores-Acosta Mario *SEM-177, NSN-49, NSN-77*  
Flores-Carrasco G. *SEM-375, THF-378, SEM-375, THF-378*  
Flores-Jiménez. J.A. *ACS-574*  
Flores-Márquez J. M. *SEM-587*  
Flores-Moreno Roberto *CHM-566*  
Flores-Ruiz Francisco J. *CHM-423*



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Fornue Francisco Leticia *SEM-404*  
Fragoso Soriano Rogelio *SEM-498, THF-224*  
Frateschi Newton Cesario *MEM-556*  
Frausto Avila Christian Mateo *CHM-379*  
Fruchart D. *NSN-208*  
Fuentes S. *NSN-229*  
Fuentes Sergio *NSN-299*  
Fuentes García Jesús Antonio *NSN-68*  
Fuentes Ramírez Rosalba *NSN-358*  
Gabriela Nieto *SEM-544*  
García Guaderrama Marco Leopoldo *SEM-186*  
Gaggero-Sager Luis Manuel *NSN-220*  
Galeazzi Reina *SEM-143, SEM-40*  
Galeazzi Isasmendi Reina *SEM-249, THF-294*  
Galicía Hernández José Mario *ACS-189*  
Galindo Hugo *NSN-277, NSN-279*  
Galindo-Velázquez Christian *LPM-253*  
Gallardo Hernández Salvador *RWE-194*  
Gallardo Sánchez Manuel *NSN-522*  
Gallardo-Hernandez Ezequiel Alberto *TRB-1*  
Galvez Lopez Maria Fernanda *SEM-341*  
García Macedo J. Antonio *TRB-202*  
García Salgado Godofredo *SEM-437*  
Garcés-Medina Emmanuel *PLV-503*  
García E. *PLV-499*  
García Ernesto *TRB-477*  
García Godofredo *SEM-143*  
García Jose Alejandro *NSN-369*  
García M. *LPM-582*  
García Miguel Ángel *THF-251*  
García Amaya Iveth Viridiana *AMC-349*  
García Cervantes Ana Laura *CHM-292, CHM-290*  
García Hipólito Manuel *AMSCR-204, NSN-184, NSN-185, LPM-218, LPM-581, LPM-257, LPM-259*  
García Jaramillo E. *PLV-529*  
García Jaramillo Efraín *TRB-489*  
García Macedo J. Antonio *TRB-79, TRB-76, CHM-290, CHM-292*  
García Rocha Miguel *NSN-403, NSN-397, CHM-180*  
García Salgado Godofredo *THF-294, SCD-347, THF-400, SEM-40*  
García Sánchez Mario Fidel *THF-3*  
García Vázquez Valentín *NSN-367*  
García-Casillas Perla Elvia *ALD-348*  
García-Cortés Elvis Anyel *MEM-445*  
García-García A. *NSN-586*  
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García-Rodríguez S. P. *AMSCR-221*  
García-Ruiz Diana Litzajaya *NSN-483, AMSCR-487*  
García-Sánchez M. F. *RWE-580*  
García-Sotelo Alejandra *SEM-557*  
García Jose Alejandro *THF-382*  
García Miguel Angel *NSN-213*  
García Alamilla Ricardo *SEM-385*  
García Martínez Amira María *RWE-474*  
García Pacheco Georgina *MEM-357*  
García Sánchez Miguel Angel *AMSCR-406*  
García-Cerda Luis Alfonso *AMC-297, THF-93, THF-91*  
García-Lozano Rodolfo *SEM-195*  
García - Ramírez Eliseo *ALD-415*  
García Miranda Maribel *THF-536*  
Garibay Alvarado Jesús Alberto *BIO-234*  
Garrafa Gálvez Horacio Edgardo *NSN-304*  
Gatin Andrey *NSN-13*  
Gaxiola Mejía Eliena *AMSCR-101*  
Gazga-Gurrión Irving *SEM-323*  
Gómez Aguilar Ramón *MEM-33*  
Gómez de Prieto María Elena *THF-459, THF-458*  
Gómez González Luis Andres *RWE-62*  
Gómez Guzmán Oscar *THF-329, THF-335*  
Gómez Pavón Luz del Carmen *NSN-507, SEM-506*  
Gómez Romero Ricardo *RWE-548, RWE-212*  
Gómez Rosales R. *THF-386*  
Gómez Rosas G. *NSN-478, NSN-476, NSN-481*  
Gómez Soberón José Manuel *BIO-391*  
Gómez Vargas Oscar A. *TRB-546*  
Gómez Vargas Oscar Armando *TRB-314*  
Gómez-Aguilar Ramón *BIO-15*  
Gómez-Esparza Cynthia Deisy *AMC-361*  
Gómez-Rosas G. *PLV-493, PLV-356, PLV-452, RWE-492, PLV-499, PLV-250*  
Gómez Vargas Oscar Armando *TRB-202*  
Gervacio Arciniega José Juan *AMC-238, AMC-237*  
Gervacio-Arciniega J. J. *CHM-423*  
Gildo Ortiz Lorenzo *NSN-231*  
Giménez G.L. *LPM-584*  
Godofredo García *SEM-544*  
Golzarri José Ignacio *BIO-90*  
Gómez Guzman Oscar *CHM-434*  
Gómez Mancilla José Carlos *NSN-239*  
Gomez-Esparza Cynthia Deisy *AMC-359*  
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González Edgar *MEM-322*  
González L.A *SEM-242*  
González María Guadalupe *NSN-384*  
González de la Cruz Gerardo *THF-224, NSN-211*  
González Domínguez José Luis *PTP-491*  
González García Pedro *THF-501*  
González Hernández Jesús *THF-501*  
González Jiménez Rodrigo Rodolfo *NSN-205*  
González - Olgún C. E. *RWE-108*  
González -Torres Cristian Alfonso *AMSCR-236*  
González Edgar *MEM-366*  
González M. A. *NSN-231*  
González Albarrán Marco Aurelio *SEM-186*  
González Flores Edgar *MEM-276*  
González López Luis A *RWE-418*  
González Lozano María Azucena *AMC-191*  
González Morones Pablo *NSN-399, LPM-510*  
González Olgún C. E. *RWE-109*  
González Tovar Luis Daniel *NSN-124, NSN-123*  
González Vizcarra Benjamin *BIO-515*  
González-López L. A. *SEM-587*  
González-Meza Gómez-Farías Cristobal *NSN-308*  
González-Morones Pablo *LPM-253*  
González-Rivera Y. A. *SEM-442*  
Gorbatchev Andrei Yu *NSN-512, NSN-577, SEM-462, SEM-534*  
Granada Daladier *SEM-498*  
Granados-Martínez Francisco Gabriel *NSN-483, AMSCR-487*  
Grishin Maksim *NSN-13*  
Guarneros Cesia *THF-382, SEM-365, NSN-369*  
Guarneros Aguilar Cesia *SEM-344, SEM-404*  
Guerra Yanín *SCD-309*  
Guerra Valdéz Wendy *SEM-389*  
Guerrero de León Jesús Alonso *PLV-250*  
Guillén Bonilla Alex *NSN-123, AMSCR-182, NSN-124, NSN-517*  
Guillén Bonilla Héctor *NSN-231, NSN-123, NSN-517, AMSCR-182, NSN-124*  
Guillén Bonilla José Trinidad *NSN-123, NSN-517, NSN-124, NSN-231*  
Guillén-Cervantes A. *PLV-270, RWE-96, NSN-151, THF-67*  
Guillen Bonilla Alex *NSN-231*  
Guillen Valdez Valeria *BIO-215*  
Guirado-López Ricardo *NSN-268, NSN-530*  
Gurevich Yuri *SEM-61, RWE-57, SEM-178*  
Gutiérrez M.P. *ACS-574*  
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Gutiérrez Z-B K. *NSN-528*  
Gutiérrez-García Carmen Judith *AMSCR-487, NSN-483*  
Gutiérrez-Juárez Gerardo *PTP-225, PTP-350*  
Gutiérrez Z-B Karla *RWE-100*  
Gutiérrez Zayas Bazán Karla *RWE-193, RWE-194, RWE-418*  
Guzmán C. *AMSCR-210, AMSCR-262, AMSCR-243*  
Guzmán Carlos *AMSCR-244*  
Guzmán José *SCD-309*  
Guzmán J. *LPM-582*  
Guzmán J.C. *LPM-582*  
Guzmán Martínez Carlos *BIO-273, AMSCR-245*  
Guzmán-Mendoza J. *LPM-581*  
Guzmán-Olguín J. C. *LPM-581*  
H'Mok H'Linh *RWE-217, ACS-227, AMC-238*  
H. Tiznado H. *CHM-25*  
Hernández Utrera Oscar *CHM-241*  
Heiras Aguirre Jesús Leonardo *SEM-451*  
Henrique Sousa Marcelo *BIO-332, BIO-589*  
Hernández C. A. *RWE-469*  
Hernández Carlos Alberto *RWE-527*  
Hernández Natiely *MEM-372*  
Hernández R. *AMSCR-210*  
Hernández Aguilar Claudia *PTP-31*  
Hernández Carabali Luz Amparo *AMSCR-200*  
Hernández Cocolletzi G. *ACS-572*  
Hernández Riesco Cedric Omar *SCD-345*  
Hernández Wong Joel *AMSCR-198*  
Hernández-Aguilar Claudia *PTP-491*  
Hernández-Arriaga Heber *ALD-415*  
Hernández-Balbuena Daniel *NSN-303*  
Hernández-Cedillo Lucero Mescli *NSN-308*  
Hernández-Como Norberto *MEM-54, SEM-195*  
Hernández-Cuevas Francisco Javier *SEM-195, MEM-54*  
Hernández-Paz Juan Francisco *AMC-538*  
Hernández-Rosas J. *NSN-528*  
Hernández Pitalua Daniel *RWE-524*  
Hernández Armando *MEM-372, RWE-355*  
Hernández José Manuel *LPM-271*  
Hernández R. *AMSCR-243*  
Hernández Roberto T. *SCD-309, THF-311*  
Hernández Aguilar Claudia *PTP-319*  
Hernández Alcántara José Manuel *AMSCR-204*  
Hernández Arriaga Heber *ALD-235*  
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Hernández Chávez Macaria *AMSCR-561*  
Hernández Cocoltzi Gregorio *ACS-380, ACS-324, ACS-444, ACS-189*  
Hernández de la Luz A.D. *NSN-455*  
Hernández Hernández Ernesto *LPM-510*  
Hernández Landaverde Martín *SEM-472, SEM-362*  
Hernández Martínez Luis *MEM-488*  
Hernández Montes Javier Edmundo *RWE-193*  
Hernández Rangel Rafael *AMSCR-245*  
Hernández Rodríguez Eric Noé *RWE-568, RWE-286*  
Hernández Sánchez Enrique *CHM-290, CHM-292*  
Hernández V. M. *NSN-293*  
Hernández Vázquez Miguel Ángel *NSN-307, NSN-258*  
Hernández Wong Joel *SEM-289*  
Hernández-Arana Andrés *AMSCR-266*  
Hernández-Arriaga Heber *ALD-348*  
Hernández-Arteaga Aida *NSN-268*  
Hernández-Flores Omar Augusto *MEM-445*  
Hernández-Gordillo Armin *AMSCR-266*  
Hernández-Gutiérrez C. A. *NSN-528*  
Hernández-Hernández A. *PLV-543, SEM-557*  
Hernández-Hernández Ernesto *LPM-253*  
Hernández-Hernández Luis A. *PLV-543, NSN-528, PLV-518*  
Hernández-Landaverde M. A. *NSN-563*  
Hernández-Marquez Jesus Alfredo *ALD-203, ALD-417, ALD-348*  
Hernández-Ochoa Manuel Alfredo *SEM-177*  
Hernández-Paz Juan Francisco *AMC-539*  
Hernández-Rodríguez Eric *RWE-340*  
Hernández-Rosas Francisco *PTP-520*  
Hernández-Rosas Juan *PTP-520*  
Hernández-Utrera Oscar *CHM-223, CHM-352, PLV-412*  
Herrera Manuel *NSN-424*  
Herrera Gomez Alberto *THF-526*  
Herrera Pérez Monserrat Alejandra *BIO-433, BIO-431*  
Herrera Perez Jose Luis *SEM-498*  
Herrera-Gomez Alberto *MEM-551, CHM-550, CHM-514*  
Higadera Andrea *RWE-327*  
Higuera Valenzuela Hiram Jesús *LPM-381*  
Horacio Edgardo Garrafa Gálvez *SEM-341*  
Huang Jiaming *THF-495, RWE-492, PLV-493*  
Huerta E. F. *LPM-298*  
Huipé-Nava Ezequiel *AMSCR-487, NSN-483*  
Hurtado Castañeda Delia *SEM-498*  
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Hurtado-Lopez Gilberto *BIO-201*  
Ievlev A. V. *NSN-208*  
Iribarren Alfonso Augusto *NSN-471*  
Isiwata-Rivera Alma Patricia *AMC-297*  
Ivanov Tsonchev Rumen *PTP-31, PTP-32*  
J. Guzmán Mendoza *AMSCR-269*  
J.J. Ortega Sigala *AMSCR-269*  
Jaime Fonseca Mónica Rosalía *CHM-321, CHM-541*  
Jaime-Acuña Oscar *NSN-299*  
Janicki Lukasz *LPM-222*  
Jaque Francisco *LPM-271*  
Jaramillo-Quintero Oscar Andrés *RWE-176*  
Jasso Ramos Luis *NSN-522*  
Jasso-Jasso M.F. *AMSCR-269*  
Jayaraman Vinoth Kumar *THF-420*  
Jiménez Barrera Rosa M. *LPM-510*  
Jiménez Olarte Daniel *THF-3, RWE-194*  
Jiménez Vivanco María del Rayo *THF-400*  
Jiménez-Barrera Rosa *LPM-253*  
Jiménez-Olarte D. *SEM-587*  
Jiménez-Sandoval S. J. *NSN-563, SEM-323, SEM-362, PLV-529, SEM-472*  
Jiménez Flores Yolanda *AMSCR-198, BIO-284*  
Jiménez Pérez José Luis *PTP-317*  
Juanico Lorán José Antonio *CHM-313*  
Juárez Héctor *THF-382, SEM-365, NSN-369*  
Juárez García José Manuel *THF-513, CHM-434*  
Juárez Santiesteban Héctor *SEM-558*  
Juarez Santiesteban Hector *ACS-326, SEM-174*  
Juárez Ignacio *MEM-372*  
Juárez García José Manuel *THF-329, THF-335*  
Juárez Gracia Antonio Gustavo *CHM-321*  
Juárez López Guillermo *NSN-465*  
Juárez Raúl *SEM-544*  
Juerez Santiesteban Héctor *SEM-190*  
Kamaraj Sathish-Kumar *RWE-383, SEM-385*  
Kar Swastik *SEM-502*  
Kharisov Boris *NSN-282, NSN-280, NSN-21*  
Kharissova Oxana *NSN-282, NSN-279, NSN-277, NSN-280, NSN-283, NSN-281*  
Klyukin K. A. *NSN-208*  
Koh Marco *RWE-395*  
Kolchenro Nikolay *NSN-13*  
Konovalenko Anatolii *NSN-331*  
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Kostromin A. *NSN-330*  
Krotova Irina *NSN-29*  
Krylova E. A. *NSN-229*  
Kudrawiec Robert *LPM-222*  
Kudriavtsev Yuri *RWE-527, RWE-469*  
Kudur Jayaprakash Gururaj *CHM-566*  
Kumar Tiwari Dharendra *NSN-435, NSN-296*  
Kuwabara Yasuhiro Matsumoto *RWE-50*  
Lamarque Frédéric *THF-206*  
Lara Castro René Homero *AMC-191*  
Lara Rodríguez Gabriel Ángel *AMSCR-468*  
Lartundo Rojas Luis *SEM-333, THF-251*  
Lashkevych Igor *SEM-288*  
López Eric *NSN-512*  
López Javier *ALD-377, ALD-376, ALD-374, ALD-371*  
López Cruz Elias *NSN-410*  
López Lazcano Carlos Augusto *THF-302*  
López López Máximo *RWE-527, NSN-416, NSN-464, PLV-140, PLV-518, NSN-571, NSN-528, RWE-469*  
López Luna Edgar *ALD-363, ALD-235*  
López Perrusquia Noe *CHM-313*  
López Urías Florentino *AMSCR-182*  
López-Fuentes Mirna *BIO-433, BIO-431*  
López-Luna Edgar *ALD-348, ALD-417*  
López-Medina K. Pamela *BIO-15*  
León Sarabia Eleazar *THF-513*  
León Cruz Elizabeth *BIO-431*  
León Sarabia E. *AMC-237, AMC-238*  
León Valiente Xairo *SEM-190*  
León- Cruz Elizabeth *BIO-433*  
León Bonilla Hugo Amilcar *RWE-523*  
Ledesma-Molinero M. *SEM-146*  
Lee Cárdenas Walther Eduardo *PLV-318, PLV-413*  
León Bonilla Ambrosio *RWE-523*  
León Sarabia Eleazar *BIO-545*  
León-Sarabia Eleazar *CHM-550*  
Leonardo Morales de la Garza *ACS-134*  
Leos-Mendez Hugo *ALD-417, ALD-348*  
Lesly-Jiménez G. *LPM-585*  
Leyva Hernández Viviana *TRB-448*  
Leyva Porras César *SEM-186*  
Licea Jiménez Liliana *NSN-494, CHM-496, RWE-504*  
Lima-García Rosa María *NSN-308*  
Limón Luna Cesar Adrian *NSN-435*



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Linares Aranda Mónico *MEM-488*  
Liu Xingxing *THF-206*  
Lizardi Vega Marina *CHM-313*  
Loeza-Poot Mariely *RWE-340*  
López López Lluvia *NSN-399*  
Lopera Wilson *THF-459*  
Lopera Muñoz Wilson *THF-458*  
López Catalina *CHM-352*  
López J. *ALD-214*  
López Javier *CHM-352*  
López Gamboa Genaro *PTP-317*  
López Lazcano Carlos Augusto *THF-285*  
López Luna Edgar *SEM-364, ALD-64, ALD-415*  
López Medina Javier Alonso *ALD-87, ALD-88, ALD-439, ALD-438*  
Lopez-Gomez Carlos Alberto *MEM-54*  
Lozada Morales Rosendo *AMC-349, LPM-535, SEM-442*  
Lozada-Morales R. L. *PLV-356*  
Luebbert Larios Octavio *ALD-261*  
Lugo Jesus *SEM-143*  
Luna Arias Juan Pedro *SEM-498*  
Luna Bárcenas Gabriel *BIO-273*  
Luna Contreras Blanca Elizabeth *ACS-380*  
Luna Guzmán José Antonio *LPM-218*  
Luna López José Alberto *NSN-440, NSN-205*  
Luna-Barcenas Gabriel *NSN-53*  
Luna-Flores Adan *AMC-457*  
Luque Morales Priscy Alfredo *NSN-304*  
Macías Aguilar Carlos Gerardo *PLV-479*  
Machorro Roberto *ALD-377, ALD-439, ALD-371, ALD-438, ALD-376, ALD-88, ALD-374, ALD-87*  
Machorro-Mejía Roberto *CHM-241, PLV-318, PLV-413, CHM-223, CHM-352, PLV-412*  
Madrigal Carrillo Karina Gabriela *ACS-27*  
Maldonado Orozco María Cristina *AMC-359, AMC-361*  
Mandujano Ruíz Araceli *TRB-448*  
Mani González Pierre Giovanni *ALD-64, ALD-348, ALD-417, ALD-363, NSN-540, ALD-415, ALD-203*  
Mantilla Ramírez María de los Ángeles *SEM-333, AMSCR-198, AMSCR-200*  
Manzanarez Eric *RWE-466*  
Marín Ernesto *PTP-450*  
Marín Moares Ernesto *PTP-31, PTP-32, CHM-321*  
Marín Romero José Alfredo *THF-470, THF-470*  
Marco A. García-Lobato *AMC-401*  
Mardegan M. *LPM-578*  
Marinez Suarez Frolan *CHM-434*  
Mariscal Antonio *LPM-525*  
Mariscal Becerra Luis *LPM-56*



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Martín A. Hernández-Landaverde *AMC-401*  
Martínez Jesús *ALD-376, ALD-374, ALD-377, RWE-355*  
Martínez Aguilar E. *AMC-238, ACS-227, RWE-217*  
Martínez Castañón Gabriel Alejandro *NSN-486, BIO-63, BIO-192, BIO-475*  
Martínez Chávez Luis Alejandro *AMSCR-245*  
Martínez Falomir Gibrán Guadalupe *THF-302*  
Martínez Guerra Eduardo *ALD-235, ALD-509, ALD-508*  
Martínez Hernández Ana Laura *THF-335*  
Martínez Juárez Javier *THF-255, NSN-455*  
Martínez Luevanos Antonia *AMSCR-393*  
Martínez Martínez Rafael *NSN-465*  
Martínez-Benítez A. *RWE-492*  
Martínez-Colunga Juan G. *BIO-219 BIO-201*  
Martínez-Luévanos A. *AMSCR-197*  
Martínez-Merlín I. *LPM-581*  
Martínez-Sánchez Roberto *AMC-359*  
Martínez-Sánchez Mitzy Victoria *RWE-194*  
Martínez-Sánchez Roberto *AMC-361*  
Martínez A. *LPM-582*  
Martínez Jesús *ALD-438*  
Martínez Falomir Gibran Guadalupe *THF-285*  
Martínez Gil Miguel *RWE-388*  
Martínez Guerra Eduardo *ALD-261*  
Martínez Juárez Javier *NSN-205*  
Martínez Maldonado Lorena *AMSCR-55*  
Martínez Pastor Juan *THF-402*  
Martínez-Guerra Eduardo *ALD-415, THF-93*  
Martínez-Landeros Víctor Hugo *THF-91, THF-93*  
Martucci A. *LPM-578*  
Mata Guadarrama Fernando *CHM-531*  
Mata-Padilla José *BIO-201, BIO-219*  
Mathew Xavier *THF-382*  
Mauricio Pacio *SEM-544*  
Mayén-Hernández S.A. *PLV-270, RWE-96*  
Mayoral García Álvaro *ALD-508*  
Mazón Montijo Dalia Alejandra *AMSCR-353, SCD-187*  
Márquez Béltran César *BIO-332*  
Márquez Herrera Alfredo *RWE-286, RWE-568, THF-228*  
Méndez V. H. *NSN-571*  
Méndez Camacho Reyna *ACS-22, NSN-416, NSN-464, NSN-542*  
Méndez García Victor Hugo *MEM-505, PLV-346, THF-386, SEM-336, NSN-342, PLV-398, NSN-569, NSN-2, NSN-416, NSN-464, NSN-512, NSN-577*  
Medina Juan Carlos *THF-207*  
Medina-Llamas V.L. *AMSCR-533*



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Mejía Silva Isarel *ALD-261*  
Meléndez-Lira Miguel Angel *PLV-543, SEM-557, SCD-230*  
Meléndrez Manuel *ALD-508*  
Mendez V. H. *RWE-469*  
Mendez-Garcia Víctor Hugo *CHM-576*  
Mendez-Gonzalez María Magdalena *NSN-384, NSN-403, NSN-397*  
Mendivil Escalante José Miguel *BIO-391*  
Mendoza Salvador *MEM-366, MEM-322*  
Mendoza Acevedo Salvador *MEM-357*  
Mendoza Álvarez Julio G. *SEM-498*  
Mendoza De la Rosa Luis Alberto *AMC-401*  
Mendoza Herrera Teodulo *TRB-314*  
Mendoza López Doroteo *NSN-312*  
Mendoza Mendoza Ingrid Marcela *CHM-434, THF-329*  
Mendoza Pérez Rogelio *RWE-418, RWE-524, RWE-523*  
Mendoza Vázquez Ignacio *CHM-290, CHM-292*  
Mendoza-Alvarez Julio Gregorio *THF-224*  
Mendoza-Galván Arturo *SEM-323*  
Mendoza-Gonzalez Zelene Patrocinio *NSN-248*  
Mendoza-Guzman J. *AMSCR-260*  
Mendoza-Herrera M. C. *BIO-431, BIO-433*  
Mendoza-Mendoza Esmeralda *AMC-297*  
Mendoza-Pérez R. *SEM-587*  
Meraz Dávila Susana *RWE-360*  
Mercado C. *NSN-577*  
Mercado Christian A. *NSN-512, NSN-569, MEM-505*  
Mercado Ornelas Christian Alejandro *AMSCR-316, NSN-571*  
Mestres Lourdes *ACS-227*  
Meza Juan Manuel *THF-272*  
Meza-Rocha Abraham *LPM-535*  
Meza-Rochab A.N. *SEM-442*  
Michournyi Viatcheslav Andreevich *SEM-534*  
Milosevic O. *THF-378, SEM-375*  
Mimila-Arroyo Jaime *RWE-216*  
Mirabal-Rojas Roberto *TRB-339, THF-453, TRB-339*  
Miranda Álvaro *NSN-441*  
Miranda Duran Alvaro *ACS-28*  
Miranda Meléndez Paulina Guadalupe *BIO-475*  
Mis-Fernández Ricardo *RWE-395, RWE-340, RWE-325, RWE-327*  
Mishurnyi Viatcheslav Andreevich *THF-255, SEM-462*  
Misiewicz Jan *LPM-222*  
Moggio Ivanna *LPM-510, LPM-253*  
Molar-Velázquez Gabriela *MEM-551*  
Molina Valdovinos Sergio *SEM-178*



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Molina-Duarte J. *NSN-530*  
Molina-Reyes Joel *ALD-415*  
Molina-Valdovinos Sergio *NSN-226*  
Monarca Serrano José Antonio *BIO-90*  
Monjarás Ávila Ana Josefina *BIO-192*  
Monroy Betsabeé Marel *RWE-62*  
Montejano Carrizales Juan Martín *NSN-12*  
Montemayor Sagrario M. *AMSCR-221, AMSCR-197*  
Montes E. *LPM-581*  
Montiel González Zeuz *SCD-188, ALD-233, AMSCR-353, THF-526, CHM-550*  
Mora Rodrigo *SEM-365*  
Mora Ochoa Fermín *SEM-558*  
Mora-Seró Iván *RWE-176*  
Morachis Galindo Diego *ACS-419*  
Morale Mendoza Javier Eliel *AMSCR-461*  
Morales Arturo *RWE-527*  
Morales Crisóforo *SEM-40, SCD-347, SEM-143*  
Morales Manuel *AMSCR-221*  
Morales Nicolás *NSN-507, SEM-506*  
Morales Acevedo Arturo *SEM-506, NSN-507, RWE-418*  
Morales de la Garza L. *ACS-573*  
Morales Garcia Sandra Soledad *RWE-383*  
MORALES HERNÁNDEZ JORGE *TRB-448*  
Morales Mendoza Javier Eliel *THF-463, THF-460*  
Morales Morales Francisco *THF-400*  
Morales Ruíz Crisóforo *SEM-437*  
Morales Valenzuela German L. *CHM-241*  
Morales Villagómez L. M. *NSN-296*  
Morales-Acevedo Arturo *RWE-421, SEM-587*  
Moran Lázaro Juan Pablo *NSN-517, THF-196, AMSCR-182*  
Moreno Mario *RWE-355*  
Moreno Armenta Ma. Guadalupe *RWE-217*  
Moreno Close Eric Rolando *NSN-408*  
Moreno García Harumi *SEM-364*  
Moreno-Amado Myriam *THF-453*  
Moreno-Bárceñas A. *NSN-586*  
Moreno-Cabrera Nidia Esther *NSN-226*  
Moreno-Coria Luis Armando *CHM-516*  
Moyeda-Martinez Francisco Argenis *THF-91*  
Muñoz Hernández Rocío Alejandra *CHM-321*  
Muñoz Saldaña Juan *AMC-409*  
Muñoz Sandoval Emilio *AMSCR-182*  
Muñoz-Fernandez L. *THF-378, SEM-375*  
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Muñoz-Saldaña Juan *CHM-254*  
Muñiz Soria Jesus *ACS-326*  
Muhl Stephen *PLV-503, TRB-477, PLV-414 THF-199 PLV-422, AMC-456, NSN-552*  
Munguía Moreno Silvia *BIO-63*  
Munguia Jacobo *SEM-195, MEM-54*  
Murias Dulce *RWE-355*  
Murillo Eduardo *ALD-377, ALD-438, ALD-376, NSN-239, ALD-374*  
Murillo Bracamontes Eduardo A *AMC-238, AMC-237, CHM-423*  
Murrieta Sanchez Héctor Octavio *AMSCR-204, LPM-271, LPM-56*  
Murrieta-Rico Fabian N. *NSN-303*  
Navarro-Contreras Hugo Ricardo *NSN-268*  
Núñez Rodríguez Diola Marina *AMC-191*  
Nedev Nicola *ALD-87, ALD-439, ALD-88*  
Neira-Velázquez Guadalupe *LPM-253*  
Niño Martínez Nereyda *BIO-475, NSN-486*  
Nieto Fabiola *SCD-347*  
Nieto Caballero Fabiola Gabriela *THF-400, SEM-437, SEM-40*  
Nikolaev Sergey *NSN-29*  
Nogal Luis Uriel *CHM-321*  
Nolasco Arizmendi Víctor *NSN-373*  
Noriega Zenteno Jorge *CHM-313*  
Novelo Peralta Omar *AMC-191*  
Nuñez-Briones Adriana Guadalupe *AMC-297*  
Nuñez-Dorantes Juan Carlos *CHM-559*  
Ocón Trejo Sergio Francisco *PLV-479, SEM-336*  
Ojeda Martinez Miguel *SEM-26, ACS-28*  
Olaya Flórez Jhon Jairo *THF-526*  
Olivares Trejo José de Jesús *BIO-590*  
Olvera Amador María de la Luz *AMSCR-182, PLV-270, RWE-100, RWE-96, SEM-146*  
Olvera Gonzalez Ernesto *PTP-31, PTP-32*  
Olvera-Rodriguez I. *AMSCR-243*  
Ordoñez Ñañez John Edward *THF-459*  
Ornelas-Soto N.E. *NSN-586*  
Oros Ruiz Socorro *RWE-212*  
Orozco Susana *SCD-309*  
Orozco Durán G. Esmeralda *CHM-425*  
Orozco Ortega P.E. *NSN-476*  
Orrantia Borunda Erasmo *AMSCR-461*  
Ortíz-Saavedra J. *AMC-265*  
Ortega Beatriz *NSN-277, NSN-279, NSN-281*  
Ortega J. J. *TRB-39, 2SEM-336, THF-386, THF-328, NSN-342, PLV-398, PLV-346, THF-553*  
Ortega Cervantes Gerardo *LPM-532, NSN-232*  
Ortega Aviles Mayahuel *MEM-357*



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Ortega Cigala José Juan *AMSCR-316*  
Ortega Sigala J. J. *PLV-529, AMSCR-533*  
Ortega Sigala José Juan *PLV-482, TRB-489, THF-490, THF-287*  
Ortega Sigala Juan José *PLV-479*  
Ortiz Belman Erick Daniel *THF-148*  
Ortiz Domínguez Martín *TRB-314*  
Ortiz Lopez Jaime *LPM-532, NSN-232*  
Ortiz Morales Alejandro *LPM-532*  
Ortiz Reyes Julia María *AMSCR-393*  
Ortiz Saavedra Juan *THF-328, PLV-479, THF-490, THF-287, PLV-346, PLV-529*  
Ortiz-Trejo A. *ACS-574*  
Oscar Adrián Lugo García *BIO-310*  
Oseguera Peña Joaquín E. *TRB-546, TRB-314*  
Osorio Diana Marcela *THF-513*  
Osorio Jaime *THF-272*  
Osorio de la Rosa Edith *SEM-190*  
Ovalle-Encinia O. *NSN-563*  
Pacio Abraham *THF-382*  
Pacio Castillo Mauricio *NSN-369, SEM-365, THF-382, SEM-404, ACS-326, SEM-190, SEM-344, SEM-174*  
Padilla Rosales Isela *LPM-564*  
Palacios López Javier *SEM-558*  
Palacios Quintas Germán *TRB-79, TRB-76*  
Palomec Garfias Abraham Francisco *BIO-332*  
Palomino M. A. *CHM-467*  
Patiño Marín Nuria *BIO-475, BIO-192, BIO-63*  
Páramo García Ulises *SEM-472, SEM-362*  
Pérez Armando *AMC-547*  
Pérez Luis Antonio *NSN-441*  
Pérez Tejada Rojas Norma Elizabeth *ACS-27*  
Pérez Arrieta María Leticia *THF-287, TRB-489, NSN-465, AMC-265, SEM-336, THF-386, NSN-342, THF-553, AMSCR-533, THF-264, AMSCR-260, AMSCR-269*  
Pérez Centeno Armando *NSN-408, THF-495, NSN-478, NSN-476, PLV-452, RWE-492, PLV-499, PLV-493, PLV-356, PLV-250, NSN-481*  
Pérez García Sergio Alfonso *CHM-496, RWE-504, RWE-30, NSN-494*  
Pérez Hernández Carlos Guadalupe *AMC-349*  
Pérez Ramos Martha Elva *NSN-263*  
Pérez Rodríguez Felipe *NSN-367*  
Pérez Sánchez Gerardo Francisco *NSN-507, SEM-506*  
Pérez Tijerina Eduardo *ALD-508*  
Pérez-Luna José Guillermo *CHM-516*  
Pérez-Luna Verónica *NSN-447*  
Pérez-Rodríguez Felipe *NSN-181, NSN-331*



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Pérez-Solano Rafael *PTP-225, PTP-350, PTP-350*  
Peña Chapa Juan Luis *RWE-340, RWE-286, RWE-325, RWE-327, RWE-549, RWE-395*  
Peña Rodríguez Gabriel *PTP-5, AMSCR-55*  
Peña Sierra Ramon *SEM-249, SEM-506, NSN-507*  
Peña-Bueno Gabriela Alejandra *AMC-252*  
Pech-Canul M.I *SEM-242*  
Pedroza Rodriguez Aura *ALD-64*  
Peláez Betsabee Marel Monroy *RWE-50*  
Peralta Arriola Miriam *CHM-241*  
Pérez Caro Manuel *PLV-140*  
Perea-Parrales Felipe Eduardo *CHM-576*  
Pérez Ladrón de Guevara Héctor *SEM-364*  
Perez-Robles J. F. *NSN-586*  
Pernot Julien *NSN-179*  
Pescador Rojas José Alfredo *NSN-560*  
Petranovskii Vitalii *NSN-229, NSN-303, NSN-299, NSN-306*  
Pola-Albores Francisco *NSN-97*  
Polcar Tomas *TRB-477*  
Ponce Victor *MEM-322*  
Ponce Cabrera Luis *SEM-389*  
Ponce Pérez Rodrigo *ACS-444*  
Ponce Peña Patricia *AMC-191*  
Porraz-Culebro Teresa Elena *NSN-209*  
Preciado Grijalva Alan *PLV-318, PLV-413*  
Prelle Cristine *THF-206*  
Prieto Pulido Pedro Antonio *THF-458*  
Priscy Alfredo Luque Morales *SEM-341*  
Privalov A. F. *NSN-208*  
Prokhorov Evgen *NSN-53*  
Puch Ceballos F.  
Puch Ceballos F. R. *AMSCR-533, AMSCR-316, PLV-482, PLV-479, PLV-346, SEM-336, PLV-398, AMC-265, AMSCR-260*  
Puente Lee Iván *AMSCR-561*  
Puente-Urbina B. A. *AMSCR-221, AMSCR-197, BIO-368, AMC-297*  
Puga A. *AMSCR-533, THF-264, AMSCR-260*  
Puga-Candelas A. *AMC-265*  
Pulgarín-Agudelo F. *RWE-580*  
Pulido Castellanos José de Jesús *AMC-457*  
Quandt A. *LPM-578*  
Quevedo López Manuel  
Quevedo López Manuel A. *THF-302, ALD-261, THF-285, THF-93, THF-91, AMSCR-41*  
Quiñones Galván J.G. *THF-495, PLV-499, PLV-493, RWE-492, PLV-452, PLV-270, NSN-408, PLV-356, PLV-250, RWE-96, NSN-481, NSN-478, NSN-476*  
Quiñonez Penagos Mario Fernando *THF-459*



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Quintana Mildred *NSN-447, NSN-446, NSN-60, NSN-497*  
Quintana Owen Patricia *THF-470*  
Quirama Alix *THF-272*  
Quiroz Germán *MEM-322, MEM-366*  
Quiroz Cardoso Oscar *RWE-212*  
Quiroz Merino Germán *MEM-276*  
Rabanal M.E. *THF-378, SEM-375*  
Radnev Nikola *ALD-374, ALD-377, ALD-376*  
Rahman Talat *ACS-189*  
Ramírez Marthen Moisés *SEM-26*  
Ramírez Bon Rafael *SEM-177, RWE-360, RWE-30, THF-329, BIO-545, THF-335, AMSCR-24, THF-501, CHM-434*  
Ramírez Dámaso G. *RWE-109, RWE-108*  
Ramírez Esquivel Obed Yamín *AMSCR-353*  
Ramírez González Francisco Sebastian *SCD-347, SEM-40*  
Ramírez López Manolo *PLV-140, LPM-222, LPM-222*  
Ramírez Platón I.E. *RWE-109, RWE-108*  
Ramírez Rodríguez O. *RWE-109*  
Ramírez Solís Jorge Fernando *AMSCR-561*  
Ramírez-Garza R. E. *AMSCR-575*  
Ramirez Giovanni *THF-453, TRB-339*  
Ramirez Medina Oscar Alejandro *THF-148*  
Ramirez Mendoza Leticia Arizbeth *NSN-399*  
Ramirez Solano Jesus *ACS-28*  
Ramirez-Rodriguez O. *RWE-108*  
Ramos Brito Francisco *BIO-320, BIO-278, AMSCR-204, NSN-184, NSN-185, LPM-259*  
Ramos Fierro Julio Gabriel *PLV-140, LPM-222*  
Ramos-Murillo Manuel Antonio *ALD-348, ALD-417, ALD-203*  
Ramos-Ortiz Gabriel *PTP-350, PTP-225*  
Ramírez-Amador Raquel *THF-536*  
Rangel M. Rosario *AMSCR-221*  
Rangel Ricardo *ALD-509*  
Rangel-Kuoppa V. T. *RWE-418, SEM-587, NSN-588*  
Raymond Oscar *NSN-303, NSN-299, ACS-227*  
Rayo Mayoral Patricia *CHM-541*  
Réyes López Simón Yobanny *BIO-234*  
Ríos Luis A. *NSN-239*  
Ríos Pimentel Fernando Francisco *NSN-403*  
Ríos-Valdovinos Edna *NSN-97*  
Rejón Víctor *RWE-340*  
Rejón Moo Víctor *RWE-286*  
Rejon V. *RWE-327, RWE-325*  
Rejon Victor *RWE-395*  
Renero Francisco *MEM-372*



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Reséndiz Muñoz Juan *THF-228*  
Resendiz-Calderon Cesar David *TRB-1*  
Restrepo Johans *THF-199, AMC-456*  
Reyes Cervantes Elia Viridiana *THF-294*  
Reyes Esqueda Jorge Alejandro *AMC-537*  
Reyes Fernández Jesús *BIO-433, BIO-431*  
Reyes Gómez Juan *NSN-123, NSN-124*  
Reyes López Simón Yobanny *AMC-521, AMC-334, BIO-215, AMSCR-246*  
Reyes Valdez Juan Jesús *SEM-344, SEM-404*  
Reyes-Ixta F.P. *AMC-265*  
Reyes-Lopez Simon Yobanny *NSN-248, MEM-556, AMSCR-247, AMSCR-236, AMC-240, AMC-252*  
Reyes-Ramirez Bartolome *PTP-225, PTP-350*  
Reynoso Soto Edgar *CHM-25*  
Ribas Ariño Jordi *ACS-227*  
Rickards Jorge *NSN-213*  
Rickards Campbell Jorge *THF-251*  
Riech Inés *RWE-340*  
Riech Ines *RWE-395*  
Righini G. C. *LPM-578*  
Rimmaudo Ivan *RWE-325, RWE-327, RWE-395*  
Rincon González Marina Elizabeth *RWE-176*  
Rios Medina Oscar Fernando *RWE-383*  
Rios Saldaña Luis Eduardo *NSN-512*  
Rivera Laura *PLV-414*  
Rivera Zacarias *LPM-56*  
Rivera Flores Bertha Luisa *SEM-249*  
Rivera Gómez Alma Rocio *THF-460*  
Rivera López J. Eduardo *CHM-425*  
Rivera Márquez José Antonio *NSN-440*  
Rivera Reséndiz L.P. *PLV-493*  
Rivera Resendiz Laura Patricia *PLV-422*  
Rivera Soto María Ana *BIO-590*  
Rivera-Márquez J. A *BIO-431, BIO-433*  
Rivera-Reséndiz L.P. *PLV-499*  
Robledo Tania *SEM-385*  
Roblero Aguilar Sandra S. *TRB-546*  
Rocha Rubio Maricruz *NSN-373*  
Rodil Sandra Elizabeth *AMC-456, TRB-339, THF-337, THF-207, THF-453*  
Rodríguez Fernando *LPM-271*  
Rodríguez Guillermo Santana *RWE-50*  
Rodríguez Jared *NSN-282*  
Rodríguez Betancourt Verónica María *NSN-123, NSN-517, NSN-231, NSN-124*  
Rodríguez Dávila Rodolfo Antonio *ALD-261*  
Rodríguez Flores Tania del Carmen *SEM-506*



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Rodríguez García Carlos Eduardo *ACS-380, ACS-324*  
Rodríguez Gattorno Geonel *BIO-590*  
Rodríguez Hernández Paola Elideth *RWE-173*  
Rodríguez Luis Osvelia *NSN-486*  
Rodríguez Melgarejo Francisco *SEM-362, SEM-472*  
Rodríguez Pulido Alicia *AMC-191*  
Rodríguez Rodríguez Carlos Iván *NSN-373*  
Rodríguez Rosales K. *RWE-492*  
Rodríguez Vargas Isaac *SEM-6*  
Rodríguez Victoria A.P. *NSN-455*  
Rodríguez-Fernández Luis *THF-251, NSN-213*  
Rodríguez-González Claudia Alejandra *AMC-359, AMC-361*  
Rodríguez-Iznaga I. *AMSCR-575*  
Rodríguez-Rosales Karen *RWE-96*  
Rodríguez-Vargas Isaac *NSN-220, NSN-226*  
Rodríguez-Vazquez A. G. *NSN-530*  
Rodríguez Carlos A. *AMC-547*  
Rodríguez Canto Pedro *THF-402*  
Rodríguez Rosales Karen *RWE-100*  
Rodríguez-Fragoso Patricia *THF-224*  
Rodríguez-Lopez Andres *SEM-195*  
Rojas Hernández E. *RWE-109*  
Rojas Ochoa Luis Fernando *CHM-180*  
Rojas Trigos José Bruno *SEM-289, CHM-321, AMSCR-198, BIO-284*  
Rojas-Chávez H *NSN-563*  
Rojas-Hernandez E. *RWE-108*  
Rojo Blanco Celia Luz *NSN-552*  
Romano Roman *SEM-40, SEM-143*  
Romero de la Cruz María Teresa *SCD-345, ACS-324, ACS-380*  
Romero Guerrero Radamés *TRB-162*  
Romero Gutierrez Esperanza Paulina *THF-148*  
Romero Huerta Berenice del Rocío *NSN-517*  
Romero Ibarra Josué *BIO-590, RWE-591*  
Romero Ortiz Guadalupe *SEM-333, AMSCR-198, AMSCR-200*  
Romero-García J. *AMSCR-221*  
Romero-Ibarra Issis C. *RWE-579*  
Romero-Salazar Carolina *MEM-445*  
Romo José Manuel *ALD-371*  
Romo-Herrera J.M. *CHM-25, NSN-239, ALD-214, ALD-390, ALD-141*  
Romo-Jimenez O. *ALD-214*  
Roque-Ruiz Jose Hafid *AMC-240*  
Rosales A. *AMSCR-262*  
Rosales Pedro *RWE-355*  
Rosano-Ortega Genoveva *AMC-457*



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Rosas-Durazo Aarón *AMSCR-41*  
Rosendo Enrique *SEM-40, SEM-143*  
Rosendo Andrés Enrique *THF-294, THF-400*  
Ruíz Facundo *BIO-192*  
Rubin Daniel *SEM-502*  
Rubio Astorga Guillermo Javier *TRB-162*  
Rubio Pereda Pamela *ACS-419, ACS-338*  
Rubio Rosas Efraín *NSN-358, CHM-559*  
Rueda Morales Gabriela Lourdes *LPM-532, NSN-232*  
Ruiz Facundo *BIO-475, NSN-486*  
Ruiz Araujo Noe Daniel *AMC-409*  
Ruiz-Marcial Daniel *THF-311*  
Saavedra Rodríguez Gerardo *LPM-381*  
Sáenz Galindo Aidé *NSN-399, SCD-345*  
Salazar Hernandez Maria Del Carmen *THF-148*  
Salazar R. Bertha S. *THF-311*  
Salazar Valenzuela Ernesto Abraham *LPM-381*  
Salcedo Reyes Juan Carlos *ALD-64*  
Saldaña Saldaña Xóchitl Ines *NSN-410*  
Saloma Ruiz Erasmo *CHM-516*  
Salomón Preciado Ana María *RWE-194, RWE-100, RWE-193*  
Salvador Jonathan *SEM-385*  
Salvador Pamela *BIO-433*  
Sampedro M. P. *SEM-506, BIO-433, BIO-431*  
San Juan Hernández Samuel *SEM-396*  
Sánchez Nestor Gabriel *NSN-384*  
Sánchez Rodolfo *MEM-322*  
Sánchez Garrido O *THF-386*  
Sánchez Matías Guadalupe *RWE-383*  
Sánchez Sosa Roberto *SEM-385*  
Sánchez Uriarte Regino *NSN-481*  
Sanchez-Castillo A. *ACS-572, ACS-573, ACS-574.*  
Sanchez-Mera T. *AMC-125*  
Sanchez-Sinencio Feliciano *PTP-491*  
Sandoval Jiménez Fátima Reyna *SEM-6*  
Sandoval Vázquez L. A. *PLV-346*  
Sandoval-Puentes Miguel Ángel *NSN-220*  
Sanginés de Castro Roberto *PLV-318, CHM-241, CHM-223, CHM-352, PLV-412, PLV-413*  
Sansores Luis E. *ACS-511*  
Santamaría Covarrubias Carlos *SEM-534*  
Santana Guillermo *RWE-469, RWE-524.*  
Santana Aranda M.A. *PLV-356, THF-495, NSN-478, NSN-476, RWE-492, NSN-481, PLV-493, PLV-452, PLV-499, NSN-408, PLV-250*  
Santana Rodríguez Guillermo *PLV-518, SEM-389, RWE-62*



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Santiago Del Angel Edgar Adrian *RWE-383*  
Santiago-Jaimes E. *RWE-580*  
Santiesteban Cos Raúl *TRB-162*  
Santos Cruz J. *RWE-173*  
Santos Morales Agustín A. *THF-287*  
Santos-Cruz J. *PLV-270, RWE-96, SEM-146*  
Santoyo Morales José *THF-3*  
Santoyo Salazar Santoyo Salazar *NSN-563, NSN-151, NSN-68, NSN-231, PLV-267*  
Sarmiento Janeth *SEM-143*  
Sastré Hernández Jorge *RWE-194, RWE-418, SEM-587*  
Sastre Hernández Jorge *RWE-524, RWE-523*  
Sato Berrú Roberto Y. *NSN-312, TRB-477*  
Sáenz Galindo Aidé *AMSCR-393*  
Sánchez Carlos William *THF-458*  
Sánchez E. *CHM-467*  
Sánchez Rodolfo *MEM-366*  
Sánchez Alarcón Raúl Ivan *LPM-257, THF-402*  
Sánchez Avalos Jazzia Michelle *RWE-568*  
Sánchez de la Rosa José *NSN-283*  
Sánchez Esperanza Elizabeth Concepción *NSN-465*  
Sánchez Garrido O. *TRB-392, TRB-489, PLV-482*  
Sánchez Martínez Araceli *SEM-186*  
Sánchez Mora Enrique *NSN-367*  
Sánchez Navarro María del Carmen *NSN-486*  
Sánchez Niño Francisco *THF-255*  
Sánchez Ramírez José Francisco *NSN-570*  
Sánchez Rodríguez Fernando J. *NSN-185*  
Sánchez Tizapa Marciano *AMSCR-182, THF-196*  
Sánchez Uriarte Regino *NSN-478*  
Sánchez-Alejo Marco A. *LPM-271*  
Sánchez-Dena Oswaldo *AMC-537*  
Söderlund Mikko *ALD-567*  
Schabes Retchkiman Pablo *RWE-591*  
Secundino Sánchez Oscar *NSN-570*  
Sepúlveda Guzmán Selene *NSN-522*  
Sergiyenko Oleg *NSN-303*  
Serna Rosalía *LPM-525*  
Serrano Juan Ramón Ramos *RWE-50*  
Serrano Orozco Fernando Adán *ACS-28*  
Shelyapina M. G. *NSN-306, NSN-229, NSN-208, NSN-330*  
Shilina Marina *NSN-29*  
Shimomura Satoshi *NSN-2*  
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Silva Galindo G.I. *SEM-275*  
Silva-López Héctor *THF-67*  
Simakov A. *AMSCR-575*  
Simón Yobanny Reyes López *BIO-310*  
Siqueiros J. M. *CHM-423, AMC-237, AMC-238, RWE-217*  
Siqueiros Beltrones Jesús María  
Skryabina N. E. *NSN-208*  
Slutsky Vladislav *NSN-13*  
Sneck Sami *ALD-567*  
Solís Pomar Francisco *ALD-508*  
Solís Romero José *TRB-314*  
Solis Andrés *NSN-283*  
Solis de la Fuente Mauricio *RWE-176*  
Solis Romero Jose *TRB-546*  
Solorio Eduardo *ALD-87*  
Soriano Corral Florentino *LPM-253, LPM-510*  
Sosa Muñiz María del Carmen *THF-196*  
Sotelo Armando *ALD-88*  
Sotelo Lerma Mérida *RWE-388, AMSCR-41*  
Soto Blanca Susana *AMSCR-449*  
Soto G. *ALD-439, ALD-371, ALD-390, ALD-214, CHM-25, ALD-141*  
Soto García Víctor Manuel *NSN-517*  
Soto Rojo Rody Abraham *AMC-409*  
Soto-Cruz B.S. *THF-378, SEM-375, THF-536*  
Sotolongo-Costa Oscar *NSN-220*  
Speghini Adolfo *LPM-535*  
Stephen Driver *ACS-134*  
Suarez Luisa *THF-459*  
Suarez Quezada Monserrat *AMSCR-200, AMSCR-198*  
Suarez Quezada Víctor Manuel *AMSCR-198, AMSCR-200, SEM-289, SEM-333*  
Suárez Gómez Amaury *THF-196*  
Suárez Quezada Monserrat *SEM-333*  
Surova L. S. *NSN-208*  
Takeuchi Noboru *ACS-419, ACS-338, ACS-444*  
Tamayo Meza P. Alejandro *CHM-425*  
Tanori Cordoba Judith Celina *RWE-466, AMC-562*  
Tapia Jesús *NSN-446*  
Tchoufian Pierre *NSN-179*  
Tejeda Adriana *AMC-191*  
Tellez Flores Dalia *SEM-437*  
Tepale-Ochoa Nancy *AMC-457*  
Tijerina-Rosa A. *AMSCR-197*  
Titov Oleg *RWE-57, SEM-61*  
Tiznado Hugo *ALD-376, ALD-374, ALD-371, ALD-377, ALD-87, CHM-352, ALD-439, ALD-438,*



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*ALD-88, ALD-390, ALD-214, ALD-141*  
Toledo-Solano M. *CHM-467*  
Tomas Diaz *SEM-544*  
Tonkikh Alexander *NSN-588*  
Torres Espinoza N.D. *NSN-455*  
Torres Jacome Alfonso *MEM-488, CHM-531, RWE-500*  
Torres Ochoa Alejandro *THF-526, MEM-551, CHM-550*  
Torres-Morales S. *ACS-573*  
Toscabo Giles José Arturo *THF-329*  
Tototzintle Huitle Hugo *TRB-392, NSN-342, THF-553, AMSCR-316, PLV-479, THF-287, PLV-482, THF-328, THF-264*  
Trave E. *LPM-578*  
Trejo Baños Alejandro *NSN-441, ACS-28, ACS-27, SEM-26*  
Trejo-Luna Rebeca *NSN-213, THF-251*  
Tsodikov Mark *NSN-306*  
Tufiño Velazquez Miguel *RWE-193, RWE-418, SEM-587*  
Turkowski Volodymyr *ACS-189*  
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Valaguez Velázquez Enrique *THF-228, SEM-274, SEM-275*  
Valdés Valdés Guadalupe *LPM-510, LPM-253*  
Valdes Madrigal Manuel Alejandro *NSN-397*  
Valdez Castro Ricardo *BIO-515*  
Valdez Núñez Karla Paola *SCD-256, CHM-254*  
Valdez Pérez Donato *NSN-464*  
Valdez Valdés Sharyl K. *LPM-510, LPM-253*  
Valdez-Garza Janett *BIO-201, BIO-219*  
Valencia Romero María del Rosario *NSN-373*  
Valencia-Resendiz E. *RWE-580*  
Valenzuela Benavides José *NSN-296*  
Vargas Ortiz Ramón Álvaro *THF-302, AMC-409, NSN-304, THF-285*  
Vargas-García Jorge Roberto *THF-315*  
Vargas Ortiz Ramon Alvaro *SEM-341*  
Vargas-Martínez Nadia *AMSCR-247*  
Vazquez Bañuelos J. *THF-553*  
Vázquez Cazares José Humberto *NSN-478, NSN-481*  
Vázquez López Carlos *BIO-90*  
Vázquez Velázquez Arturo Roman *NSN-494, CHM-496, RWE-504*  
Vázquez Zubiarte Lizeth *NSN-411*  
Vega Marina *AMSCR-244*  
Vega Chavez Karla Edith *NSN-373*  
Vega Hierro Andrés *NSN-12*  
Velarde Escobar Oscar Jesús *NSN-184, BIO-320, BIO-278*  
Velasco Soto Miguel Angel *NSN-494*  
Velázquez Cruz Evaristo Isac *NSN-465*



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Vera-Robles L. Irais *AMSCR-266*  
Verde Gómez José Ysmael *NSN-263*  
Verduzco Martínez Jorge Alejandro *AMSCR-468*  
Vidal Borbolla Miguel Angel *ALD-363, ALD-235, SEM-364, ALD-415*  
Vigil Galán Osvaldo *RWE-38, SCD-45, THF-3, RWE-580*  
Vigueras-Santiago Enrique *AMC-539, AMC-538*  
Villa Hernández José de Jesús *PTP-31, PTP-32*  
Villafan Vidales Heidi I. *AMC-562, RWE-466*  
Villagrán Ocadiz Marco Antonio *NSN-507*  
Villaneda-Saldívar B. *THF-264*  
Villanueva Ángeles *NSN-540*  
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