

Sociedad Mexicana de Ciencias y Tecnología
de Superficies y Materiales A.C.



XIV
*International Conference on
Surfaces, Materials and Vacuum*



October 18-21 , Virtual Meeting. México

Book of
ABSTRACTS





**XIV INTERNATIONAL CONFERENCE ON SURFACES,
MATERIALS AND VACUUM**
SOCIEDAD MEXICANA DE CIENCIAS SUPERFICIES Y
MATERIALES AC
VIRTUAL CONFERENCE OCTOBER 17-22TH, MEXICO.

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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 this occasion due the sanitary emergency that we are well aware for first time we implemented a full virtual meeting, and we congratulated of having received a enormous support from all the members of the SMCTSM which made the XIV-ICSMV possible.

The scientific program of the Conference is divided into plenary conferences, short courses and the different symposia with oral and poster contributions. 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 XIV ICSMV

Organizing Committee SMCTSM

October 2021



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PLENARY TALKS



MARIA BERNECHEA



DAVIDE BONIFAZI



ANOUK GALTAYRIES



ARMANDO ENCINAS



MÁXIMO LÓPEZ LÓPEZ



MANUEL QUEVEDO



RONY SNYDERS

5 PLENARY TALKS



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MARIA BERNECHEA

ARAID, Instituto de Nanociencia
y Materiales de Aragón, Spain

BIO

I obtained my PhD (Cum laude) with European mention in 2006. The research was developed at Universidad de La Rioja, through a FPI (Formación Personal Investigador) fellowship, and focused on the synthesis, characterization and study of the properties of organometallic complexes of Pt, Rh, Ir and Ru.

During this period I also worked for 6 months at the Laboratoire de Chimie de Coordination (LCC-CRNS), in Toulouse, thanks to a Marie Curie fellowship, where I studied the potential of the new ruthenium organometallic complexes to act as precursors in ROMP reactions. After that, I was selected for a research contract to develop a collaborative project between Universidad de Alcalá (UAH) and Instituto de Catálisis y Petroleoquímica (ICP-CSIC), focusing on the synthesis of metallic nanoparticles and their use as catalysts: in C-C coupling reactions in aqueous medium and as electrocatalysts for fuel cells.

In 2010, I moved to the Institute of Photonic Sciences (ICFO) to work on the synthesis and characterization of colloidal nanocrystalline semiconductors for their use in solution-processed optoelectronic devices, such as photodetectors and solar cells. I mainly focused on solar cells

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and more precisely on the development of new materials composed of earth-abundant non-toxic elements.

In 2016 I was hired as Lecturer in Energy Materials at Cardiff University where I was involved in several modules of BEng and MEng of Medical and Mechanical Engineering, and MSc in Sustainable Energy and Environment. My research on that time focused on nanomaterials for clean energy applications.

Since October 2017 I'm ARAID researcher at the Institute of Nanoscience and Materials of Aragón-INMA (CSIC-Universidad de Zaragoza) where I perform research on the development of nanomaterials for clean energy. Since then, I'm leading several national and international projects.

As a summary, I'm interested in the synthesis and characterization of functional nanomaterials for their use in energy-related applications, such as solar cells, electrochemical energy storage devices, (photo)catalysis, or thermoelectric devices.

Ideally these nanomaterials can be obtained as colloidal solutions, which allows an easy processing, and low-cost fabrication of devices. The development of materials composed of earth-abundant elements further reduces costs, while the use of non-toxic elements reduces health and environmental concerns.

My work has given rise to several communications in conferences (3 as plenary/Keynote), 2 patents, and the publication of more than 30 articles, among them 3 Nature family papers.



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DAVIDE BONIFAZI

University of Vienna, Austria

BIO

Davide Bonifazi was born in Guastalla (Italy) in 1975. After obtaining the “Laurea” in “Industrial Chemistry” from the University of Parma (1994-1999) working with Prof. Enrico Dalcanale (organic synthesis and metal-directed self-assembly of cavitands derivatives), he joined the group of Prof. François Diederich as doctoral fellow (organic functionalization of [60] fullerene and porphyrin derivatives) at the Swiss Federal Institute of Technology, Zürich (2000-2004). During his doctoral studies he has been also visiting scientist at the Weizmann Institute Scientist working with Prof. David Cahen. He was awarded the Silver Medallion of the ETH for his doctoral dissertation (2005). After a one-year postdoctoral fellowship with Prof. Maurizio Prato at University of Trieste (organic functionalization of carbon nanotubes), he joined the Department of Pharmaceutical Science at the University of Trieste as a research associate first and then as a part-time Researcher/Professor (2012-2016). In 2006, he joined the Department of Chemistry at the University of Namur (BE) as Junior Professor (2006-2011) and as Associate Professor of Organic Chemistry (2012-2015). Since 2016 he is Chair Professor of Organic

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Supramolecular Chemistry in the School of Chemistry at Cardiff University (UK). In 2010, he was awarded with the “Ciamician Medal” from the Organic Division of the Italian Chemical Society and in 2011 he gained an ERC starting grant.

His activities are focused on the creation of functional organic architectures in interdisciplinary projects through targeted organic synthesis, self-assembly and self-organization of organic architectures in solution and on surfaces, physical-organic studies, and material- and bio-based design.



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ANOUK GALTAYRIES

French Dean at Paris Curie Engineering
School/Chimie Pékin
Invited Professor

@Beijing University of Chemical Technology
(BUCT)

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BIO

- Since 1999: Associate Professor in Materials Chemistry
@ Ecole Nationale Supérieure de Chimie de Paris (Chimie Paristech)
@ Institut de Recherche de Chimie Paris (CNRS)

Research Group: Physico-Chemistry at Surfaces

- 2019-2022: President of the International Union of Vacuum Science, Technique and Applications, 35 countries, www.iuvsta.org
- Member of International Scientific Committee @EVC-15, Geneva, 2018
- Member of International Scientific Committee @SIMS21, Krakow, 2017
- Co-Chair of ECASIA'17 in Montpellier, 2017



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RESEARCH

- Surface reactivity of model catalysts and passivated metals and alloys: oxidation, corrosion, biointerfaces, $h=30$, more than 2845 citations (Google Scholar)
- Chemical surface characterisations under UHV (XPS, ToF-SIMS)
- Member of the Editorial Board of the Biointerphases Journal (AVS)
- Member of the Société Chimique de France (Member of the Board of Chemical Physics Division)
- Member of the Board of the French Vacuum Society (Past-President)
- Collaborations: Université de Technologie de Compiègne (F); Sorbonne Université (F); École Normale Supérieure de Paris (F); Université de Paris (F); University of Cádiz (S); Politecnico Torino (I); University of Ferrara (I); Bulgarian Academy of Sciences (Sofia, BLG); Romania Academy of Sciences (Bucarest, ROM); Federal University of São Carlo, (BRA)
- Collaborations: Solvay; CEA; Areva; TOTAL; Saint-Gobain; EDF; Alveole (Paris)



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ARMANDO ENCINAS

Instituto Potosino de Investigación Científica y Tecnológica

BIO

Since 2002, Armando Encinas is a professor of Physics and Materials Science, first at Physics Institute of the Universidad Autónoma de San Luis Potosí, UASLP, and since 2015 in the Advanced Materials Division, IPICYT, in Mexico. He is the responsible of the Magnetism and Sustainable materials Lab. His work has centered around the properties of magnetic materials such as multilayers and thin films, arrays of nanowires and nanoparticles, as well as macroscopic materials. More recently his work has shifted towards studying more sustainable approaches to produce materials using greener fabrication methods using renewable and more abundant feedstock.

Armando obtained his doctorate in physics of materials science from the Univeristé de Paris Sud, France, in 1999. Working under the supervision of Prof. Alan Schulh at the Unité Mixte de Physique THALES-CNRS 137. He later held postdoctoral appointment at the Unité de Physico-Chimie de Materiaux at the Universite Catholique de Louvain, at Luvain-la-Neuve, Belgium in the group of Prof. Luc Piraux. Dr. Encinas' research has been recognized through national and international awards and honors such as the National Research System, SNI 3, CONACYT-

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México and the UASLP Research Prize to the best young researcher in 2007. He has presented more than 50 international invited talks in France, Belgium, Portugal, Chile, Brasil, United States of America, and Mexico.



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MÁXIMO LÓPEZ LÓPEZ

Department of Physics

Centro de Investigación y de Estudios Avanzados
del Instituto Politécnico Nacional (CINVESTAV-IPN)

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BIO

Máximo López López received his PhD from the Toyohashi University of Technology, Japan, in 1992. His thesis was a study on the initial growth process and interface formation of Si-GaAs heterostructures grown by molecular beam epitaxy. After that, he joined the optoelectronic technology research laboratory for 4 years as researcher at Tsukuba city, Japan. Since 1995, he is full professor of the department of physics at Cinvestav-IPN and is head of III-V Molecular Beam Epitaxy (III-V MBE) and III-N Materials Processing Laboratories. In 2011, he became chairman of the Department of Physics (2011-2019). In 2019, he took a sabbatical leave at the Quantum Technology Centre at Lancaster University UK (2019-2020).

Professor Lopez's research has centered on the physical properties of semiconductor, thin films, nanostructures and multi-layered structures grown by MBE. Fields of research activity include MBE growth of III-V compounds, III-V-nitrides, II-VI compounds, heteroepitaxy on Silicon, optoelectronic devices, low dimensional structures, diluted magnetic semiconductors. He has directed 17 PhD and 19 master's thesis. He has published more than 140 articles in

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refereed journals, his works has been cited over 1000 times. Professor Máximo has received a variety of national and international awards, and is member of professional organizations and societies of high prestige, as Mexican Physical Society, Sociedad Mexicana de Ciencia de Superficies y Vacío (Mexican Vacuum Society), Sistema Nacional de Investigadores (National Researcher Sistem, level III), American Vacuum Society, Materials Research Society, Japanese Society of Applied Physics.



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MANUEL QUEVEDO

Department Head, Department of
Materials Science and Engineering
The University of Texas at Dallas, USA

BIO

Prof. Manuel Quevedo is Professor and Department Head in the Materials Science and Engineering Department at the University of Texas at Dallas. Dr. Quevedo is also member of the scientific board of Nanoholdings LLC and CTO of WAND LLC. Dr. Quevedo has published more than 250 papers, 4 book chapters, and holds 15 US patents with 8 more pending. His current research includes nanostructured materials and devices for flexible electronics, large area sensors and energy harvesting. He currently directs a research group of about 25 members. Prof. Quevedo's research is supported by the The National Science Foundation (NSF), The Air Force Office of Sponsored Research (AFOSR), Defense Advanced Research Projects (DARPA), Domestic Nuclear Detection Office (DNDO), Conacyt, Department of Homeland Security, Texas Instruments, etc



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RONY SNYDERS

Universidad de Mons, Belgium

Chimie des Interactions Plasma-Surface, ChIPS
Chemistry Department/Science Faculty
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BIO

Rony Snyders received his PhD in Science from the University of Mons in 2004. Then, he spent 18 months at Polytechnic School of Montreal and 18 months at RWTH Aachen University as a postdoc. In 2007 he became associate Professor at the University of Mons and since 2009, he is head of the Chimie des Interactions Plasma-Surface (ChIPS) group and one of the Scientific Director of Materia Nova R&D, Mons, Belgium. Since 2017, he is full Professor and is a visiting Professor of the Technical University of Tianjin, Tianjin, China thanks to a “Thousand talents” grant from the Chinese government. He is the present President of the Belgian Vacuum Society, Belvac and members of several boards: IONICS, IVT, INISMA, Materia Nova. His interests are on the utilization of low pressure plasmas for the synthesis of materials and for gas conversion with a special attention to the characterization of the plasma phase during these processes. He has been promoting 17 PhD thesis and co-authored more than 225 peer-reviewed papers in the fields of thin films synthesis (magnetron sputtering, plasma polymerization), of plasma functionalization, and of plasma chemistry. His present H factor is 39.



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ATOMIC LAYER DEPOSITION

Chairmen:

Dr. Edgard López Luna: (UASLP), edgar.luna@uaslp.mx

Dr. Pierre Giovanni Mani González: (UACJ), pierre.mani@uacj.mx

Dr. Hugo Tiznado:(CNYN-UNAM), tiznado@cryn.unam.mx

The purpose of this symposium is to provide a forum for the discussion about basic issues and state the art applications of atomic layer deposition (ALD). The topics include:

- Simulation, Modeling and Theory of ALD
- Precursors and Chemistry
- Surface Functionalization
- Structural, chemical and electrical characterization.
- Growth and Nucleation in the Ultra-Thin Regime
- Novel Materials
- Plasma-Enhanced ALD
- Molecular Layer Deposition
- Others.



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**[ALD-205] Zirconium infiltration on P4VP brushes for oxide obtaining:
HAXPES and conventional XPS analysis.**

Pierre Giovanni Mani Gonzalez (pierre.mani@uacj.mx)², Jesus Alfredo Hernandez Marquez², Matthew Snelgrove⁴, Lilián Andrea Garay-Cervantes², Lorena Rivera Rios², Joseph Woicik³, Gregory Hughes⁴, Pravind Yadav¹, Robert O'Connor⁵

¹ *AMBER Research Centre and School of Chemistry, Trinity College Dublin, Dublin 2, Ireland*

² *Institute of Engineering and Technology, Department of Physics and Mathematics, Autonomous University of Ciudad Juárez, Cd. Juárez 32310, México*

³ *Materials Measurements Science Division, Material Measurement Laboratory, Gaithersburg, Maryland, 20899, USA.*

⁴ *School of Physical Sciences, Dublin City University, Glasnevin, Dublin 9, Ireland*

⁵ *School of Physical Sciences, Dublin City University, Glasnevin, Dublin 9, Ireland. Advanced Processing Technology Centre, Dublin City University, Glasnevin, Dublin 9, Ireland*

Polymer thin films infiltration is an overstudied area which offers a wide range of solutions to problems in optoelectronic devices industry. The study of polymer structures known as block copolymers due to its molecular accommodation infiltrated with metals (active sites). Obtaining metal oxides represent a huge advance in area selective deposition techniques and a way to reduce time and investment cost in lithographic area. In this work, organo-metallic precursor was used as a mean to diffuse metal ions into a poly 4-vinylpyridine (P4VP) polymer brush layer (~4 nm) which was deposited by spin coating on a silicon or corning glass as substrate. Thin P4VP films infused with zirconium nitrate by a wet chemical process was analyzed with hard x-ray photoelectron spectroscopy (HAXPES) and conventional X-ray photoelectron spectroscopy (XPS). The characterization technique XPS has been applied to evaluate both different energy of X-Ray source due to their affinity for chemical analysis. The results can be obtained according to binding energy of chemical states and stoichiometric values of the samples. Chemical states are the objects of study and also associated to the linking of uncertainty to the variables such as: inelastic mean free path (IMFP), elastic attenuation length (EAL) and cross section which are related to the material and source energy of the X-ray beam. The uncertainty of the background spectra from signal adjustment applied is considered. The overall calculation involves Poisson statistics, chi-square, ANOVA, and uncertainty propagation. Completely comparison from XPS and HAXPES have to be considerate on structure carefully in terms to chemical analysis and structure of the films. The system currently evaluated is zirconium infiltration into PVP deposited via spin coating and drop casting but this comparison could be used at any structure.



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[ALD-4] Non-quarter-wave dielectric mirror prepared by thermal atomic layer deposition

Javier López (javierlo21@ens.cnyun.unam.mx)³, Jorge Vázquez¹, Heriberto Márquez¹, Mario Farías², Hugo Tiznado²

¹ Centro de Investigación Científica y Educación Superior de Ensenada - CICESE

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³ Cátedra CONACYT - Centro de Nanociencias y Nanotecnología - CNYN UNAM

In this work, we design and fabricate from $n(\lambda)$ and $k(\lambda)$ experimental data for both Al_2O_3 and TiO_2 single-layer materials, an optical coating as “dielectric-mirror” following the non-quarter-wave stack formula $(\text{H}_x\text{L}_y)^8\text{H}_x$. The optical coating based on multilayer film on BK7 glass and Si(100) wafer substrates, were grown by thermal atomic layer deposition at 150 °C. Optical constants and optical properties of the TiO_2 - Al_2O_3 multilayer stack, before and after thermal treatment at 450 °C, were studied via spectroscopy ellipsometry and UV - Vis measurements in the spectral range from 200 to 1100 nm. Also, similar samples were studied by means of TEM, SEM, and AFM at room temperature in order to obtain information about the morphological properties. From optical studies, we found absorption due to carbon impurities related to organometallic precursors used in the ALD process; to reduce carbon related absorption, samples were submitted to an annealing process at 450 °C under air atmosphere. A reject zone or “stopband region” between 381 and 451 nm, with a maximum reflection around 99.9%, cut-off points at 371 and 455 nm after thermal treatment. This reject zone presents an acceptable bandwidth at $\lambda_0 = 420$ nm reference wavelength. Results open the possibility to fabricate dielectric-mirrors on complex geometry substrates without the restriction of direct evaporate exposed-view, due to the conformality advantage of ALD technology and its affinity with nanophotonics and integrated optics.

Keywords: Optical coating; Multilayer stack; Dielectric mirror; Atomic layer deposition.

Acknowledgments: This work was partially supported Basic Science projects 2017 - 2018 A1-S-21323 and A1-S-21084, FORDECYT - CONACYT 272894 and DGAPA-UNAM, through research projects: PAPIIT IN103220, IG200320, IN110018, IN113219. Authors would like to thank valuable technical support by Eloisa Aparicio, Eduardo Murillo, David Dominguez, Israel Gradilla, Francisco Ruíz, and Jaime Mendoza.



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**[ALD-268] Effect of Oxygen Source on the Various Properties of SnO₂ Thin
Films Deposited by Plasma-Enhanced Atomic Layer Deposition**

Mario Alberto Hidrogo Rico (mario.hidrogo@cimav.edu.mx)¹, Eduardo Martínez Guerra (eduardo.martinez@cimav.edu.mx)¹, Marcelo Martínez Puente¹, María Isabel Mendivil Palma¹, Francisco Servando Aguirre Tostado¹

¹ Centro de Investigación en Materiales Avanzados, S.C. (CIMAV-Sede Monterrey), Alianza Norte 202. Parque de Investigación e Innovación Tecnológica, C.P. 66600, Apodaca, Nuevo León, México.

Recently, the use of tin oxide as electron transport layer (ETL) has been widely used in perovskite solar cells (PSC). In terms of fabrication, PSCs with inorganics electron transporting layers are highly promising due to electrical, optical properties and low-temperature processing of tin oxide films. In this study, atomic layer deposition (ALD) and plasma-enhanced atomic layer deposition (PEALD) of 10 and 40 nm SnO films were performed using tetrakis(dimethylamino)tin (TDMASn) as the tin precursor and water (H₂O), oxygen (O₂) and ozone (O₃) as co-reactant at 80 and 200°C on fluorine-doped tin oxide (FTO) and glass. The growth per cycle (GPC) depends on the substrate and oxidant agent, respectively. At 80°C, the GPC is higher on FTO (0.5 to 1.45 Å/c) than glass (0.1 to 1.4 Å/c) and at 200°C the GPC is favored on glass with a GPC of 1 Å/c for all samples, but on FTO it dependent on oxidant agent, with H₂O the GPC is around 0.5 Å/c and with O₂ or O₃ is 1.3 Å/c, respectively. X-ray photoelectron spectroscopy (XPS) measurements showed that exists a dependence of chemical characteristics on the surface with oxidant agent. The relation of O/Sn confirms trend to stoichiometry and OH species on the surface. The optical transmittance was obtained from the UV-Vis analysis and show the high transparency (>90%) on the visible region of the electromagnetic spectrum. Electrical properties were performed with the four points method and Hall effect. Through the four points method, the electrical resistivity of the SnO films was low (1 to 8x10⁻⁴ ohm-cm) and show sheet resistance around >80 ohm/sq for all films. Hall effect confirmed the resistivity of all films. Also, high carrier concentration was ~x10¹⁹cm⁻³, and a high mobility (>10 cm² V⁻¹s⁻¹) from all SnO films synthesized by ALD.

Keywords: Tin oxide, atomic layer deposition, perovskite solar cells, inorganic electron transport layer.



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BIOMATERIALS AND POLYMERS

Chairmen:

Dr. César Márquez Beltrán (BUAP), cmarquez@ifuap.buap.mx

Dr. Amir Maldonado Arce (USON), amir.maldonado@unison.mx

The symposium on Biomaterials and Polymers consist on themes related with: 'Emerging Technologies and Scientific Advancements in polymers and Biomaterials Engineering.

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[BIO-18] Development of a microsensor for the rapid detection of SARS-CoV-2

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The COVID-19 disease is generated by a type of coronavirus identified as SARS-CoV-2. Infected people present late symptoms of disease, thus delaying the treatment time and consequently the survival possibility. Therefore, are necessary expeditious actions to allow an efficient diagnosis of SARS-CoV-2. The diagnostic tests accepted by the *U.S. Food and Drug Administration* (FDA) are based on molecular diagnosis and antigen testing. However, disadvantages have been evidenced, such as the time of sample treatment in molecular diagnosis, while rapid antigen tests have a decreased sensitivity in samples with the low viral load as well as the risk of cross-reaction. Under the context of prevention, identification, and precise diagnosis of SARS-CoV-2 and COVID-19, a strategy is based on the use of impedance biosensors due to its simplicity, speed, accuracy, high detection sensitivity without the need for pre-sample preparation, low cost, and ease of miniaturization. In combination with nanotechnologies, biosensors are a promising alternative to increase the chances of early diagnosis of COVID-19. Au nanoparticles (AuNPs) are widely used in biological systems research due to their characteristics such as size and shape-related properties, surface-to-volume ratio, excellent biocompatibility, and low toxicity. Additionally, the biomolecular functionalization of AuNPs provides a versatile platform for nanobiological assemblies with oligonucleotides, antibodies (Ab's), and proteins. For the present project, the synthesis of AuNPs and their surface modification with specific Ab's (Au-Ab's NPs) was proposed for the specific detection of antigens present in the transmembrane Spike protein of SARS-CoV-2. Hence, pseudo viral particles (VLPs) present structural proteins similar to SARS-CoV-2 without the presence of genetic material inside, and the stimulus of interaction with the RBD domain of the Spike protein attached to a green fluorescent protein (rGFP) were used as antigen detection. Through various characterization techniques (UV-vis, Potential Z, DLS, HRTEM, EDS, fluorescence spectroscopy, and ELISA), the interaction of Au-Ab's NPs with VLPs and rGFP was evidenced. Consequently, due to the optoelectronic characteristics of AuNPs, it was proposed that Au-Ab's NPs act as a conductive interface in the impedance biosensor. Preliminary results have indicated that such characteristics can be enhanced for the correct identification of the SARS-CoV-2 analysis.



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[BIO-231] alumina-hydroxyapatite-silver spheres with antibacterial activity

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The researches is currently looking for materials that are stable, functional, aesthetic, biocompatible and that are not susceptible to infection, therefore, there is great interest in obtaining a material that has a balance between aesthetic, biological, mechanical and functional factors, which can be used as an infection control material for example in the dental industry. Nanotechnology has played an important role in the search of new ways to prevent and treat infections, including the use of metallic nanoparticles with antibacterial properties. On this study we worked on the design of a composite of silver nanoparticles (AgNPs) in an alumina-hydroxyapatite matrix and evaluate its antimicrobial properties against various Gram-positive and Gram-negative microorganisms associated to drug-resistant infections. The union of hydroxyapatite to the alumina to make highly bioactive scaffolds with increased mechanical strength. Antimicrobial susceptibility was verified with the agar diffusion and turbidimetry methods in Gram-negative (*Escherichia coli*, *Klebsiella oxytoca* and *Pseudomonas aeruginosa*) and Gram-positive (*Streptococcus mutans*, *Staphylococcus aureus* and *Bacillus subtilis*) bacteria. All the bacteria used were susceptible to the Alumina- hydroxyapatite-silver (Al-HAp-AgNPs) spheres even at lower silver concentration, the higher susceptibility is found for *E. coli*, *P. aeruginosa* and *S. aureus* bacteria. The composites have a higher possibility for medical applications focused to the control of microorganisms with drug-resistance.



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**[BIO-236] In-vitro and in-vivo test of bioactive silica-hydroxyapatite
composites**

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Different characteristics ensure the success of a bioactive material such as microstructure, morphology, and chemical composition. Hydroxyapatite and silica are used extensively in the biomedical field because of their capacity to elicit a positive response on osseous tissue, allowing its regeneration. However, both materials, lack structural strength and can be improved through combination and processing. In this study, different iterations of fibrous membranes composed mainly of hydroxyapatite and silica were obtained using the sol-gel method and the electrospinning technique. The materials were characterized using X-ray diffraction, infrared spectroscopy, and scanning electron microscopy, to observe their chemical composition and microstructure. The fibers in the membranes had diameters roughly over 200 nm in green and around 100 nm sintered. The membranes were tested *in-vitro* with fibroblasts using the MTT assay to observe viability and *in-vivo* in rats implanting the material to observe the histological response. The membranes promoted cell proliferation, and the response on the test subjects was not harmful.



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**[BIO-20] Self-Normalized Photoacoustic Technique, a novel methodology
for quantification in polymer films**

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A Self-Normalized Photoacoustic Technique for pigment's quantification in polymer films is presented. Tangent of the difference of photoacoustic phases in both configurations (rear and transmission configurations), as a function of the pigment concentration and at a fixed modulation frequency, is involved. This novel photothermal methodology was tested on polymer films based on carob gum and k-carragenan at different concentrations of a green pigment, taking advantage of their optical properties at a wave-length of 660 nm.



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**[BIO-77] Thermal and Thermomechanical properties of starch-based
biocomposites with Hibiscus sabdariffa**

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The current consumption of plastics has increased in the last decades but also the awareness about reducing the exploitation of limited fossil resources and the desire to prevent damage to the environment. Therefore, scientific investigations have directed their interest towards a special type of materials: bioplastics. The manufacture of a product using 100% renewable resources is an area with a great future and the trend to use a greater proportion of available renewable resources is increasingly important. The present research focuses on developing biopolymeric starch films reinforced with natural fibers such as Hibiscus flower fibers. For the experimental procedure, different reinforcement and plasticizer formulations were made. The morphological, thermal, and thermomechanical properties of the films obtained by casting were performed through the following techniques: dynamic mechanical analysis (DMA), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA) and scanning electron microscopy (SEM). The results obtained were compared with the matrix without reinforcement and showed synergy and significant differences in the thermal and thermomechanical values attributed to the reinforcement and the amount of it. Finally, the development of this research contributes to the environment through the formation of a reinforced and sustainable polymer, the reuse of solid waste and the generation of biodegradable materials.



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**[BIO-94] Improving corrosion resistance of Mg with addition of TiO₂ by
plasma electrolytic oxidation technique**

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Magnesium (Mg) is a biocompatible material, however, applications of this material and its alloys are very limited in bioengineering area, due to their low corrosion resistance in physiological environments. A route to improve the corrosion and wear resistance is to use a surface treatment, such as the one provided by the plasma electrolytic oxidation (PEO). This technique is used to apply ceramic coatings on light metals, and it is widely applied in biomedical area.

Based on the above, in this work we carried out a study in order to improve the corrosion resistance of the AZ31 Mg alloy by applying TiO₂-based coatings through the PEO technique. Anatase-TiO₂ powders were incorporated into the electrolytic solution due to their good biocompatibility. Coatings were developed by varying the TiO₂ concentration from 0.08 g to 0.18 g, and the current density from 180 to 220 mA/cm². The distance between electrodes was set to 2 cm and the pH was 11.9.

The presence of TiO₂ in the coatings was confirmed by optical reflectance tests. Surface morphology and chemical composition were studied by Scanning Electron Microscope (SEM). SEM images at 500x magnification showed that TiO₂-based coatings have formed a porous surface. The porosity increases as density current increases. The open-circuit potential (OCP), electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization curves (Tafel) were employed to investigate the corrosion resistance of the AZ31 substrate with and without coatings in Hanks' balanced salts. Preliminary results show that I_{corr} is reduced in one order of magnitude when a TiO₂-based coatings were used, indicating an improve on the corrosion resistance.

Results demonstrate that the process developed in this work can be applied to improve corrosion resistance of Mg and its alloys to expand their applications.

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**[BIO-121] Osteoblastic adhesion due to the addition of amphiphilic
peptide nanoparticles**

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The addition of nanoparticles of amphiphilic peptide to the Ti4Al6V coatings of bone implants promotes the proliferation of osteoblastic cells, allowing obtaining a bioactive interface that promotes osteoblastic adhesion. Due to the difficulty for the amphiphilic peptide nanoparticles to solidify, was used a base of the polyhydroxyethylmethacrylate hydrogel as it is a biocompatible material.



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[BIO-133] Meniscus prosthesis by 3-D printing using Hydrogel with Carbon nanotubes and Gentamicin

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Articular cartilage injuries are one of the main causes of attention in health systems and have become a real public health problem. Millions of people suffer from injuries or tissue damage, transplantation being the solution to this problem. Currently, different biomaterials have been developed to replace damaged organs or tissues. One of the most innovative biomaterial manufacturing techniques is 3D printing of materials such as hydrogels, in a personalized medicine concept using image segmentation. Despite the unique properties of this type of biomaterial, hydrogels present problems that limit their use in 3D printing, motivating the incorporation of nanomaterials that improve these limitations. Multiwalled Carbon Nanotubes (MWCNT), exhibit unique atomic structure, aspect ratio, electrical and mechanical properties, making them an ideal reinforcing fiber. Through the functionalization of MWCNT, changes in physical properties can be obtained, such as solubility and dispersion, which are important because it allows having a better interaction with biological molecules. On other hand, Gentamicin (GENT) is used for its antibiotic properties to prevent possible infections. The objective of this work is to synthesize a hydrogel with MWCNT and GENT, in order to be used as biotin in 3D printing of meniscus prosthesis, through the use of monomers as chitosan (CS) and Sodium 2-acrylamide-2-methylpropanesulfonate (AMPS). To obtain a double network hydrogel, Bentonite (BENT) was dispersed in acetic acid (AA) and PBS (saline sulfate solution), subsequently, the monomers (CS, AMPS) are mechanically mixed with crosslinker NMBA (N, N' - methylenebis (acrylamide)), photoinitiator I2959 (2- Hydroxy - 4' - (2- hydroxyethoxy) - 2-methylpropiophenone), MWCNT or functionalized MWCNT (f- MWCNT) and finally GENT was added. The hydrogel will be used to build a meniscus prosthesis by 3D printing, carrying out its polymerization by UV radiation to provide rigidity to the piece. The functionalization of MWCNT was characterized by Raman spectroscopy obtaining the characteristic phonons at 1337 and 1564 cm^{-1} , furthermore, the polymerization process of the hydrogels was monitored, finding 48 hours as optimal polymerization time. To establish interactions between GENT and CS, as well as the activation of BENT, the samples were characterized by FTIR-ATR. Finally, a swelling factor of 300% was obtained in the synthesized hydrogels. The materials were characterized by resazurin essay obtaining cellular metabolic activity values of 73%. The viscosity of the material was obtained between 24-56 kPa that guarantees the ideal viscosity to be extruded by 3D printing.

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Mantenimiento de Infraestructura Científica en Laboratorios Nacionales 315911 and 2020-314931, FAI-UASLP and the access to Laboratorio Nacional de Análisis Físicos, Químicos y Biológicos-UASLP. During the course of this research, Grecia Aranzazú Guerrero Martínez with CVU: 1008586 acknowledges the financial support of CONACyT through a Master scholarship.

Keywords: Hydrogels, Multiwalled Carbon Nanotubes, Gentamicin, 3D Bio-printing.



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**[BIO-134] 3D printing of meniscus prosthesis based on hydrogel synthesized
with silver nanoparticles (Ag NPs), Collagen and Hyaluronic Acid**

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Materials science is immersing in all branches of knowledge, one of these areas is medicine, which tries to find materials that can interact with the human body, known as biomaterials. The most important characteristic of biomaterials is the interaction with biological systems without creating an immune response, denominated Biocompatibility. Hydrogels are commonly used due to their properties of being accepted in the human body as a structure containing water, being inert in biological processes, and permeability to biological substances. Nanocomposites, such as silver nanoparticles (Ag NPs) are useful in biomedical applications due to their antibacterial and fungicidal spectrum, while, Collagen and Hyaluronic Acid, provide properties of mechanical resistance, coagulation, and non-toxicity for humans. The objective of this work is to synthesize a hydrogel with Ag NPs, Collagen, and Hyaluronic Acid to create a network with antibacterial properties and well cellular viability, to be applied in meniscus prosthesis by 3D printing. As methodology, a first solution is obtained when AMPS monomer is dispersed under rigorous stirring, adding MBBA (crosslinking agent), I2959 (photo initiator) and Ag NPs previously synthesized. For a second solution, bentonite (BENT) is dispersed in acetic acid (AA) and PBS (Saline Sulfate Solution) and mixed with the first solution. To create a double network hydrogel, hyaluronic acid/collagen are used as monomers. The hydrogel obtained is applied in 3D printer employing a design created by image segmentation and performing the curing by UV radiation to provide rigidity to the piece. Size and morphology of Ag NPs were characterized by Scanning transmission electron microscope (STEM), Dynamic light scattering (DLS), Zeta Potential, and Ultraviolet-visible spectroscopy (UV-VIS), obtaining semi-spherical Ag NPs from 18-29 nm and negative charge of -53 mV. The functionalization of the hydrogel and BENT is studied by FTIR to find the interactions between Hyaluronic acid/Collagen/BENT, between 1232-1634 cm⁻¹. The polymerization process, is characterized by Raman spectroscopy obtaining characteristic phonons at 181, 684, 1046, 1412 and between 1600-1700 cm⁻¹, corresponding to the vibrational modes of the hydrogel. Finally, with the synthesized hydrogel a meniscus prosthesis was built by 3D printing.

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Key Words: Hydrogel, Collagen, Hyaluronic Acid, Ag NPs, 3D printing.



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[BIO-135] Controlled release systems for bioherbicides in weed control

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The results of the encapsulation of secondary metabolites of *Streptomyces sp.* with controlled release properties and their evaluation as pre-emergent bioherbicides in weed control. The biosynthesis of the bioherbicide was carried out using the fermentation method in liquid state. Absorption maxima at a wavelength at 452 nm and color changes were used to monitor bioherbicide production. Through the drip extrusion technique, the bioherbicide was encapsulated surrounded by a polymeric alginate shell. The shell was developed to protect and control release properties. By varying the concentration percentage of the sodium alginate precursor, well-defined capsules were prepared with a spherical shape, an average diameter of 4.5 mm and shell thicknesses around 180 µm. Formation of compact and porous shells were obtained with higher concentrations of the alginate precursor of 2%. The characterization of the structural properties of the capsules was carried out using optical microscopy. The release properties were quantified using the intensity values of the absorption spectra at 452 nm wavelength as a function of time, showing better values for the more compact capsules. The extraordinary phytotoxic properties of the encapsulated bioherbicide were verified by evaluating its activity in the pre-emergent application in *Amaranthus retroflexus*, *Bidens pilosa* and *Lolium perenne*.



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**[BIO-136] Cellulose nanofibers fabricated by electrospinning technique
and their use as seed coatings of *Solanum Lycopersicum***

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The development of nanotechnology has had great progress in recent years along with the manufacture of nanofibers using the electrospinning technique [1], its use has been highly exploited in the textile industry, medical, environmental and agriculture, in agriculture has been used mainly to bring pesticides and fertilizers to crops, has also been used to cover pruning wounds, to cover seeds and provide support for germination [2], [3]. In this work, cellulose fibers extracted from agro-industrial waste were manufactured by the electrospinning technique, the electrospinning technique is a process to form fibers of nanometric to micrometric diameter, whose basic principle consists of applying a high voltage (between 5 KV and 30 KV) to a generally polymeric solution [4] that, when electrically charged, deforms into threads that intertwine when directed towards a zone of lower potential, which is generally grounded to earth. Control over the preparation parameters makes it possible to have fibers with desirable characteristics. These fibers were used as support in the germination of *Solanum Lycopersicum* seeds; the fibers were made from a solution of cellulose in trifluoroacetic acid at different concentrations (4%-10% W/V), the fibers were characterized morphologically by SEM and thermogravimetrically by TGA. Once the fibers were obtained, they were used as a support for tomato seeds to see how they affected their germination.

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**[BIO-233] Biocompatibility studies of poly- ϵ -caprolactone/silver
nanofibers in Wistar rats.**

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Over the years, there has been a need to correct problems related to tissue loss due to trauma, disease or deterioration. This has oriented research to the development of materials that can be used to reproduce the function of living tissues in biological systems in a safe and physiologically acceptable way. Biocompatibility tests of poly- ϵ -caprolactone nanofibers, embedded with silver nanoparticles manufactured by means of the electrospinning technique, were carried out in Wistar rats to be used as oral dressings for the eradication of bacteria. Solutions of 12.5, 25, 50 and 100 mM of silver nitrate were made using *N*-dimethylformamide (DMF) and tetrahydrofuran (THF) as reducing solvents with 8% of poly- ϵ -caprolactone (PCL) polymer. The solutions were electrospun, and the nanofibers obtained in the process were characterized by infrared spectroscopy, Raman spectroscopy, scanning electron microscopy and X-ray scattering spectroscopy. The nanofibers had an average diameter of 400 ± 100 nm. Once the characterization of the material was done, three implants of each concentration of the nanofibers were formed and placed in the subcutaneous tissue of the rats. Three experimental subjects were used, leaving the material in them for a length of two, four and six weeks, respectively. The rats showed good healing, with the lesions completely healed at four weeks after implantation. After that time, biopsies were taken, and histopathological sections were made to evaluate the inflammatory infiltrate. The tissues of the rats presented chronic inflammatory infiltrate composed mainly of lymphocytes and giant multinucleated cells. The material was rejected by the rats when a layer of collagen and fibroblasts was produced, coating the material, a process characteristic of a foreign body reaction.



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**[BIO-257] Antimicrobial effect of mesoporous silica nanoparticles loaded
with antimicrobial peptides against *Clavibacter michiganensis* subsp.
*michiganensis***

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Solanum lycopersicum L. is affected among other pests and diseases, by the actinomycete *Clavibacter michiganensis* subsp. *michiganensis* (*Cmm*), causing important economic losses worldwide. Antimicrobial peptides (AMPs) are amphipathic cationic oligopeptides with variable length, sequence, and structures that protect their host from a broad spectrum of bacteria, fungi, viruses, and protozoa. However, AMPs are inactivated and/or degraded by different factors, an alternative that has been proposed to avoid these effects it is your nanoencapsulation. Mesoporous silica-based materials have been gaining ground in recent years; structural characteristics such as uniform distribution of pore size, high specific surface area, high pore volume and tunable pore size (2-50 nm) make them excellent candidates for the encapsulation and delivery of biologically active molecules. Therefore, in this study, we evaluate antimicrobial activity of mesoporous silica nanoparticles (MSN5.4) loaded with human β -defensin-2 (h β D2) and two mutants (TRX-h β D2-M and h β D2-M) against *Cmm*. h β D2, TRX-h β D2-M and h β D2-M presented a half-maximum inhibitory concentration (IC₅₀) of 3.64, 1.56 and 6.17 μ g/mL, respectively. MSNs had average particle sizes of 140 nm (SEM) and a tunable pore diameter of 4.8 up to 5.4 nm (BJH). AMPs were adsorbed more than 99% into MSN and a first release after 24 h was observed. The MSN loaded with the AMPs inhibited the growth of *Cmm* in solid and liquid media. It was also determined that MSNs protect AMPs from enzymatic degradation when the MSN/AMPs complexes were exposed to a pepsin treatment. An improved AMP performance was registered when it was adsorbed in the mesoporous matrix. The present study could expand the applications of MSNs loaded with AMPs as a biological control and provide new tools for the management of phytopathogenic microorganisms.



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**[BIO-262] Sensing parameters evaluation of polymeric compounds with
MWNT, respect to the composition of the polymeric matrix based on
xylitolated and epoxidized linseed oils**

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Nowadays, the pollution caused by oil derivatives and their depletion have led to numerous investigations in the search for alternative materials. In this context, Linseed oil is susceptible to be functionalized with epoxy rings or hydroxyl groups, to be used later as polymerizable monomers. The epoxy resins could be used as matrices in conductive bio-polymeric composites (CPC), presenting promising electrical properties in the sensing area. The objective of the present work is to analyze the influence of the composition on polymeric matrix in the detection of solvents, by mixing epoxidized linseed vegetable oils (ELO) and functionalized with xylitol (XELO) in different proportions. The sensing was carried out with nano-composites with multi walled carbon nanotubes (MWCNT) content of 0.5% and 1% w/w, considering the mixtures in molar ratios 1:0, 4:1 and 1:1 (mixture A, B and C, respectively) of the oils as matrices and with the polymerization of all of them as close as 100%, monitored through DSC and FT-IR. The behavior sensing of the composites for equal amounts of solvents (60 μ L), with different polarities (methanol, ethanol, acetone, ethyl acetate, tetrahydrofuran, chloroform and toluene), is affected with the increase of XELO in the matrix, since by increasing the content of this, the compounds increase their sensitivity to polar solvents, specifically methanol. The sensing experiments were carried out under the same conditions (air flow, time, number of pulses and volume of solvent) simultaneously with compounds containing each of the matrices and the same amount of CNT, due to the fact that performed simultaneously by means of a sample holder designed in the LIDMA to contain three sensors in a single sensing chamber.



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**[BIO-278] Extraction and characterization of purple sweet potato starch
(Ipomoea spp.)**

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The objective of this study was focused on the extraction and characterization of starch extracted from purple sweet potato (*Ipomoea* Spp.). The tubers were obtained from the municipality of Charo in the state of Michoacán, Mexico. The starch was obtained by wet milling and its chemical composition, physicochemical, functional properties, morphology, and crystallinity were analyzed. It was determined that the starch extraction yield was 16%. The sample had 21.7% amylose and 78.3% amylopectin. The starch granules exhibited spherical, oval and some polygonal shapes with smooth, flat surfaces and no visible cracks with an average size of 13.6 μm . The maximum viscosity of the sample was 3364 cP while the viscosity in the process of breaking the granules through gelatinization was 2011 cP with a decay difference of 1353 cP. The starch-water system showed the typical DSC endothermic transition between 59 and 75 °C with well-defined temperatures: start temperature (59.69 °C), maximum temperature (63.99 °C), end temperature (70 °C), and enthalpy. gelatinization (13.64 Jg⁻¹). In addition by X-ray diffractio, it was observed that purple sweet potato starch showed a crystallinity (%) of 37.39 with signals around 11.1 °, 14.4 °, 17.2 °, 19.5 °, 22.2 °, and 24 ° for the 2 angle. The properties found in this starch source make it a candidate to be used in different technological applications, such as in the new materials industry, particularly as a main or secondary ingredient in polymer formulations.



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CHARACTERIZATION AND METROLOGY

Chairman:

Dr. Roberto Machorro (CNYN-UNAM), roberto@cnyun.unam.mx

Optic and electronic spectroscopy and microscopy are very important and relevant fields of knowledge when it comes to fundamental and applied research in materials science. Materials and surfaces have been widely studied and characterized by using linear optics through reflectance, transmittance, absorbance, and scattering properties. By contrast, nonlinear optics are closely related to the understanding of materials and surfaces, since such phenomena for example, second harmonic generation, wave mixing, parametric up and down conversion to mention only a few are directly related to material features, such as, crystallinity, centrosymmetry, anisotropy and quantum properties.

This symposium is dedicated to the presentation and discussion of characterization and metrology within the following topics:

- Materials
- Surfaces
- Linear and nonlinear optical properties
- Raman characterization
- Nonlinear optical microscopy
- Ultrafast light-matter interaction
- Laser processing of materials: micro and nanostructures
- Laser-tissue interactions
- Laser-induced cavitation
- Photonics
- Biophotonics
- Opticaltrapping



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[CHM-74] Establishment of the surface required for MoS₂ electrocatalytic activity towards hydrogen peroxide to surpass the potential barriers formed between a metal & TMD junction

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Two-dimensional materials have been recognized for their extraordinary features that enable the fabrication of biosensing platforms. Its remarkable electronic properties allow to evaluate specific biochemical reactions for targeted molecules detection. 2D molybdenum disulfide (MoS₂) that belongs to the transition metal dichalcogenides (TMDs) family, have attracted great attention in the fields of bio-sensing and nanoelectronics due to it has proven to have an interesting surface-area-to-volume ratio, high carrier mobility and low noise level. While 2D MoS₂ interacts with hydrogen peroxide (H₂O₂) its whole structure is affected by exhibiting highly electrocatalytic activity towards the H₂O₂ reduction as a consequence of its atomical thickness. Due to the fact that interaction between analyte-detector on the superficial area plays a key role in the development of highly sensitive sensing platforms, in this work we propose to establish the surface that requires the TMD to interact with H₂O₂ and displays electrocatalytic activity to surpass the potential barriers formed in a junction between a metal and a TMD such as MoS₂. It is essential to consider the thickness for each material because the electronic properties change as function of the atomic layers (n) that affects the entire system. These measurements help us to know the minimum thresholds that the structure requires to have for the heterojunction to be able to detect a biochemical phenomenon with the lowest power consumption and resources.



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[CHM-88] Simulation of inhomogeneous film growth monitoring

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An inhomogeneous filter, a special kind of varying refractive index film, has a continuous modulation of refractive index along the stack axis. It is also known as a rugate filter. Compared with a traditional filter, made of homogeneous layers, it has some advantages, such as suppression of harmonics, reduced sensitivity to angle variation of the incident light, a wide range of potential applications. However, preparation of the rugate filter is relatively difficult because of the requirement for accuracy in realizing the continuous refractive index profile. Several techniques are reported to grow this kind of filter. Performance of manufactured coatings might differ from spectral characteristics of theoretical designs due to errors in the parameters of manufactured layers. It is convenient to have a preproduction simulation to estimate the feasibility of the theoretical design. In this paper, we describe the simulation of the process with reactive magnetron sputtering of a semiconductor Si target. Changes in refractive index are made by mass flux variations of Oxygen and Nitrogen, to obtain from SiO₂ to Si₃N₄, and SiO_xN_y in general. Target poisoning must be taken into account to be a realistic simulation. We discuss the convenience or not to monitor the thickness during deposition via quartz crystal monitor, reflectance/transmittance, and ellipsometry. We introduce a reproducibility or robustness factor of the filter. We calculate the performance when we introduce refractive index and thickness random errors.



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[CHM-91] Plasma emission spectroscopy and its relation to the refractive index of SiN_xO_y deposited by reactive magnetron sputtering for the construction of inhomogeneous filters

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Nowadays, the synthesis of inhomogeneous filters such as rugate filters is a complicated task. The complexity of these filters lies in their refractive index profile, requiring a high control during the manufacturing process. In order to achieve the desired optical performance, several theoretical design methods, manufacturing techniques and monitoring systems have been studied. One of the most common fabrication methods for rugate filters is reactive magnetron sputtering. This technique allows the synthesis of different compounds using a metallic target in a reactive atmosphere. Different properties can be obtained with the variation of the deposition parameters such as power supply, reactive gas flow and working pressure. Silicon oxynitride is commonly used for the synthesis of rugate filters, different refractive indices can be obtained depending on the oxygen/nitrogen reactive gas mixture [1]. Nevertheless, slightly different optical properties and deposition rates are presented even if the same deposition parameters are used. Different monitoring systems have been developed to address this control-related drawback, e.g. in situ reflectance [2] and transmittance [3]. The optical emission spectroscopy (OES) has been used to study the synthesis of silicon nitride thin films, reporting an association between the emission lines, the deposition parameters and the refractive index [4]. In this work, the refractive index, the emission lines and the reactive gas mixture were correlated to establish a monitoring system for the synthesis of rugate filters using principal components analysis (PCA), aiming to enhance the reproducibility and performance of rugate filters.

[1] H. Bartzsch, S. Lange, P. Frach, and K. Goedicke, "Graded refractive index layer systems for antireflective coatings and rugate filters deposited by reactive pulsed magnetron sputtering," *Surf. Coatings Technol.*, vol. 180–181, pp. 616–620, Mar. 2004.



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[CHM-125] The magic angle for XPS monochromated X-ray sources

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Bragg diffraction is employed as a means for monochromatizing X-rays in various spectroscopies such as X-ray photoelectron spectroscopy (XPS), X-ray absorption, X-ray diffraction, etc. The Bragg reflection causes a partial polarization of the beam impinging the sample. In fact, Bragg-reflection is commonly employed as a means for polarizing X-ray beams [1]. It was not until year 2010 that the partial polarization caused by the monochromator in XPS instruments was reported as a required correction in the calculations of the electron core-level photoelectric cross section [2]; the associated correction could be up to 10%. The partial polarization also affects the so-called “magic angle”, which refers to the angle at which the photoelectric cross section does not depend on the core-level asymmetry factor. The quantification of the change on the magic angle is reported in Ref. [3]. The correction on the photoelectric cross-section was done by *averaging over initial polarizations* [2]. This is the rule employed when calculating cross-sections in optical and electron physics [4–6]. An issue that is not discussed in the textbooks is that this assumption implies that Bragg-reflected photons imping the sample as either with s-polarization or with p-polarization with probabilities depending on the polarization direction of the photon before reflection [3]. The other possibility is that the reflected photons are elliptically polarized (referred as *case b*). This is assumed in important works such as that described by Hart in 1978 [7]. In the first case, the magic angle (58.7°) differs by 4° from the value usually employed (54.7°). In the second case, the magic angle only changes by 2°.

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**[CHM-142] Time evolution of the shape of the analyzing volume of
spectrometer and of the monochromatized X-ray beam of an XPS
equipment.**

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The angular dependence of the X-ray photoelectron spectroscopy (XPS) signal is determined not only by the electron take-off angle, but also by instrument-related geometric factors. In fact, the XPS signal is originated from the overlapping region of the X-ray beam, the analysis volume of the spectrometer and the sample surface, which depends, therefore, on the size and shape of the analysis volume of the spectrometer and the X-ray beam, as well as on their relative orientation. This work describes how the use of models and protocols for the characterization of the parameters that define the geometry of an XPS instrument [1] have allowed for maintaining a high measurement standards of a XPS instrument for more than 10 years, reducing the uncertainty in data acquisition for XPS and ARXPS. The protocols include methods for evaluating the area of analysis of the spectrometer and the dimension of the X-ray beam spot, as well as numerical modeling of the overlapping region (software XPSGeometry [1]). The method allows the prediction of the experimental intensity of the XPS peaks, thus eliminating the need to normalize the areas of the peaks to the area of a given substrate peak. The associated reduction in uncertainty is of particular importance.

The equipment has received constant maintenance since 2010 through this methodology; in this paper we report the time evolution along eleven years of the geometrical parameters defining the shape of the spectrometer analyzing volume and of the X-ray beam.



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[CHM-217] Niobium addition in electrodes for SMAW process: electrode efficiency, welding heat input, and microstructure analysis

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Hard Coatings Applications (Hardfacing) have multiple and varied uses in the mining and maintenance industry, related to the recovery of parts that have suffered severe wear, mainly by abrasive or adhesive wear and corrosives process. The electrodes used in SMAW welding (Shielded Metal Arc Welding) for hard coating applications have as one of its main alloying elements the chromium, which helps in the formation of carbides primaries of type M_7C_3 . These carbides improve the wear properties of the coating. The addition of Niobium has been studying to produce a reinforcement in the matrix of the deposited material, as a consequence of the formation of niobium carbides, that could improve the corrosion performance of the coating. In this research, Niobium is added in 0-8% in mass, and the coatings were deposited on ASTM A36 steel. The welding processes were controlled, and parameters as electrode efficiency and welding heat input were estimated. The microstructure of coatings was analyzed by XRD and its morphology was studied by SEM. The results allowed us to observe that higher niobium concentration had effects on electrode efficiency and heat input, and a reduction in the grain size of chromium carbides also was observed.



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**[CHM-49] Optical properties of P3HT and 2D materials based photoactive
layers for semitransparent organic solar cells obtained by spray coating
deposition in air.**

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Optical properties of the photoactive layer in organic solar cells represent one of the most important characteristics, playing a key role in the performance of the photovoltaic device. To make the most of the solar radiation, materials with high and broad absorption within the solar spectrum are desired, while keeping good transparency. Both conjugated polymers and 2D materials have shown promising potential for solar cell applications due to their outstanding electronic properties and excellent compatibility. Besides the great properties of the materials, the processing has also a great impact on the optical properties of the films. Spray coating has arisen as a low-cost scalable method for the realization of organic solar cells. Therefore, the characterization of the optical properties of thin films obtained from this method is of great relevance. In this work, UV-Vis spectroscopy along with fluorescence measurements and Haze analysis are used to characterize the effect of the addition of selectively oxidized graphene and molybdenum disulfide to a P3HT matrix in binary and ternary blends.



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**[CHM-50] AFM topography study of P3HT and 2D materials thin films
photoactive layer for semitransparent solar cells by Spray coating
deposition in air.**

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Topography characterization of the bulk heterojunction (BHJ) in photoactive layers is crucial to understand solar cell performance and optimize its efficiency. Moreover, transparency is greatly affected by the increment on surface roughness. Topography is affected at the same time during the deposition process and the properties of the materials, arising as a challenge to obtain the desired properties. Spray coating is a scalable deposition technique that holds a great potential to produce large areas and low-cost solar cells. To use this deposition method, it is crucial to produce a good dispersion of the donor and acceptor materials in a proper solvent, facilitating that after the deposition the materials will arrange in domains of a certain length. Here, we propose the use of P3HT along with 2D materials namely selectively oxidized graphene and molybdenum disulfide to obtain the binary and ternary photoactive layers, also, the 2D materials were subjected to functionalization to enhance the dispersion in the polymer matrix. The AFM technique reveals the impact of the number of spray passes onto the roughness of the film, the influence of the 2D materials addition, and the effect of the functionalization.



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**[CHM-68] Uncertainty calculations in the photoemission process in X-ray
photoelectron spectroscopy on hard energies**

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The seizing of nanometric dimension structures brings a broader perspective to materials analysis in comparison to bulk materials. Considering surfaces, which have local distribution of atoms with electronic properties, physical responses, and chemical behavior distinguishable from bulk the assessment of their properties under different parameters becomes a plausible issue. The system currently evaluated is hafnium infiltration into poly 4-vinylpyridine deposited via spin coating and PEALD. The characterization as angle resolved hard energy electron spectroscopy, ARHAXPES, has been applied to evaluate both surfaces and interfaces due to their affinity for chemical analysis. The results can be divided in binding energy of chemical states and stoichiometric values of the samples. As both are established as continuous data obtained from signal adjustments, the possibilities are open for determining uncertainty with levels of confidence (95% as commonly used) become not just plausible but an alternative way to deliver concise results. Because the object of study are chemical states there is also the linking of uncertainty to the variables such as: inelastic mean free path (IMFP), elastic attenuation length (EAL) and cross section which are related to the material and source energy of the x-ray beam. The uncertainty of the background spectra from signal adjustment applied is considered. The overall calculation involves Poisson statistics, chi-square, ANOVA, and uncertainty propagation.



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**[CHM-210] Photothermal Z-Scan model fitting in the complex plane for
thermal diffusivity determination in liquids**

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Thermal properties of liquids are obtained by fitting various complex photothermal models of the pyroelectric signal in the Z-Scan configuration, also known as Thermal Wave Resonator Cavity. The proposed methodology involves the fitting in the complex plane, using both amplitude and phase, which increases accuracy of the calculated thermal diffusivity, and also, the fitting procedure is in the whole sample thickness range, without approximation to differentiate between thermally thin or thick regimes. It is shown that using our approach the obtained thermal diffusivity of liquids was in good agreement with those reported in the literature with a reduction in the measurement error, due to the advantage of the analysis methodology since it is not required any cumbersome procedures, because it is not necessary to start the sample thickness scanning in the thermally thick regime or to decide whether to use amplitude or phase to calculate the thermal diffusivity.



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**[CHM-225] Analysis of the cementitious materials used in the restoration
work at the Toriles archaeological site, Iztlán del Río Nayarit**

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Spectroscopic techniques are widely used in various areas of archeology. These include different materials, environmental media, and life sciences. In this work, the energy dispersive spectroscopy (EDS) technique was used for the analysis of five samples of cementitious materials that were applied in different structures in the restoration work at different times from 1947 to 2015 in the archaeological site that are located in areas A, B, C in Los Toriles, Iztlán del Río Nayarit, Mexico. Of the different cementitious materials, the origin and composition of these materials is not known, and there is no full knowledge of the materials that were used in their restoration. Of the five samples that were analyzed, the elemental composition of each cementitious was determined and compared with the historical literature of the interventions of restoration works, which are in agreement with other studies that relate its composition and technology to the restoration of the site.



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**[CHM-265] A comprehensive multiparametric Raman analysis of graphene
evolution under prolonged near-IR femtosecond laser irradiation**

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Laser processing is a promising technique for graphene modification and patterning, with applications in the development of several electronic devices. *In-situ* Raman spectroscopy allows monitoring laser processing, providing information on numerous perturbations of the graphene lattice, such as disorder, strain, and doping, among others. This work focuses on the study of a graphene layer under prolonged irradiation with a femtosecond near-infrared laser at different average powers below the ablation threshold. The temporal evolution of the Raman spectral parameters is analyzed, including the central position, width, and area of the main Raman bands attributed to graphene and silicon substrate, as well as the background signal. In addition, we present the correlation curves between most of these parameters. Our results show an initial *instantaneous effect*, linear with irradiation power, in which mainly p-type doping occurs. With prolonged fs-laser irradiation, the evolution of the spectral parameters can be divided into several intervals associated with different doping and strain stages. At each stage, the parameters present multiple time dependencies, nevertheless, several correlations between them are revealed. This work highlights the complexity of the evolution of the complete Raman spectrum of graphene and the relevance of a comprehensive multiparametric analysis.



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**[CHM-272] Analysis and control of porous silicon dioxide thin films
synthesized by reactive sputtering**

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In the glass industry, thin film coatings can have different applications such as anti-reflective, self-cleaning and energy saving filters [1]. Some of these can be achieved with transparent materials such as porous silicon dioxide [2]. In this work, it is proposed to study the degree of porosity in silicon dioxide films grown by reactive sputtering. Optical emission spectroscopy (OES) was employed to monitor the spectral lines of the plasma as a method to control the degree of porosity. Particularly, a spatial analysis of the plasma was performed in the vicinity of the sputtering target surface and the substrate to relate the plasma emission lines to the optical properties of the film obtained by spectro-ellipsometry and spectrophotometry [3]. Different properties of SiO₂ films were achieved by changing deposition parameters such as working pressure, supplied power and partial pressure of O₂ within the deposition chamber. The optimal deposition conditions to grow porous SiO₂ are reported.

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LUMINESCENCE PHENOMENA: MATERIALS AND APPLICATIONS

Chairmen:

Dr. Gilberto Alarcón Flores: (CICATA-IPN), galarcon@ipn.mx

Dr. Salvador Carmona Téllez: (CONACyT-BUAP), scarmonat@fcfm.buap.mx

This symposium centers on the science and technology of luminescence, in its broader sense, including photo-, thermo-, electro- and mechano-luminescence. The aim is to gather international experts as well as students to discuss the recent progresses in this highly inter- and multi-disciplinary area, with particular attention to the synthesis characterization, and applications of materials exhibiting advanced luminescence properties.

The scope of the conference will cover the following areas:

- Photoluminescence
- Cathodoluminescence
- Ionoluminescence
- Bioluminescence
- Thermoluminescence
- Electroluminescence
- Mechano-, Sono- and Chemi-Luminescence
- Theoretical aspects of luminescence
- Nanophosphors: Physics and materials
- Crystalline, amorphous and glass-ceramic materials
- Polymeric and hybrid materials
- Novel Synthesis
- Materials Characterization
- Quantum cutting and up-conversion
- Combination of luminescent and plasmonic effects
- Light emitting devices



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- Displays
- Solar cells



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[LPM-80] Down-conversion from UV to NIR in CaF₂:Nd/Yb/Li phosphors.

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The capability to obtain two or more low energy photons from one high energy photon through Down-conversion (DC) process in rare-earth doped materials, have taken attention, especially in Silicon solar cells, since this represents reduction of loss energy. In this work, down-conversion process is confirmed in CaF₂:Nd/Yb/Li phosphor upon UV light excitation by DC efficiency analysis and effective quantum yield measurements. A DC efficiency up to 150% was obtained, while value of $81 \pm 10\%$ of effective quantum yield was measured.



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**[LPM-123] Gadolinium-based phosphors; a comparative study of
properties and synthesis methods**

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In the present work, $\text{Gd}_2\text{O}_3:\text{Tb}^{3+}$ and $\text{Gd}(\text{OH})_3:\text{Tb}^{3+}$ phosphors synthesized by simple evaporation (SET) and microwave assisted solvothermal (MWS) methods respectively are studied. For SET $\text{Gd}_2\text{O}_3:\text{Tb}^{3+}$ (0.25 at. %) phosphor under 229 nm excitation, luminescence peaks observed are associated with inter-level transitions within the electronic energy states of Tb^{3+} ions, particularly those corresponding to transitions among levels $^5\text{D}_4 \rightarrow ^7\text{F}_6$, $^7\text{F}_5$, $^7\text{F}_4$ and $^7\text{F}_3$, located at 484, 542, 583, and 621 nm respectively. The dominant peak for these spectra is the one associated with the transition $^5\text{D}_4 \rightarrow ^7\text{F}_5$ at 542 nm, which gives the characteristic green light emission identified with the presence of Tb^{3+} ions. On the other hand, emission spectrum under 262 nm excitation wavelength for MWS $\text{Gd}(\text{OH})_3:\text{Tb}^{3+}$ green phosphors consists of an intense green emission, corresponding to $^5\text{D}_4 \rightarrow ^7\text{F}_5$ transition at 545 nm, three other emission bands are found at 490 nm ($^5\text{D}_4 \rightarrow ^7\text{F}_6$), 586 nm ($^5\text{D}_4 \rightarrow ^7\text{F}_4$) and 622 nm ($^5\text{D}_4 \rightarrow ^7\text{F}_3$). In addition, a complete comparison between SET and MWS phosphors' properties which includes luminescent, optical, morphological and structural characteristics are also presented. Furthermore, these phosphors were functionalized using Benzene-1,4-dicarboxylic acid (BDC), and then the treated powders were incorporated into polystyrene (PS) and polymethylmetacrilate (PMMA) films, whose properties were also compared.



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**[LPM-162] Novel non- aqueous fluorolytic sol gel synthesis of Mn⁴⁺ doped
K₂SiF₆ red phosphor for WLED applications**

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Mn⁴⁺ doped metal fluorides have been used in commercial warm white light emitting diodes (WLED's) devices in the last years, because of their unique properties as broad excitation band in the ultraviolet and blue region, its high photoluminescent quantum yields and good thermal stability. Among them, Mn⁴⁺ doped K₂SiF₆ have drawn attention owing to its sharp emission bands centered in 630 nm and PLQY > 90%. Although these phosphors exhibit good optical properties for LED based illumination devices, its synthesis involves the use of highly toxic HF. In this way, we report a novel and fast synthesis for Mn⁴⁺: K₂SiF₆ phosphors using NH₄F as a fluorine source. Thermal decomposition of ammonium salts above 150 °C give rise to formation of ammonia and HF, which reacts with metal organic precursor in solution (Tetraethoxysilane and potassium ethoxide) in benzyl alcohol. Fluorolytic synthesis was carried out inside a microwave reactor Monowave 300 from Anton Paar, controlling HF pollution to the atmosphere. This phosphor is polycrystalline, and their diffraction peaks could be indexed in the cubic phase (JCPDS 85-1382). Mn⁴⁺ doping was carried out by cation exchange reaction in solution phase using K₂MnF₆ at different molar concentrations and aqueous HF solutions. As synthesized Mn⁴⁺: K₂SiF₆ phosphor showed a high intensity red-light emission centered at 631 nm and a PLQY near to 90 %. Photoluminescence, quantum yield and kinetics measurements carried out.

Keyword: Fluorolytic sol gel synthesis, microwave assisted synthesis, photoluminescence



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**[LPM-185] Analysis of the luminescent properties of magnesium
pyrophosphate doped with thulium ions.**

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In this work Thulium (Tm^{3+}) doped magnesium pyrophosphate powders ($\text{Mg}_2\text{P}_2\text{O}_7$) doped were synthesized by the solvent evaporation method and their luminescent properties were studied by photoluminescence (PL) and thermoluminescence (TL). The $\text{Mg}_2\text{P}_2\text{O}_7:\text{Tm}$ powders was characterized by X-ray diffraction (XRD). It was found the formation of two phases, $\text{Mg}_2\text{P}_2\text{O}_7$ and TmPO_4 . The excitation and emission spectrum show two transitions at 452 and 458 nm, corresponding to the characteristic $^1\text{D}_2 \rightarrow ^3\text{F}_4$ transition of Tm^{3+} in the $\text{Mg}_2\text{P}_2\text{O}_7$ lattice. For the TL measurements, the samples were irradiated with a source of beta particles from ^{90}Sr , the TL glow curves are complex, with a well-defined peak of higher intensity at 199 ° C, the material shows a better TL response at a concentration of Tm^{3+} of 8 mol%.



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**[LPM-248] Synthesis and characterization of a Nd-YAG material for laser
applications**

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Materials known as YAG are crystalline materials of the cubic system made from yttrium and aluminum garnet, which have excellent physical, chemical, thermal, mechanical and optical properties. One of the applications of this type of materials is its widespread use in the manufacture of white light emitters. In this study it was proposed a simple and inexpensive alternative to manufacturing YAG materials, through solid state reactions following powder processing routes. For this, an intense mixture of the precursor materials (Al_2O_3 and Y_2O_3) be carried out, in which there will also be the addition of neodymium atoms, with the purpose of improving the optical properties of the resulting material. After high energy mechanical mixing of the precursor powders, the average particle size is less than 1 micron, having a good size distributions of the powders. The advance of YAG formation was monitoring by intermediate phase formation during heat treatment through interrupted tests at different temperatures and analysis by XRD. From this analysis it was found that reaction for the formation of the desired YAG is completed at 1500 °C. Analysis by TG also was carried out in order to follow any change in the weight of the powders mixtures. The microstructure of the resulting material is fine and homogeneous.



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[LPM-287] Antisolvent enhanced luminescence of lead halide perovskite films deposited by AACVD

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Most solution-based synthetic routes for perovskite film deposition take place under highly controlled atmospheres and cannot be easily escalated for mass production. Here, the control in situ over luminescent, morphological, and structural characteristics of hybrid and inorganic perovskite films deposited on top of hot glass substrates by multi-source AACVD is reported. The crystallization of the films was performed in situ by the implementation of an anti-solvent stream source during deposition which in turn, yielded films with superior luminescence properties. The high degree of control on the final properties of the films indicates that AACVD could be a breakthrough for low-cost, scalable, high-throughput metal-halide perovskite film deposition.



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**[LPM-44] Dominant non-radiative recombination in perovskite CsPbBr₃-
xI_x quantum dots**

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Colloidal perovskite (cesium lead bromide-iodide) quantum dots (PQDs) with different iodine concentration were prepared. These PQDs show excellent optical properties with high light absorption and high photoluminescence. Light absorption is in the range between 500 and 550 nm and extending into the ultraviolet. The photoluminescence spectra show peaks from 490 to 675 nm. Charge carrier lifetime measurements, obtained with the time-resolved photoluminescence technique, indicate that the dominant mechanisms for recombination are the non-radiative recombination processes. Finally, increasing the iodine content, increases defect concentration in the PQDs.



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**[LPM-117] NIR emitting perovskite films, deposited by spray from
aqueous solutions.**

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CsPbCl₃ perovskites doped with Yb have recently been the target of intense research due to PLQY's have been found up to 190 % in thin films and 170 % in powders. The large PLQY's is explained by the large absorption coefficient of the CsPbCl₃ matrix, followed by an ultra-fast energy transfer to the 4f levels of the Yb, in a phenomenon known as *quantum cutting*; where the absorption of a photon with an energy equal to the band gap of perovskite CsPbCl₃ (420 nm) results in the emission of two photons characteristic of the typical emission of Yb in the infrared (984 nm).

In this work, films of CsPbCl₃ perovskites doped with Yb were synthesized in situ using the ultrasound-assisted spray deposition technique from aqueous solutions. This technique introduces several advantages: a) the fact of being able to deposit the films starting from a solution in water, something that could not be done with other deposit techniques, due to the low solubility of the precursor salts in common solvents, b) it is possible to incorporate an antisolvent stream that is simultaneously injected as an assistant in the crystallization of the films, which can result in an increase or decrease of the PL depending on the antisolvent to consider, c) the low cost of the technique combined with the high rate of film production per minute (a 1 micron thick film every 2 minutes), makes this industrially scalable technique for the possible manufacture of CsPbCl₃ perovskite films doped with Yb for their future application in photovoltaic cells, sensors, and solar concentrators.



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[LPM-156] Luminescent study of HfO₂:Tb³⁺ synthesized by two different techniques

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In the last decades, have arise an interest in the materials with nanometric size, this due their unique physical, chemical, and optical properties, etc., compared with the materials in bulk. Among the different nanoparticles (NPs), the nanophosphors appeared as promising candidates for the industry due the broad use for the manufacturing of different optoelectronic devices (LEDs, bio-sensors, biomedical applications). The phosphors are luminescent materials which emits in the visible region when they are irradiated by ultraviolet light (UV), electron beams, visible or infrared sources. Some materials acts as luminescent materials by themselves and emits radiations however usually the spectral emissions are broad and diffuse. On the contrary there are some materials that needs dopants which acts as the luminescent materials. The dopants are impurities/ions intentionally added which are incorporated into the system to obtain luminescent desired properties. The phosphors consists of two main components, the host matrix and the dopant. The host can be any oxide, borate, sulfate or aluminate, a good host material should have a stable crystalline structure, low phononic energy, chemical and thermal stability, broad bandgap, etc. The dopants can be any of the transition metals or ions of rare-earths.

In this work, there was synthesized hafnium oxide (HfO₂) doped with terbium (Tb³⁺) by two different techniques, solvent evaporation and microwave assisted, for a photoluminescent and microstructural comparative analysis. Showing the potential application for luminescent devices.



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[LPM-157] Spectroscopy properties of CdO-B2O3:Nd³⁺ glasses

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Nd³⁺-doped cadmium-borate glasses were synthesized by the melt-quenching method. Spectroscopy studies of Nd³⁺-doped cadmium-borate glasses were performed, due to the potential applications since the transition $^4F_{3/2} \rightarrow ^4I_{11/2}$ present high efficiencies being the most used for the fabrication of near-infrared lasers. Raman spectra displayed vibration modes mainly constitute by borate groups. By optical absorption, band gap (E_g) values (~ 2.5 eV) were determined. The emission spectra of the Nd³⁺-doped glasses upon 585 and 808 nm excitation displayed the Nd³⁺ transitions $^4F_{3/2} \rightarrow ^4I_{9/2}$, $^4F_{3/2} \rightarrow ^4I_{11/2}$, $^4F_{3/2} \rightarrow ^4I_{13/2}$ associated with the emission bands 880, 1060, 1335 nm respectively. Both spectra beyond 1.4 mol% of Nd³⁺ are quenched. The emission decay profiles at 1061 nm are shortened with the Nd³⁺ content, suggesting an increment of the non-radiative rate.



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**[LPM-161] Luminescent emission in ZnO: RE (Tm + 3 / Eu + 3) thin films
obtained by the ultrasonic spray pyrolysis technique**

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ZnO is a one metal oxide that has been widely studied since ago many time due its interesting properties, such as its band gap value of 3.37 eV, great chemical stability, and optical properties, among others. In recent years great contributions about the different properties in rare earths doped ZnO has been observed. The rare earths give improved electrical, optical and magnetic properties to a great extent in ZnO. These also used like as a photoactive material to obtain white light emissions. Due to this fact we are interest in some rare earth elements to doped ZnO and to obtained photoluminescence in the visible region of electromagnetic spectrum. In particular the ions of Eu + 3, Tm + 3, Tb + 3 show luminescence in the region of the visible spectrum, red, blue and green respectively. This work focuses on determining the conditions to obtain ZnO thin films doped with RE = Eu + 3, Tm + 3, Eu + 3 / Tm + 3, searching the concentration of impurities (doping) that favor an increase in luminescence. The films were prepared using the Ultrasonic Spray Pyrolysis technique, studying the influence on the variation of the europium and thulium concentration from 0.5% at to 3% at separately. Subsequently, a co-doping (Eu + 3: Tm + 3) was carried out, choosing the concentrations that presented the highest luminescent intensity.

The samples were characterized by X-ray diffraction (XRD), UV / Vis and photoluminescent spectroscopy (PL) techniques. The XRD pattern showed a Wurtzite structure (hexagonal) in the thin films obtained. The results of UV / Vis transmittance indicate a varied band gap interval from 2.88 to 3.10 eV according to different percent doping of Eu + 3. In the case of doping with Tm + 3 we obtained values of 2,97 to 3,22 eV. The analysis of photoluminescence emission bands in the films prepared was analized in the range of 300 to 1100 nm using an excitation wavelength of 285 nm showing the transitions of the excited levels for both the Eu + 3 and Tm + 3 ions.



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**[LPM-166] The Study of the Effect of the Luminescence of europium doped
calcium tungstate, Synthetized by the Spray Pyrolysis technique**

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Rare earth doped Wolframates have been widely studied due to their luminescent properties. The calcium tungstate has the highest emissions among alkali tungsten, since the intensity of Photoluminescent emission is greater if the ionic radius is smaller. The calcium tungstate is a luminescent material that acts as a host for a variety of rare earth ions. The wolframates in calcium tungstate structural units absorb light in the short and medium wave UV range through the charge transfer of oxygen to tungsten and the absorbed energy is transferred to rare earth ions, which subsequently undergo f-f transitions and produce sharp emission peaks.

In this work, nanometric and micrometric size particles of europium doped calcium tungstate were synthesized using the spray pyrolysis technique, the nanoparticles and microparticles synthesized technique has spherical morphology, the Europium (Eu) doping concentrations that were used in this project, are: 0.5, 1, 3, 4.5, 6, 10 and 15 mol%, subsequently a silicon oxide covering was made to observe the change in the crystallinity of the material as it is expected that with this covering there will be a rearrangement of the crystalline structure.

The excitation photoluminescence spectra, as expected, show a maximum at wavelength of 241 nm, which is found in the ultraviolet visible (UV) range, since both; the matrix calcium tungstate and Europium have the property to emit in the visible region of the spectrum when it is stimulated with ultraviolet light. The before mentioned, is an important property that allows us to observe emissions from both, the matrix and Europium, in the emission spectra at excitation wavelength of 240 nm, a growth in the emission that goes from a wavelength of 400 nm to 500 nm in Gaussian form that has a maximum at wavelength of 445 nm can be observed. These emissions are associated with the electronic transitions of the ions wolframates. Their emission range belongs to blue in the visible region, furthermore peaks are also observed in wavelengths 612 nm, 615 nm, 702 nm, 622 nm and 655 nm, which are associated to the transitions corresponded to Europium, Finally, the most intense emission corresponds to 612 nm that is associated to the transition the ions Europium.



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**[LPM-218] Optical recombination dynamics induced by potential
fluctuations in AlGa_N thin films**

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The optical properties of III-V semiconductors have been intensively investigated over the past 30 years enabling the development of diverse optoelectronic devices like light emission diodes, lasers, and solar cells with optical performance on the ultraviolet, visible, and infrared wavelengths of the electromagnetic spectrum. However, the effects of the interfaces and their bulk structural properties on the optical performance are not yet fully understood for semiconductors grown on non-native substrates. Carrier generation and recombination rates are affected by the crystalline quality of the sample, which influences the emission intensity and the full width of a half maximum (FWHM) of the spectral peaks, however, there are limited studies of the effect of potential fluctuations induced by composition variations on the carrier dynamics during luminescence spectroscopy. This work presents a detailed description of carrier dynamics in AlGa_N thin films grown on Si substrates by the MOCVD technique. Five samples were grown at Si(111) substrate temperatures of 950, 980, 1010, 1040, and 1070 °C, maintaining the nominal stoichiometry of Al at 8%. The samples were characterized by high-resolution X-ray diffraction, scanning electron microscopy, reflectance, and temperature-dependence photoluminescence techniques. The FWHM of (002) diffraction peak decreases from 710.2 to 457.6 arcsec as growth temperatures were increased, which indicates that dislocations density and point defects are reduced as the thermal energy increases during the synthesis. Surface morphology of the samples measured by SEM indicates a wide morphological and compositional uniformity in the detection limits, however, reflectance spectroscopy points to a variation in the effective bandgap for each sample correlated with its respective growth temperatures. It was identified that samples grown at the lowest temperatures presented limited incorporation of aluminum inducing compositional and potential fluctuations. Photoluminescence spectra show the near-band-emission and yellow and blue bands of AlGa_N samples, whose intensity evolution as a function of temperature indicates a carrier delocalization caused by potential fluctuations due to the variation of the concentration of Al,



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with a high dependence on growth temperature. This work was partially supported by SIP-IPN projects No. 20211386 and 20210341. The authors are grateful for the grant from the BEIFI program.

Keywords: potential fluctuations, AlGaN, photoluminescence, delocalization.



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[LPM-251] Systematic characterization of the crystalline phase transformation of annealed electrospun TiO₂ nanofibers for photocatalysis applications

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TiO₂ nanofibers were synthesised by the electrospinning technique, which were annealed at high temperatures to achieve the crystalline phase transformation. The stoichiometry of annealed TiO₂ nanofibers was estimated by EDS, finding that at low annealing temperatures there is excess oxygen and at high temperatures excess titanium. By TEM corroborates the presence of TiO₂ nanofibers and their surface morphology that present a homogeneous and continuous form without the presence of crystalline defects, which depends strongly on the annealing temperature. The crystalline phase transformation was studied by Raman dispersion, which revealed that annealed TiO₂ nanofibers showed a crystalline phase transformation from pure anatase, anatase-rutile mixed and pure rutile as the annealing temperature increased, which was corroborated by X-ray diffraction and High-resolution transmission electron microscopy. The grain size is increased with the crystalline phase transformation from 10 to 24 nm for anatase and from 30 to 47 nm for rutile, estimated by the Scherrer-Debye equation. The band gap energy, obtained from optical absorption spectra, decreases monotonically but a local minimum is observed at 700 °C, which ranged from 3.75 to 2.42 eV, caused by the crystalline phase transformation anatase→rutile. The photoluminescence shows that radiative bands redshift as the temperature increases due to the reduction of the band gap energy.



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**[LPM-264] Dominant non-radiative recombination in perovskite CsPbBr₃-
xI_x quantum dots**

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Colloidal perovskite (cesium lead bromide-iodide) quantum dots (PQDs) with different iodine concentration were prepared. These PQDs show excellent optical properties with high light absorption and high photoluminescence. Light absorption is in the range between 500 and 550 nm and extending into the ultraviolet. The photoluminescence spectra show peaks from 490 to 675 nm. Charge carrier lifetime measurements, obtained with the time-resolved photoluminescence technique, indicate that the dominant mechanisms for recombination are the non-radiative recombination processes. Finally, increasing the iodine content, increases defect concentration in the PQDs.



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MICROELECTRONICS AND MEMS

Chairmen:

Dr. Norberto Hernández Como, (Centro de Nanotecnología, IPN), nohernandezc@ipn.mx
Dr Israel Mejia Silva (CIDESI), israel.mejia@cidesi.edu.mx

Internet of Things (IoT) is providing several stand-alone internet-connected sensors that can be monitored and/or controlled from a remote location, this is an example of how silicon-related technology is changing the world for human benefit.

In this regard the mission of this Microelectronics and MEMS (MicroSystems) Symposium is to bring together scientists and technologists interested in these two interrelated fields. The program will highlight recent advances in the design and fabrication of integrated circuits (IC's), Microelectronics Technology, Materials Science for Micro and Nanoelectromechanical devices and systems (NEMS), as well as the different strategies for the integration and packaging of MEMS and NEMS.

Microelectronics; which in its widest conception includes the design, fabrication, characterization, and modeling of micro- and nano- devices, and circuits, has emerged as the fundamental technology for the fabrication of Microsystems. In this field, it is interesting to analyze the scaling laws and size regimes in which macro theories start requiring further non-linear analysis. The purpose is to obtain a deeper understanding of the physical consequences of downscaling electrostatic, electromagnetic, fluidic, optical, thermal, chemical devices, and some combinations of them. It is of great importance to study the non-linear behavior of miniaturized devices and systems, which apart from reason involving economics, volume and weight, can lead to new operating principles and even to increase the system performance. All of them is the basis for current technology trend.

Main Topics:

The Microelectronics and MEMS Symposium is focused on the integration of materials and processes for developing MEMS/NEMS devices. Invited Talks, Oral and Poster



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Session will include the following topics:

- Internet of things
- Design, characterization, and modeling of IC's
- Amorphous Materials and compound Semiconductors
- Characterization and Modeling of Circuits with Sensors/Actuators
- Microsystems design (MEMS/NEMS)
- Bulk and Surface Micromachining
- Radio Frequency CMOS-MEMS
- Integrated Optics
- BioMEMS and Lab on a Chip
- Aerospace Applications
- Chemical Sensors Applications
- Automotive Applications



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**[MEM-26] Ultra-dry air plasma treatment for enhancing the dielectric
properties of Al₂O₃-GPTMS-PMMA hybrid dielectric gate layers in a-IGZO
TFT applications**

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We assessed the effects of ultra dry-air plasma surface treatments on the properties of Al₂O₃-GPTMS-PMMA hybrid dielectric layers for applications to high-performance amorphous Indium Gallium Zinc Oxide (a-IGZO) thin film transistors (TFTs). The hybrid layers were deposited by an easy dip coating sol-gel process at low temperature and then treated with dry-air plasma at 1, 2 and 3 consecutive cycles. Their properties were analyzed as a function of the number of plasma cycles and contrasted with those of the untreated ones. The dielectric characteristics of the hybrid layers were determined from I-V and C-f measurements performed on metal-insulator-metal and metal-insulator-semiconductor devices. The results show that the plasma treatments increase the surface energy and wettability of the hybrid films. There is also a reduction of the OH groups and oxygen vacancies in the hybrid network improving the dielectric properties. The incorporation of nitrogen into the hybrid films surface is also observed. The plasma-treated hybrid dielectric layers were applied as dielectric gate in the fabrication of a-IGZO TFTs. The best electrical performance of the fabricated TFTs was achieved with the 3 cycles plasma-treated hybrid dielectric gate, showing high mobility, 29.3 cm² V⁻¹ s⁻¹, low threshold voltage, 2.9 V, high ION/OFF current ratio, 10⁶, and low subthreshold swing of 0.42 V dec⁻¹.



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**[MEM-42] Low-toxicity Chemical Solution Deposition of Ferroelectric
doped-HfO₂ for Energy Applications**

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Hafnium oxide, HfO₂, is an insulating material with a band gap of 5.5 eV and a high dielectric constant. It has been studied, for decades, as a high-k dielectric to replace SiO₂ in silicon-based transistors. However, in 2011 Böscke et al. found that piezoelectric and ferroelectric response can be produced with the introduction of dopants to stabilize the orthorhombic phase of HfO₂. Although the high piezoelectricity of PZT systems (Pb(Zr_xTi_{1-x})O₃) is well known, lead is highly toxic. Therefore, HfO₂ has been regarded as a material with great potential for information storage devices, electromechanical systems, piezoelectric-power generation, and energy storage. Techniques such as sputtering, atomic layer (ALD) and pulsed laser (PLD) deposition have produced highly ferroelectric doped-HfO₂ thin films with P_r up to 45 μC/cm². However, they have some disadvantages such as high operating cost and toxic precursors. To achieve a large-scale application of HfO₂ at low cost, on large areas and with non-toxic raw materials, new synthesis, and optimization of HfO₂ film-fabrication methods are required. Chemical solution deposition methods recently achieved a P_r of 15 μC/cm² in doped-HfO₂, but they still need to be optimized. Nevertheless, current chemical approaches make use of highly unstable and toxic compounds as hafnium chlorides and alkoxides, and corrosive solvents as carboxylic anhydrides among other poisonous precursors; all of which require restrictive inert-atmosphere conditions. In our work, we have focused on the sustainable synthesis of good-quality Zr-, or Ca- doped-hafnia films by employing much less or non-toxic chemical precursors such as stable hafnium organic salts, low toxicity solvents as alcohols and some stabilizing agents. As a consequence, no special synthesis conditions are required, which makes the processing simpler, cheaper and more flexible. We have produced metal-insulator-metal structure micro-capacitors with high-k values by employing the hafnium-based oxide films deposited by spin-coating. For these devices, we have calculated dielectric constants of 22 - 29 at 1 MHz and current leakage as low as 1.6X10⁻⁷ A/cm² for 100 nm thick films, which is in the range of good high-k dielectrics for CMOS technology. Depending on the rapid annealing treatment, the films have also showed ferroelectric behavior after wake-up cycling, which is evidence of the stabilization of the polar orthorhombic phase. In order to study and optimize the piezoelectric properties of HfO₂ based devices for energy harvesting applications, current work is being done to improve the ferroelectric response and the remnant polarization of the films. Our final goal is to produce piezoelectric hafnia-based devices by spray-coating for MEMS implementation.



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**[MEM-111] Low temperature solution synthesis route for the fabrication
of CdS/TiSiOx-PVP thin film transistors.**

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This work describes a low-cost method for fabricating a complete solution processed field effect transistor (TFT) at low temperature without the need of a clean room. This study illustrates the solution deposition of semiconductor and dielectric layers. To create a hybrid material with a flexible characteristic, silicon oxide and titanium oxide were utilized as inorganic phases and polyvinyl phenol (PVP) as an organic phase. To achieve a thin layer, the dielectric hybrid was synthesized using a low temperature sol gel method and coated by spin coating. A morphological study using FTIR was performed to verify the Ti-O-Si phase and the organic phase's connection. At 0.1MV/cm, the leakage current density is in the order of 10^{-9} and the dielectric constant is 7.3 at 1kHz. The TFT was fabricated using a bottom gate and top contacts architecture, and the CdS semiconductor was coated using chemical bath deposition at 70°C over the hybrid dielectric. The fabricated TFT shown exceptional electrical properties, i.e., The mobility, on/off ratio, subthreshold swing (SS), and threshold voltage of the devices were determined to be $80 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$, 10^3 , 0.4 and -0.4, respectively, using family curves and transfer characteristics. Chemical synthesis's ability, their low temperature solution processing, and their mechanical flexibility all provide the opportunity for device manufacturing at a low cost, as well as large-area and flexible applications.



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**[MEM-263] Characterization and properties of Al₂O₃/ZnO thin film
transistors prepared by PE-ALD at low temperature**

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Thin film transistors (TFT) were fabricated by plasma-enhanced atomic layer deposition (PE-ALD) of zinc oxide (ZnO) and aluminum oxide (Al₂O₃) on glass substrates at 70 °C. The thicknesses of the Al₂O₃ (gate dielectric) and ZnO (n-type semiconductor) were 25 and 60 nm, respectively. Prior to Al₂O₃ deposition Cr/Au gate contacts were deposited by e-beam evaporation and patterned using photolithography. Aluminum layer with thickness of 200 nm was used for source and drain contacts defined by photolithography. TFTs with W/L ratios between 8 and 1 were fabricated by varying the channel length L (5, 10, 20 and 40 μm), while the channel width W was kept constant at 40 μm. Additionally, serpentine resistors with various lengths and capacitors with various areas were prepared as control structures. Capacitance-voltage measurements revealed good uniformity of the Al₂O₃ layer seen as a linear dependence between the capacitor area and capacitance. The obtained dielectric constant of Al₂O₃ has a value of ~ 8 in the frequency range of 5 kHz to 5MHz. The sheet resistance of the ZnO layer was found to be ~ 2400 Ω/sq. The TFT electrical characterization showed that the saturation mobility (μ_{sat}) does not depend substantially on W/L ratio and had values between 1.4 and 1.5 cm² V⁻¹s⁻¹, while the slope subthreshold swing (SS) varied between 190 and 225 mV/dec. Moreover, a high on/off current ratio of 10⁸ was determined. The threshold voltage was obtained in the order of 2.2 V for all the W/L ratios. The excellent properties of the Al₂O₃ and ZnO layers deposited by PE-ALD at low temperature allowed fabrication of TFTs, capacitors and resistors promising for application in transparent flexible electronics.



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**[MEM-10] Electrical Behavior of Hafnium Oxide Gate-Dielectric under
Temperature and Electrical Stress for Flexible Electronics**

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Hafnium oxide have been previously reported as gate dielectric on flexible electronic devices towards biomedical applications, where thin-film transistors (TFTs) are the main circuitry component. In this work the electrical behavior and lifetime of hafnium oxide (HfO₂) -based metal-insulator-metal (MIM) capacitors are presented. The MIM capacitors where fabricated on top of a flexible and softening polymer as mechanical substrate by atomic layer deposition technique and photolithographic processes, at 100 °C. The electrical behavior for capacitance-frequency, current-voltage, and time dependent dielectric breakdown (TDDB) were analyzed in this work. Posteriorly, the capacitors were subjected to different temperatures in order to compare the relationship between temperatures conditions and electrical performance. The TDDB analysis with different temperatures shown the changes of the electrical behavior which allows to estimate the lifetime and reliability of the HfO₂ for gate-dielectric on TFTs, and therefore complex circuits on bioelectronic applications.



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[MEM-54] Synthesis of binary compound semiconductors (tin oxide and zinc oxide) as thin films by SILAR method and the influence on the deposition parameters

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Metallic oxide materials commonly obtained by solution-processes for electronics application have attracted interest in the last years due to unique conditions as low cost and low process-temperature. These oxides have been used to improve the electrical characteristics of p-n junctions in microelectronic devices. The solution-processes have been recognized as potential substitutes of vacuum deposition methods by a huge cost reduction and enrichment on structural, optical, and electrical properties. Tin (IV) oxide (SnO₂) and zinc oxide (ZnO) thin films were wet chemically synthesized over glass substrates using the Successive Ionic Layer Absorption and Reaction (SILAR) method, which is economical, simple, and easy-processing method. SnO₂ material was obtained from 2 solution precursors: tin sulfate as cationic source and sodium sulfate as anionic source along with 2 rinsing baths in deionized water after each precursor immersion. ZnO material was obtained from: zinc chloride and ammonium hydroxide as cationic source and deionized water at 90°C as anionic source along with 2 rinsing baths in deionized water after each precursor immersion. The resulting thin films were studied through settings in the deposition parameters as: molar concentrations, pH, time, bath temperature and thermal treatments, etc. This is to search the feasibility and reproducibility in the several devices fabrication of technological interest. The structural, optical, morphological, chemical, and electrical properties of the thin films were analyzed by x-ray diffraction (XRD), ultraviolet-visible spectroscopy (UVvis), scanning electron microscopy (SEM), energy-dispersive x-ray spectroscopy (EDS) and current-voltage, respectively. Both materials were characterized with and without thermal treatments at 200 and 400°C. Later, these properties were tuned according to deposition parameters to implement thin films with ideal characteristics inside solar cell devices.

Keywords: metallic oxides, tin oxide, zinc oxide, semiconductor material, successive ionic layer adsorption and reaction (SILAR) method.



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**[MEM-84] Design, manufacture and characterization of a thin film photo
sensor device**

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Thin film device fabrication technologies have been a topic of constant interest and development in recent years. Microelectromechanical systems with a variety of functions including optical sensors, photovoltaic structures, biosensors, and other interesting MEMS devices have been successfully developed by some national institutions. In this work, we report the progress in the development of a radiation detector device, based on a photo resistive sensor and a voltage divider conditioned circuit. This design is proposed for the detection of luminous light energy from the variation of electrical resistance of PbS thin film obtained by the Chemical Bath Deposition (CBD). In the system, the electrical resistance change signals are transformed to one sign for the excitation/unexcitation voltage change output signals that reach the base of a transistor and finally to a controller of the luminous load in the system, the variation of the electrical resistance is transformed into a binary voltage signal (on / off) connected to the base of a transistor which finally controls a light charge controller.. The electrical characterization of the PbS films is reported as part of the evaluation of their potential as the optical sensor of this system. The difference in the electrical properties of the materials measured in light exposure with respect to their measurement in darkness is clearly seen, the PbS films become less resistive when exposed to light, enough to appreciate this response in the developed device. What is interesting about this proposal is the simplicity of its design, the low cost of fabrication with a minimum of laboratory infrastructure and its functionality as a radiation detector.

Keywords: thin film devices, semiconductor, optical sensors.



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**[MEM-128] Quantitative Surface Stress determination in microcantilevers
using a fiber-based Fabry-Perot Interferometer for BSA protein detection**

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Molecular binding over a biosensing surface promotes a change onto the surface stress that can be used for biological detection. This is the key mechanism for a suspended biosensor array operating in static mode. In that case, the sensing surface is functionalized with a bioreceptor film that exhibit high binding affinity to the target molecules, which lead to a proportional bending. This work is focused on the experimental analysis and extraction of surface stress onto silicon microcantilevers ($500 \times 90 \times 1 \mu\text{m}^3$ and $750 \times 90 \times 1 \mu\text{m}^3$) which are used for biological detection of Bovine Serum Albumin (BSA) proteins and the pesticide carbaryl. The experimental setup is developed for achieving a detectable concentration below of $20 \mu\text{g/L}$, according to the resulting mechanical deflection with an out-of-plane displacement resolution of 1nm. This scheme is validated by the well-known Stoney and Tamayo equations. In order to monitor the changes in the microcantilever surface stress, when targeted molecule is detected, an optical technique has been implemented consisting of a pair of extrinsic optical fiber Fabry-Perot interferometers (EFPI) in parallel. The deflection of the microcantilever modifies the length of the Fabry-Perot cavity, formed between the fiber tip and the microcantilever surface, producing a phase shift of the interference pattern.



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**[MEM-200] pH Sensor Based on Mesoporous Silica Extended Gate Field-
Effect Transistor**

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In recent decades there has been unprecedented interest in the development of analytical devices for the detection of different biological and chemical compounds. Sensors based on semiconductor structures have received considerable attention. In this study, mesoporous silica was prepared and tested as a modification of the gate surface on ion-sensitive field-effect transistors (ISFETs) for pH sensing. The mesoporous silica has pore sizes in the range of 20 to 50 nm. The results of testing for hydrogen ion sensing in different pH buffer solutions in the range of 4 to 9 reveal that has a sensitivity value of 51 mV/pH at 25 °C, the pH current sensitivity obtained was 0.49 $\mu\text{A}^{1/2}/\text{pH}$. The higher surface-to-volume ratio with a larger effective surface area of the mesoporous silica is the main reason for the good pH voltage sensitivity, this reveals a promising application in the field for detecting hydrogen ions in different solutions



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MULTIFUNCTIONAL AND MAGNETIC MATERIALS

Chairmen:

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Materials capable of performing two or more primary functions, either simultaneously or sequentially, are called multifunctional. Those can be hybrid materials, that is, a mixture or combination of two materials of different compositions or crystalline phases (alternating layers of thin films, for example) or single-phase materials that may behave multifunctional under applied electric and/or magnetic fields. Besides, the technology around us has a fundamental basis in magnetic materials. They are one of the key materials for mechanical energy conversion to electrical power.

Between the multifunctional materials, there is a great assortment of ceramics, which are used in electronic devices such as actuators, sensors, switches, capacitors, oscillators and may also be used to make engines. Magnetic, piezoelectric, pyroelectric and ferroelectric materials are extensively studied in present days not only for their potential technological applications but also because the understanding of the behavior and properties involves many phenomena that are in the frontier of knowledge such as "magnetoelectricity", a property present in some multiferroic materials. For example, the fascinating magnetic spiral and helical structures that give place to an electrical polarization in some ceramics (making them multifunctional) are a real challenge for the theoretical and experimental researchers in this field.

This symposium is a forum to present the results of theoretical and experimental research that may include synthesis routes, sintering procedures, analysis, and characterization of the properties, as well as practical applications of the multifunctional and magnetic materials. Regarding the theory, we are interested in studies that allow a deep understanding of the involved phenomena, to design new materials, to predict their behavior, and as a guide to improve on existing ones.



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**[MUL-70] Contrasting experimental and simulated piezoresponse loops of
Bi_{0.9}Ba_{0.1}Fe_{0.94}Ta_{0.05}Cr_{0.01}O₃ films as a function of compressive stress
and internal electric field**

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The behaviors of the remanent polarization, the coercive electric field, and the piezoelectric coefficient of a ferroelectric under different conditions of uniaxial stress and internal electric field (E_{in}) were numerically simulated. The simulation takes into account the temporal evolution of the polarization (P) and the strain (ϵ) triggered by the variations of an external electric field (E_{ext}) that emulates on-field and off-field experimental conditions. The dynamic equations were derived from the Landau-Khalatnikov equation, which in turn involves the free energy density of the system. The free energy density was expressed as a series of even powers of P , according to the Landau-Devonshire theory, plus strain-dependent terms. A term representing the coupling between E_{in} and P was also added to the energy density. E_{in} represents the electric field of a real ferroelectric system due to its synthesis process or by injection charges. The P and ϵ vs. E simulated loops were compared with experimental results. The experimental hysteresis loops were obtained from piezoresponse force microscopy measurements with switching configuration on ferroelectric Bi_{0.9}Ba_{0.1}Fe_{0.94}Ta_{0.05}Cr_{0.01}O₃ films deposited by pulsed laser deposition. The loops were obtained at points of areas with an electric field induced by injection charges. The qualitative similarity between the experimental and simulated hysteresis loops



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confirms that the simulation reproduces the ferroelectric behavior. The shape of the ϵ - E loops is discussed in terms of compressive stress and internal electric field.



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**[MUL-180] Antimicrobial effect of Vicugna pacos "alpaca" fibers
functionalized with silver nanoparticles**

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Vicugna pacos "alpaca" is the main source of animal textile fibers that can be found in the Peruvian mountain range due to its excellent characteristics. Currently, nanotechnology allows us to modify the surfaces of compounds through functionalization with nanoparticles. The objective of this research was to evaluate the antimicrobial activity of brown alpaca fibers functionalized with silver nanoparticles synthesized by chemical means, with different concentrations of TCS. The functional fibers were characterized using UV-vis and Raman spectroscopy, and the modified AATCC 100 methodology was applied to determine the antibacterial effect. The average particle size could be determined by absorbance and reflectance techniques through the resonance of the surface plasmon. The antimicrobial effect was expressed as a percentage reduction with 96.073 and 99.990% for *E. coli* and *S. aureus* as the highest values, the statistical analysis did not find significant differences due to the groups of bacteria, as well as between the treatment of 6 and 10mg by TCS. Therefore, we can conclude that functionalized alpaca fibers have a high antibacterial activity against both bacteria equally and increases with the content of TCS until reaching a maximum of 6 mg.

Keywords: Alpaca fibers, functionalization, antimicrobial, nanotechnology, silver nanoparticles.



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**[MUL-213] Looking for magnetocaloric effect in superparamagnetic Ni-Zn
based ferrite around its blocking temperature**

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The coprecipitation method was used to produce superparamagnetic Ni_{0.3}Zn_{0.7}Fe₂O₄ ferrite nanoparticles using nickel, zinc, and iron nitrates as raw materials. Sodium Hydroxide was the precipitating agent and distilled water as the solvent. Subsequently, high-temperature calcination was used to obtain the powders with the desired phase. Through scanning electron microscopy, the morphology of the powders was observed. Later, X-ray diffraction patterns verified that the calcination parameters were adequate for forming the single crystalline phase. The magnetization behavior of the samples was determined by measuring the hysteresis loops with a vibrating sample magnetometer. The blocking temperature, T_B, was determined from the ZFC curve as T = 229 K. The temperature range from 230 to 345 K was defined to measure the thermoremanence curves to determine the maximum value of ΔSm by numerical integration of the Maxwell equations. Finally, data shows that the variation of magnetic entropy around TB is higher enough to research the magnetocaloric effect for these superparamagnetic materials.



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**[MUL-3] Magnetic Nanostructured Based On Cobalt - Zinc Ferrites
Designed for Photocatalytic Dye Degradation**

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This work focuses on the design and manufacture of multifunctional materials for the degradation of dyes contained in effluents of the textile industry. The design is based on $\text{Co}_{0.25}\text{Zn}_{0.75}\text{Fe}_2\text{O}_4$ ferrite nanoparticles with super-paramagnetic behavior used as seeds of the Stöber process to produce spherical SiO_2 particles. The SiO_2 bead works as a template where the $\text{Co}_{0.25}\text{Zn}_{0.75}\text{Fe}_2\text{O}_4$ ferrite is mechanically stabilized to avoid particle agglomeration and the loss of the super-paramagnetic behavior. After that, the SiO_2 bead is coated with ZnO ultrathin layer via an atomic layer deposition technique (ALD). The materials were characterized for morphology, size, composition, magnetic response, and photocatalytic activity using different techniques. The final $\text{Co}_{0.25}\text{Zn}_{0.75}\text{Fe}_2\text{O}_4$ nanostructured material showed good mechanical stability, excellent magnetic response, and high efficiency in the catalytic degradation of toxic red amaranth dye under UV irradiation. The results showed that these materials are suitable to be used as efficient photocatalysts and recovered from wastewater using magnetic separation protocols.

Keywords: Multifunctional materials; magnetic nanostructures; photodegradation; atomic layer deposition.

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**[MUL-63] Interphase effect on the effective magneto-electro-elastic
properties of periodic three-phase fiber-reinforced composites using a
semi-analytical approach**

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The effective properties knowledge of composite materials is an important problem. The characterization of multi-phase fiber-reinforced composites (FRC) has been studied by means of theoretical modelling, simulation or experimentally techniques due to their wide field of applications. These tools support the design of experiments in the search for new materials with desired and optimized properties as a guide to improvement. In this work, a semi-analytical method is developed to predict the effective magneto-electro-elastic properties of a three-phase periodic FRC. The fibers are infinitely long unidirectional concentric cylinders distributed in a periodic square array. The analytical formulation of the local problems and effective properties are obtained by means of the two-scale asymptotic homogenization method (AHM). Local problems are solved by finite element method (FEM) via the principle of minimum potential energy. The effect of interphase thickness and the fiber material properties on effective moduli is analyzed. The results obtained by the application of AHM, solved via potential theory, are compared with those of a semi-analytical method. Very good agreement is obtained. The use of the combined AHM and FEM allows the treatment of more complex microstructures.



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**[MUL-71] Synthesis of BiFeO₃ doped with Al³⁺ obtained by the
conventional solid state route using high energy milling**

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Barium titanate (BaTiO₃ or BTO) and lead zirconate titanate (Pb[Zr_xTi_{1-x}]O₃ or PZT) are ferroelectric ceramics widely used in devices, however this materials have some disadvantages. Such as low Curie temperature (CT) of 130 °C for BTO and high lead content in PZT. Ceramic bismuth ferrite (BiFeO₃ or BFO) is one of the most important material of the multiferroic family with a perovskite ABO₃ structure. BFO can be synthesized by a large number of techniques and has excellent photovoltaic, electrical and magnetic properties above ambient temperature. It has a CT of 830 °C and is lead-free, but has drawbacks in technological applications derived from a high leakage current density. Aluminum (Al) was used as a doping for BFO due to the excellent dielectric, piezoelectric, ferroelectric and optical properties of bismuth aluminate (BiAlO₃ or BAO). However, BAO has only been synthesized at high pressures and high temperatures simultaneously, making its study significantly difficult. In this work, the microstructure, relative density and crystal structure of BiFe_{1-x}Al_xO₃ ceramics with x = 0, 0.015, 0.030, 0.045 and 0.060 obtained by the conventional solid state route were investigated. In addition, Rietveld refinement was performed on each of the samples. To obtain the ceramics, bismuth oxide (Bi₂O₃), iron oxide (Fe₂O₃) and aluminum oxide (Al₂O₃) powders were first mixed in stoichiometric proportions for 3 hours using a SPEX high-energy ball milling and later they were calcined and sintered at 725 °C. X-ray diffraction data (XRD) indicated distorted rhombohedral perovskite formation. With the increase of Al in the BiFe_{1-x}Al_xO₃ system, the decrease of secondary phases was promoted and the relative density of the samples decreased from 95.02 to 86.20% for x = 0 and x = 0.060, respectively. The images obtained by scanning electron microscopy (SEM) indicated a reduction in grain size: 544, 478 and 258 nm for the samples with 3, 4.5 and 6% of Al, respectively.



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**[MUL-72] Effect of co-doping on structural, optical and ferroelectric
properties in lead-free perovskites**

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Advanced ceramics have a wide variety of properties, such as mechanical, electrical, thermal, magnetic and optical. Among those with outstanding electrical properties are ferroelectric materials. These are characterized by having a high dielectric constant, presenting the piezoelectric effect and possessing ferroelectric properties. Due to these properties, they have a large number of applications such as actuator devices, sensors, and in general, all those areas of electronics and microelectronics, that is, from cell phone components, medical equipment, computers, cars, airplanes and satellites. BiFeO₃ base ceramics with small doping of titanium oxide (TiO₂) and zinc oxide (ZnO) were manufactured by the solid state route in order to evaluate the effect that substitution has on the structural, optical and ferroelectric properties in this system. The ceramics obtained were characterized by X-ray diffraction (XRD) to determine the crystalline structure which was perovskite type, scanning electron microscopy (SEM) for microstructure and grain size behavior, in addition to the presence of secondary phases rich in Fe and Bi, ferroelectric polarization - electric field hysteresis curves (P - E) were used to determine remanent polarization values, where ceramics with 7% of Ti and Zn had a Pr = 0.863 μC / cm³, the identification of electrical behavior was studied through current - voltage curves (I - V). The coexistence of phases in the co-doped samples (rhombohedral and tetragonal) was determined, which improved the ferroelectric behavior by allowing a partial reorientation of domains, in addition, a modification was observed in the band gap of powders of this system, from 2.26 to 2.35 eV, which was attributed to the deformation of the Jahn-Teller octahedron.



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[MUL-186] Soft magnetic properties in Fe-Co-Ni low entropy alloy

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Nowadays magnetic materials have attracted great attention due to their versatility in diverse technological applications, the modern application of soft magnetic material with low Curie temperature is magnetic refrigeration based on magnetocaloric materials. a modern magnetocaloric material is the so-called high entropy alloys which consist of a mixture of five elements at the same proportion, these alloys exhibit soft magnetic properties with a Curie temperature at room temperature, these properties are essential in a magnetocaloric material. This work is presented a low entropy alloy based on Fe Co Ni at different proportions, the objective of this work is to obtain a low entropy alloy with a Curie temperature closer to room temperature. The experimental results show that the elaborated alloys by electric arc furnace have an FCC crystal structure with no secondary phase. EDS analysis confirms each element's proper elemental content, magnetic properties confirm soft magnetic properties in the alloys. In conclusion, the alloys have their Curie temperature above room temperature, so it's possible to diminish the temperature by adding a fourth or fifth nonmagnetic element to create a dilutional effect in the ferromagnetic order of the alloy to reduce its Curie temperature at 298 K to make them attractive for magnetic refrigeration.



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**[MUL-280] Photosacoustic spectroscopic of thin films of Gd₃Fe₅O₁₂ and
SrFe₁₂O₁₉**

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The demand to develop new materials with outstanding magnetic properties for magneto-optical, microwave and electrochemical, etc. applications has brought up a great variety of studies of new and well-known materials alongside with their intrinsic experimental techniques of synthesis. In this work, we report the synthesis of Gd₃Fe₅O₁₂ and SrFe₁₂O₁₉ by means of the pulsed laser technique. Briefly, the growth of the thin films was conducted by considering targets of the materials mentioned above using a fluence of 2.5 J / cm² with a repetition time of 10 Hz in an oxygen atmosphere of 100mT. During the growing stage of the thin films, the substrate was heated to reach a temperature of 700 °C. Derived from previous photoacoustic studies, the annealing process of the thin films was conducting at 500 and 1000 °C during 2 hours under air and Argon atmosphere separately. Finally, the characterization of the materials obtained was performed by Raman, photoacoustic and XRD spectroscopies as well as by scanning electron microscopy.

Keywords: thin films, laser ablation, Photoacoustic.

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The symposium scientific program will cover a wide spectrum of topics including physical phenomena, materials sciences, and applications of nanostructures. The diversity of topics provides an opportunity to broaden the knowledge on latest developments and future perspectives in nanostructures research. Current development in the nanostructured materials includes: (i) Synthesis, functionalization, processing and self-assembly of nanoparticles, (ii) Nanotubes, nanowires, quantum dots and other low dimensional structures, (iii) Bio-active nanomaterials and nanostructured materials for bio-medical applications, (iv) Carbon nanostructured materials, Nano-structured membranes, nano-porous materials, functional coatings, (v) Nanomaterials for photo-catalysis, solar hydrogen and thermoelectric, (vi) Nano-fabrication, characterization and manipulation techniques for nanostructures, (vii) Magnetic and nano-semiconductor materials, (ix) Industrial development and application of nanomaterials and (x) Theoretical studies of nanostructured materials.

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[NSN-12] Particle aggregation and gelation in nano-colloidal dispersions

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Particle aggregation or clustering is an obligatory step for the initiation of the phase separation or the large-scale formation of materials that exhibit a heterogeneous structure, such as gels and porous media. Nevertheless, even though the macroscopic structure of such materials depends on the shape and size of the resulting clusters or aggregates, the cluster formation at equilibrium and its corresponding morphology are not fully understood. The local morphological information is also important for the identification of the physical mechanisms for arrested states of matter, especially gels and glasses, which remains a hotly debated research topic in condensed matter physics. Due to the complex nature and different microscopic details of each particular system, a general, consistent and unified definition is of paramount importance from both scientific and technological viewpoints. Combining molecular simulations, experimental characterizations and theoretical calculations: 1) we conclusively demonstrate that the cluster morphology in short-ranged attractive colloidal systems (SRACS) at equilibrium conditions can be uniquely determined by the reduced second virial coefficient; our findings link the reversible colloidal aggregation with the extended law of corresponding states, and 2) we show that gelation in nano-colloidal dispersions is the result of the rigidity percolation with coordination number equal to 2.4; these results connect the concept of critical gel formation in SRACS to the universal concept of the rigidity percolation.



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**[NSN-28] Recent advances on bulk and supported transition metal sulfide
catalysts**

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Transition metal sulfides have been used as hydrotreating catalysts since the first half of the past century due to their properties for double bond hydrogenation as well as hydrogenolysis of C-S, C-N, C-O and C-M bonds. These catalytic properties are particularly relevant when the presence of sulfur compounds causes metal catalysts to become poisoned. Such a behavior made them very attractive for industrial applications and therefore, the refining oil industry uses them in various processes. Important issues for hydrotreating catalysts such as the use of promoters, the effect of alumina as support, the nature of active sites, and the dependence on reaction conditions (P, T, SV) have been intensively investigated for a long time and are now very well established, however, recent advances about the morphology and electronic properties of TMS nanoparticles bring new insights that may help to optimize and improve their catalytic properties. Recent advances in morphology and electronic properties of bulk TMS as well as the effect of non-traditional supports such as meso porous silica, zeolites and alumina nanorods will be presented.



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**[NSN-29] Evaluation of the optical and structural properties of NiCo₂O₄
obtained using the sol gel technique**

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The synthesis of Co_{3-x}Ni_xO₄, x = 0.01, 0.04, 0.10, 0.16 was carried out using the sol gel technique with final heat treatment at 1000 °C. The samples were characterized by X-ray Diffraction (XRD) indicating the appearance of the characteristic peaks of NiCo₂O₄, as well as CoO product of the phase transition by temperature. Results of Fourier Transform Infrared (FT-IR) indicate the appearance of characteristic peaks of nickel cobaltite with visible displacements due to doping, being higher for 16% of nickel. Scanning electron microscopy (SEM) analysis indicates that the smallest particle size is 269 nm for the lowest nickel concentration and 376nm for the highest. Visible ultraviolet spectroscopy analysis allowed determining the Band Gap (*E_g*) values in the two regions of the samples for the different doping, indicating variation between 1.92 eV and 2.18 eV. The final objective of the synthesis of cobalt oxide with nickel doping is to determine the best condition for the deposit of samples for application in the detection of acetone, used as a biological marker for the detection of diabetes.



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**[NSN-37] Modification of multiwalled carbon nanotubes structures with
natural and synthetic porphyrins for the removal of heavy metals**

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The present work describes how three types of multiwalled carbon nanotubes (nitrogen doped and pristine and acid-oxidized multiwalled carbon nanotubes), were modified with protoporphyrin IX and natural porphyrins extracted from hibiscus tiliaceus. The purpose of the synthesis was to use them to remove heavy metals from water. Two different methods were used to combine the carbon nanotubes and porphyrins, the first was done by sonication and the second heating while stirring. Once obtained the composites, they were characterized by Raman spectroscopy, field emission scanning electron microscopy, ultraviolet-visible and fluorescence spectroscopy.

In all cases, the interaction between both compounds was confirmed by the significant quenching of signals measured by optical techniques, also we found the formation of covalent bonds indicated by the shifting of the absorbance peaks, showing the formation of J or H aggregates. The nanotube thickness increased and it was more significant in the multiwalled carbon nanotubes vs. the doped ones, also we found that in the case of the natural compounds, the interaction between both materials increased as the time went on so that the coating grade make us believe that this new material can be used in fields as gas sensing as for the water remediation for which they were initially synthesized.



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[NSN-48] Optical transmission of periodic dielectric multilayers

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Periodic structures made of dielectric thin films exhibit sharp optical transmission spectrum. Applications of these structures may include optical filters as well as optical mirrors. In this work, we study the transmission spectrum of periodic systems made of dielectric-dielectric thin films. We examine different dielectric-dielectric configurations starting from experimental dielectric functions and refractive index in the visible and infrared region. The combination includes a low and high contrast in the dielectric functions with values from 1 to 2000. The results show that a reduction in thickness and increase in the bilayers number, holding constant the total multilayer thickness, causes shifting on the transmission spectrum to short wavelength. On the other hand, the fill factor can be tunable to get a wide passband filter up to 1 micron in the infrared region. The study of these systems allows an easy analysis of the optical response before performing efforts in experimental manufacturing.



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[NSN-102] Molecular beam epitaxial growth and doping of cubic GaN

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The zinc-blende structure of GaN is a meta-stable phase with important advantages over the wurtzite counterpart, which makes it a promising material for applications in microelectronic and optoelectronic devices [1]. For example, spontaneous and piezoelectric polarization are not present along the cubic (100) orientation, in addition due to its high symmetry the mobility of holes should be greater than those obtained for the hexagonal phase [2]. Moreover, because cubic GaN (c-GaN) has a smaller band-gap energy, less Indium concentration is required to achieve lower band-gap energies in InGaN alloys. In the first part of this talk, I will present details of the growth of cubic GaN on GaAs (100) substrates by molecular beam epitaxy (MBE) equipped with a radio-frequency (RF) plasma source to produce reactive atomic nitrogen [3]. In particular I will show the method that we used to control the very early stages of heteroepitaxy to obtain cubic phase GaN with high crystalline quality. Then, I will discuss our results of the growth of p-type GaN with magnesium as a dopant. Employing appropriate growth conditions, we were able to obtain p-type c-GaN with a hole concentration higher than $5 \times 10^{19} \text{ cm}^{-3}$. The high p-type doping efficiency in c-GaN is due to the low Mg activation energy. Employing DFT calculations and a variety of experimental techniques, we found that the Mg ionization energy in c-GaN is around 100 meV, which is lower than that of the hexagonal phase (around 200 meV).

[1] Y.L. Casallas-Moreno, et al. Appl. Surf. Sci. 353 (2015) 588–593.

[2] C.A. Hernández-Gutiérrez, et al. Sci. Rep. 10 (2020) 1–7.

[3] M Pérez-Caro, et al. J. Appl. Phys. 128 (2020) 215304.



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**[NSN-103] Biomedical applications of magnetic and non-magnetic
nanomaterials**

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Nanomedicine is an interdisciplinary field focused on the design, synthesis and application of nanomaterials to solve health related problems. It has been estimated that nearly 16 % of materials used in biomedical and biotechnological applications will contain nanomaterials. The market for nanomaterial applications in health is calculated to be in the range from 750 to 2,000 million dollars annually. The versatility in unique composition, size, morphology and physical properties for nanomaterials, added to their surface chemical modification to improve biocompatibility and target specific recognition (cells, tissues, organs), make very promising the therapeutical, drug delivery, diagnostic and medical imaging applications. Magnetic nanomaterials in particular have interesting properties, as they can be easily manipulated under an external magnetic field; depending on their chemical composition they can be biocompatible and their biodistribution can be monitored using magnetic resonance imaging (MRI). In this seminar, we will discuss some recent advances on the development of biocompatible magnetic –and some non-magnetic- nanomaterials, their potential use for cancer therapy, brain drug delivery, colorimetric biosensors for viral infection, among other potential uses.



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**[NSN-115] Immobilization of glucose oxidase onto self-supported gold
nanowires array for amperometric glucose biosensors**

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In this work, we present different methodologies to immobilized glucose oxidase (GOx) onto self-supported gold nanowires (AuNWs) as support to promote electron transfer reactions of GOx. The primary motivation is the great significance that glucose detection implies in biomedical applications. Diabetes Mellitus is one of the leading causes of death in the world, and this disease is caused by an insulin deficiency, causing abnormal (elevated) blood glucose concentrations. For that reason, many scientists are focusing on investigating new alternatives of bio-sensors, highly sensitives and selective. GOx enzyme is widely utilized as a bio-element in most available glucose sensors because of its low cost and selectivity [1]. Nevertheless, immobilized GOx onto nanostructures is still challenging due to maintain the entire catalytic activity after immobilization. We propose four methodologies based on the modified cross-linking and physical adsorptions technics for immobilizing GOx into AuNWs, and their performance was compared. This nanowires array was synthesized by electrodeposition using a porous membrane as template, which was subsequently removed to leave only the self-supported nanowires. The pre- and post-immobilization nanowire arrays were characterized by SEM, TEM, UV-VIS, and amperometric tests varying glucose concentrations for each methodology. Characterization by UV-VIS results in a continuation of the enzyme's catalytic activity and an apparent acceleration in the catalysis reaction. By SEM and TEM, it was possible to observe the morphology of the nanowires and how the enzyme adheres to the nanowire surface from the different methodologies proposed for GOx immobilization. The amperometric tests using approximately 0.15 enzyme units (U), comparable to commercial sensors with ~ 3U, were obtained.

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**[NSN-120] ZnSe nanoparticles prepared by coprecipitation method for
photocatalytic applications**

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Pure zinc selenide (ZnSe) nanoparticles (NP's) and ZnSe NP's with traces of elemental selenium (ZnSe:Se) were synthesized by the coprecipitation method. The results from the physicochemical characterization were analyzed and correlated with the photocatalytic efficiency in hydrogen production and degradation of rhodamine b (RhB) for each sample. From X-ray diffraction (XRD) analysis the formation of a zinc blende type ZnSe with the presence of elemental Se was detected and a crystallite size of ~6 nm was calculated. The scanning (SEM) and transmission (TEM) electron microscopies showed ZnSe NP's with a spherical morphology. From ultraviolet-visible (UV-Vis) spectroscopy a red shift of absorption edge was observed when Se traces are present in ZnSe-NP's. The enhanced photocatalytic activity of ZnSe:Se NP's obtained from hydrogen production and RhB degradation was attributed to elemental Se acting as a co catalyst efficiently separating the photogenerated charge carriers.



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**[NSN-143] Influence of anthracene and benzene as precursors in the
carbon spheres synthesis**

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Carbon nanomaterials research has been dominated by CNTs studies, however spherical carbon bodies must also be considered, because they have improved properties compared to their discrete components. Carbon Spheres (CSs) are classified according to size, growth kind and graphitization degree. Several authors have reported synthesis of different types of carbon spheres such as core-shell spheres, hollow or completely solid carbon spheres in different sizes. The chemical vapor deposition (CVD) methods are commonly used for CSs synthesis. Spheres could have several applications such as reinforcement material in polymeric matrix composites, nanodevices, absorbent materials, energy storage and catalysts, due their chemical and physical properties. The aim of this research was analyze the influence of precursors in the carbon sphere synthesis by CVD method. CSs were grown on stainless steel core in to a tubular quartz reactor. The synthesis temperatures were 750, 800 and 850 °C. Reaction time was 60 minutes. Argon was used as carrier gas at 10 ml/min. The samples were analyzed by Field Emission Scanning Electron Microscopy (FESEM), Fourier Transform Infrared Spectroscopy (FTIR), and Raman Spectroscopy. FESEM micrographs confirmed a spherical morphology for all samples obtained from anthracene with 0.8 - 3 micrometer diameters. However, for benzene it was not possible to observe spheres at 750 °C, just some CNTs, but at 800 and 850°C there are spheres with diameters around 0.8 - 1.4 micrometers. The CSs center was solid and presented concentric orientation formation for all the samples, this kind of growth is associated with solid-gas interphase. CSs with small diameters tend to form chains. FTIR spectra showed a peak around 3400 cm⁻¹ corresponding to OH vibrations and also the presence of C = O in a range among 1590 and 1706 cm⁻¹. The D and G bands were observed by Raman spectroscopy around 1300 and 1600 cm⁻¹ respectively. These results are similar for all samples obtained from the two



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precursors. In conclusion, the characterization techniques showed that carbon spheres produced from benzene and anthracene are completely solid with similar characteristics. For this temperature conditions, anthracene is better in the production of the spheres than benzene, however, the smaller diameter range was obtained with benzene as precursor. The importance of carbon spheres size depends of the application. Acknowledgement to Scientific Research Coordination of UMSNH and CONACyT for the financial support.



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[NSN-232] Acicular growth of copper structures on Titania-Silica fibers

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The development of ceramic materials with copper nanoparticles has generated interest improving the properties and possible applications in catalysis. Sol-gel, electrospinning, and electrodeposition techniques allow obtaining materials with improved surface areas, with manipulation of the composition, size, and shape of the nanoparticles. In this investigation, a fibrillar material of TiO₂-SiO₂ doped with microstructures of Cu₀, CuO, and Cu₂O was elaborated and characterized. The particles presented morphologies of spheres, dendrites, and needles; using a copper ammonia electrolyte solution, a potential of 19.27 V, and different electrodeposition times.



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[NSN-253] Study of the optical and structural properties of cubic $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ quantum wells for optoelectronic applications

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III-V semiconductors have been used successfully in optoelectronic applications such as light-emitting diodes (LEDs), photodetectors (PD), laser diodes (LD), and solar cells, due to their properties. InGaN has been widely used for the growth of quantum wells (QWs), these nanostructures are used as active regions for LEDs. In this work, cubic $\text{In}_x\text{Ga}_{1-x}\text{N}$ (QWs) with GaN barriers were grown on GaAs (001) substrates varying the In content (x) by plasma-assisted molecular beam epitaxy (PA-MBE), with the aim to analyze the effect of the In content on the optical and structural properties of the QWs. 10 nm-thick QWs were grown and 30 nm-thick GaN barriers. The optical characterization was carried out with the Photoreflectance (PR) and Photoluminescence (PL) techniques. Excitonic transitions in the visible spectrum range from violet (414 nm) to green (544 nm) wavelengths were found in the QWs, with varying In content. These excitonic emissions are in good agreement with the theoretical calculations performed, where the excitonic binding energy was calculated according to the Mathieu model. These results agree with the reported literature. The chemical characterization was performed by secondary ion mass spectroscopy (SIMS) and X-ray photoelectron spectrometry (XPS). The chemical composition and binding energies in the QWs were found, which allows us to appreciate the formation of these two-dimensional nanostructures.



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**[NSN-259] Synthesis of SPIONs with direct surface polyphenol attachment
and their possibilities in magnetic hyperthermia therapy**

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The magnetite (Fe₃O₄) nanoparticles (MNPs) are the most promising superparamagnetic iron oxide nanoparticles (SPIONs) for the development of specific functions such as drug release, diagnosis, and therapy. Their addressable single magnetic domains, particle size (< 30nm), shape, composition, and surface properties have been the key tailoring the magnetic triggering of physicochemical functions in biological systems. The SPIONs have been formulated as core-shell from direct attachment with hydroxyl groups (Fe-OH). Green synthesis and wet-chemistry routes such as coprecipitation and sonochemical processing with some modifications have opened new horizons in the SPIONs processing with polyphenols, which are aromatic compounds that bear one or more hydroxyl groups. Their phytochemical features exert important biological functions like, free radical scavenging, antioxidant and anti-inflammatory effects. Direct SPIONs coating with polyphenolic surfaces is an effective alternative to improve their biocompatibility and attachment to the cell membrane, which is consistent with the different stages of an active uptake process, increasing their therapeutic possibilities. The specific biological properties of polyphenols have been recognized because of their potential for the alternative and prevention of chronic diseases such as neurodegenerative, cardiovascular, and cancer. In this work, preliminary results from the synthesis of SPIONs below 20 nm coated with polyphenols and their potential applications in magnetic hyperthermia therapy are showed.

Keywords: SPIONs, Magnetic Single Domain, Polyphenol, Hyperthermia.

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**[NSN-5] Determination of the barrier height of Pt - Ir Schottky nano-
contacts on Al-doped ZnO thin films by conductive Atomic Force
Microscopy**

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By means of the I-V characteristics measured at room temperature, the height of the Schottky barrier established by the conductive Pt-Ir tip of an Atomic Force Microscope on the aluminum doped ZnO thin films were estimated in the range of 0.58 - 0.64 eV. The ideality factors were in the range of 2.11-1.39, respectively. These values are in accordance with those reported by other authors that measured the height of the Pt Schottky barrier on ZnO by means of several methods. The procedure detailed in this work suggests that the scanning time for obtaining I-V Schottky characteristics is of the order of 2 ms.



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[NSN-9] Synthesis of hydrophobic carbon sponges from MOF type HKUST and melamine-formaldehyde sponges for the absorption of oil dispersed in water

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Currently, numerous investigations have focused on generating highly hydrophobic materials (1,2), low cost and high absorption capacity to eliminate oil dispersed in water from accidents caused during the transport of oil by sea (3,4), for this reason in this work the production of a series of carbon sponges with hydrophobic characteristics decorated with spherical metal nanoparticles on its surface is presented. The carbon sponges were synthesized using commercial melamine-formaldehyde sponges coated with HKUST type MOF, using trimesic acid as a binder and nickel, cobalt as a cations and the combination of the two mentioned cations, subsequently the coated sponges were subjected to a pyrolysis treatment in a nitrogen atmosphere at 300, 500 and 700°C. Hydrophobicity tests were performed by measuring the contact angle of the synthesized sponges and their oil absorption capacity was measured using the standardized method of ASTM F726-99, additionally, the synthesized materials were characterized with scanning electron microscopy (SEM), Spectroscopy Fourier transform infrared (FT-IR) and X-ray powder diffraction (XRD), the results obtained show that the carbon sponges obtained are promising candidates to be applied in the remediation of oil dispersed in water.

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**[NSN-14] Application of Pt and Ir catalysts supported on solid cerium-
ruthenium solutions in CO oxidation reactions**

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High surface area catalytic systems were evaluated for the carbon monoxide oxidation reaction at low temperature. Metal particles of Pt and Ir were deposited at 3% w/w on a solid solution of $\text{Ce}_{0.97}\text{Ru}_{0.03}\text{O}_2$. CO oxidation was studied under operating conditions using FTIR spectroscopy. These catalysts were characterized by BET, XRD, XPS and HRTEM. The obtained specific surface area was promising, since values greater than $140 \text{ m}^2/\text{g}$ were obtained, which are above to average values reported in the literature for CeO_2 . In addition, from the X-ray diffraction studies, we were able to verify the incorporation of ruthenium in the structure of CeO_2 , impurifying it by substituting Ce atoms, we verified this by calculating the parameters of the crystal lattice, whose value increased from 5.38 to 5.61 Å. XPS photoelectron spectroscopy let us to know the oxidation state of the Pt and Ir particles, which were found on both, metallic state and also as oxides. On the other hand, ruthenium was also superficially detected in the form of RuO_2 , as well as doping element, $\text{Ce}_{0.97}\text{Ru}_{0.03}\text{O}_2$. Among the obtained results, it was found that the Pt and Ir particles dramatically improved CO oxidation compared to pure cerium oxide, being the Pt/ $\text{Ce}_{0.97}\text{Ru}_{0.03}\text{O}_2$ system that provides the best results. From the in-situ studies, it was possible to propose a route by which the oxidation reaction takes place. This mechanism considers that CO was absorbed in the Ce and Ru sites, while O_2 is absorbed at the superficial vacancies, being activated near the Ru species. Following this, the oxygen reacts with the bound CO producing CO_2 . The reason why the system with Pt was the most efficient is because the particles promoted oxygen vacancies, increasing the activation-absorption of molecular oxygen.



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**[NSN-27] Synergistic effect of Ni doping on cobalt oxide spinel
nanostructures using the hydrothermal technique.**

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In the present investigation, synthesis of Co_3O_4 doped with nickel $\text{Co}_{3-x}\text{Ni}_x\text{O}_4$ with a percentage of Ni $x = 0.4\%$ was carried out using the hydrothermal method and subsequent calcination process at temperatures of 600°C, 700°C, 750°C and 800°C. The product obtained was characterized through XRD showing a pure nanocrystalline phase of Co_3O_4 with complete replacement of nickel in the lattice. Rietveld refinement was performed with GOF main values between 1.09 and 1.26 as well as values of X^2 between 1.28 and 1.57 indicating a good correspondence between the simulated and the experimental pattern. The particle size for temperatures from 600°C to 800°C without doping is 23.5nm and 43nm with doping. The SEM images for both types of samples are composed of assembled agglomerated particles that indicate uniform homogeneity and good connectivity between the grains. A good thermal stability can be observed since the general structures in each of the calcination temperatures are intact. The characterization means Raman spectroscopy indicates that there are five active Raman modes ($A_{1g} + E_g + 3F_{2g}$) corresponding to the phase of the spinel structure of Co_3O_4 , there are five, depending on the calcination temperature.



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**[NSN-53] Zeolite-synthesized nanostructured materials with
antimicrobial properties for water treatment applications**

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The synthesis of metal and metal oxide nanoparticles has been increasing in the last decade due to their unique physicochemical properties and nanotechnological applications such as catalysis, optoelectronics, sensors, coatings, and photothermal therapies. A novel bottom-up synthesis method for obtaining metallic and metal-oxide (Ag, Cu, CuO) nanostructures at room temperature in colloidal suspension and zeolites is presented in this work. The nanostructures were analyzed using different characterization techniques. Morphological and structural parameters were analyzed by TEM microscopy. The images corroborated the presence of silver nanoparticles in solution and powder with average sizes between 10-20 nm approximately. EDS spectrum showed evidence of the chemical composition of the synthesized nanoparticles. In the optical absorption measurements, a rightward shift of the surface plasmon resonance (SPR) absorption peak was observed as the number of milliliters of silver nitrate in the experimental process increased. According to literature reports, the band shifts may be due to structural or size changes of the nanoparticles. The obtained nanomaterials showed antibacterial activity against *Escherichia coli*.



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**[NSN-55] Recycled polystyrene coatings with low-layer graphene to
prevent damage to historical monuments by acid rain**

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Acid rain has become a potential problem that largely affects different materials and ecosystems. It is considered a type of pollution and the most appropriate term is acid deposition because acidity can be released as gas or as dust, and these particles are carried to the ground by means of rain. The effect that acid rain causes on stone monuments has been studied for several years now, but there is very little information on how to avoid this damage and maintain protection on them. On the other hand, the recycling of plastic waste is an alternative to reduce pollution due to the large amount of waste that is had. The discarded products made from expanded polystyrene have various shapes that generate many empty spaces, a ton of discarded polystyrene covers a volume of 200 m³, which is a large volume for so little material and this because it is composed of 98 % of air and 2% of the raw material: polystyrene. Although the production of plastics does not represent a problem for the environment, it does represent a greater problem because they do not degrade in their environment, their elimination is therefore a problem of great dimensions, since it is cumulative. Taking a problem that is the deterioration of stone structures caused by acid rain and an alternative in recycling, the use of polystyrene; what is desired is to find a material with the characteristics suitable to serve as a protective barrier to agents present in acid rain with the addition of a nanomaterial, graphene, which has hydrophobic properties, which are favorable in a protective barrier chemical agent. In this work, the surface properties that graphene provides implemented with a plastic base will be used, which will be obtained from the recycling of expanded polystyrene, to create a varnish that can withstand the conditions that simulate acid rain, protecting to the rocks of historical monuments, avoiding their material and aesthetic wear.



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**[NSN-62] Addressing of graphene oxide and graphite exfoliations for its
applications as membrane materials.**

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2D materials has been broadly proposed for different purposes as membrane materials such as sensitive materials for hybrid membranes or in separation membranes for high water flux permeation.

The membranes enabled by 2D materials could be classified as was proposed by Hyun et al. 2019, where they propose 3 classes according to the microporosity involved in each class. In this work we aim to know more about the possible outcomes for class 1 membranes made with graphene oxide and exfoliated graphite.

These materials sintesized by exfoliations in liquid media by ultrasonic energy are expected to have only extrinsic microporosity that may be suitable for nanofiltration purpose.

Water and DMF time filtration is notoriously different for each composition for heterostructures of grafene oxide and exfoliated graphite. This first observations combined with literature lead to know more over the expected microporosity of this easy made heterostructures.



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**[NSN-64] Ag Nanoparticles Incorporated on PMMA Opals: Synthesis and
Optical Properties Study**

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Photonic crystals are ordered structures where periodicity in the refraction index gives rise to diffraction effects of photons on dielectric lattice planes, resulting in a photonic band gap (PBG) that avoids propagation of the light in specific wavelengths ranges. Opals are distinguished as a class of photonic crystals mainly obtained by a self-assembly approach. The materials most widely used for obtaining opals are polymers because the preparative process is simple, easy, and cheap. In this regard, polymethylmethacrylate (PMMA) microspheres were synthesized and used to obtain opals. Monomer and initiator concentrations were varied systematically to monitor the size of PMMA microspheres. From SEM and DLS measurements it is observed that as the monomer and initiator concentrations increased, the average diameter of PMMA microspheres increases, except when a minimum monomer concentration is reached. We estimate the energy bandgap (Eg) by means of the Kubelka-Munk treatment; also, we estimate Urbach Energy of the PMMA microspheres. With these results, we infer that the PMMA microspheres present an indirect transition. In SEM micrographs, it is seen that PMMA opals photonic crystals are formed by microspheres in a uniform periodic face-centered cubic (fcc) array. Variable-angle specular reflectance measurements show that the opals possess a pseudo photonic bandgap (PBG) in the visible and near-IR regions. These results confirm the photonic nature of the opals. Furthermore, it was found that PBG shifts toward larger wavelengths as the average diameter of the PMMA microspheres increases. Finally, the incorporation of silver nanoparticles (Ag NPs) with an average diameter of 35 nm in PMMA opals is reported. The results showed an effect on PBG, because it shifts at longer wavelengths compared to PMMA opals. The importance of the study of these systems is mainly because they have shown an increase in the Raman signal when used as SERS substrates.



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**[NSN-76] Covalent union of N-naphthoquinonyl aminobenzoic acids to
functionalized multi-walled carbon nanotubes**

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Carbon nanotubes (CNT) have been widely used in many technology fields for their unique physical and chemical properties. In nanomedicine, the employ of this material as drug delivery system is promising. The use of both single-walled CNT (SWCNT) and multi-walled CNT (MWCNT) in cancer therapy is advantageous due to its shape as it facilitated transmembrane penetration, also they exhibit higher accumulation in tumor tissues, and the large superficial area allows it to attach small molecules and biomolecules. On the other hand, Naphthoquinones are nature occurring molecules that exhibit a wide range of therapeutic properties, among them anticancer properties. The main mechanism of cytotoxicity of naphthoquinones is the generation of reactive oxygen species (ROS) which damage cellular components. In this work we attach different N-naphthoquinonyl aminobenzoic acids to MWCNT functionalized using the diazonium salt-based arylation reaction.



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**[NSN-78] Optical response of pure metal and metal nitride films by
numerical simulation**

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The study of metal nitrides has aroused great scientific interest due to their integration in nanostructured multilayers. Transition metal nitrides (TMN) of groups IVb-Vb-VIb constitute a unique family of conductive ceramics due to their rich physical properties. In this work, we calculate the Reflectance, Transmittance, and Absorbance of smooth monolayers of elemental Nb and Ti, as well as of their respective nitrides NbN and TiN. The numerical simulation was carried out by using the Discrete Dipole Approximation (DDA) implemented in the DDSCAT (Discrete Dipole Scattering) code. Optical bands were found for Nb in the reflectance spectrum below 350nm, corresponding to the near UV region. The analysis of the dielectric function indicates that these observed bands correspond to contributions from interband electron transitions. Comparison with experiment for the case of Nb thin films is also presented.



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**[NSN-93] Synthesis of G-SO₃H for application in ketone biosensor for
diabetic patient monitoring**

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In order to synthesize and implement an enzyme-like material in a biosensor for the detection of ketone groups in human breath and, in order to have an auxiliary in blood glucose monitoring, we propose an experimental protocol of functionalization of reduced graphene oxide with hydrogen sulfide as an alternative to 4-aminobenzenesulfonic acid to produce -SO₃H radicals or sulfo groups promoting and ensuring the anchoring of ketone groups present in breath and thus monitoring the health status of diabetic patients and avoiding a referral to diabetic ketoacidosis. The reduced graphene oxide used in the previous functionalization is obtained by chemical vapor deposition (CVD) where ethanol is used as a carbon source and whose product is called rGO; in this process thin films of graphene oxide (GO) deposited on quartz are used, using the drop-casting technique, which are obtained from an aqueous dispersion of commercial graphene oxide (supplier ID-nano) synthesized by chemical exfoliation. Finally, the GO thin films are exposed to an ethanol vapor flow for 35 minutes at 700°C in the CVD process. The functionalization of the G-SO₃H material is studied by SEM and Raman, where the latter indicates the presence of the functional groups of our interest.



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**[NSN-106] Study in the Au seeds effect on ZnO nanostructures grown by
hydrothermal synthesis method**

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In this work, the growth of Zinc oxide (ZnO) nanostructures through solvothermal synthesis influenced by Au coated on Si substrates was studied. Two-step experiments were performed to provide an overview of ZnO growing based on Au seed. First, four different time conditions were tested to observe the influence of temperature in the seed growth. Subsequently, four thermal treatments at different times were explored to determine the influence of Au seeds on ZnO nanostructures morphology. Two types of experiments were conducted: a) varying time (15, 30, 45 and 60 min) with a temperature of 450 °C and b) varying temperature (350, 400 and 500 °C) for 15 min. Once the Au seed formation was completed, ZnO nanostructures were grown by a solvothermal method the synthesis goes as follows: 0.11gr of zinc acetate dihydrate was dissolved in 10 ml of distilled water, then 0.3gr of sodium hydroxide were added to the solution and stirred by 10 min. then, 2 ml of this solution were loaded into a Teflon container, which was then filled with 5 ml. of ethylene glycol and 20 ml. of ethanol. The container was placed inside an autoclave which was heated at 140 °C by 1, 2, 4 and 6 hours. Both, the seeds and the Au-ZnO film were characterized by AFM, SEM and XRD. The results showed that both time and temperature play a substantial role in influencing the grain size, producing a reduction of height and diameter. Average diameters of the Au seeds varied 60nm. to 100 nm.



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**[NSN-112] Optical characterization of CdTe nanoparticles embedded in a
nanoparticulate SnO₂ matrix**

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Cadmium telluride (CdTe) nanoparticles were grown in the interior of a SnO₂ 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 SnO₂ 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 several broad bands in the range 100 – 200 cm⁻¹, on which deconvolution allows separate five modes in the 100 – 200 cm⁻¹ interval. The bands correspond to CdTe and tetragonal Te. The transversal optic (TO) and longitudinal optic (LO) modes of CdTe at the G point of the first Brillouin zone, for phonons in nanoparticles, follow the expected behavior if the radius of crystal decreases, taking into account that the selection rules for momentum conservation are relaxed.



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**[NSN-130] Improving Self-Supported Nanowire Arrays Using the Response
Surface Methodology**

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In this work, we present a formal approach for optimizing the response of a class of sensors, namely, self-supported nanowire arrays developed by electrodeposition in restricted nanoporous membranes. In contrast to most nanosensor development strategies, which rely on phenomenological models and insights by simulations on ideal conditions, we propose a data-driven program. This proposed scheme allows conceiving an accurate model of the sensor by considering its actual behavior. Besides, the data-driven formulation provides an adequate framework for obtaining a response surface, i.e., the sensor's behavior as a function of the design variables. Consequently, we apply the response surface methodology, a statistical approach widely used in the industry, for the optimization stage. In this form, it is possible to maximize the sensor's response while having the pore density, length of the nanowires, the concentration of a substance for detection, and the metal ion used for electrodeposition as decision variables. The optimized sensor test validates our proposal's feasibility, obtaining a device of improved capabilities and performance.



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**[NSN-131] Effects on the mechanical and electronic properties of the Li
and Na at the surface of [111]-Si nanowires**

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In this work, we present a density functional theory study of the mechanical and electronic properties of hydrogen (H) passivated silicon nanowires (SiNWs) with diamond structure, grown along the [111] crystallographic direction. The model considers the systematic substitution of H atoms for sodium (Na) or lithium (Li) ones for concentrations since one up to 22 Li/Na atoms in four morphologies of SiNWs. The study is performed applying the supercell method, within the Local Density Approximation incorporated in the SIESTA code. The results indicate that the nanowire presents a semiconductor behavior, and the size of the energy band gap reveals the known quantum confinement effect as a function of the diameter of the nanowire, and a second effect in the size of the band gap due to concentration of Na and Li atoms that is stronger than the first one for a critical concentration. All studied systems present an energetic stability according with the formation energy results. Likewise, the binding energy values for the SiNWs with Li and Na atoms reveal a complicated behavior as a function of the concentration. The population Hirshfeld analysis, reveals that both Li and Na atoms give up charge to the surface Si atoms of the nanowires. The Young's modulus results seem to indicate, that the values remains almost constant for all studied concentrations of Li and Na atoms, and the obtained values are less than the value of the bulk silicon along the [111] crystallographic direction. These results open the possibility to incorporate the SiNWs as anodic materials in Na and Li in energy storage devices as rechargeable batteries.

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**[NSN-132] Theoretical study of the electronic properties of [110]-Ge
nanowires with surface Li**

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In this work, we present a density functional theory study of the electronic properties of hydrogen (H) passivated germanium nanowires (GeNWs) with diamond structure, grown along the [110] crystallographic direction. The model considers two morphologies of nanowires (M1 and M2), and the systematic substitution of H atoms for lithium (Li) ones, for concentrations since one up to 12 Li atoms at the unit cell. The study is performed within the Local Density Approximation incorporated in the SIESTA code. The results indicate that all studied nanowires presents a semiconductor behavior, and the size of the energy band gap is a function of the concentration of the Li atoms. Likewise, both studied nanowires present an energetic stability according with the results of the formation energy. Particularly, for concentration less than 6 Li atoms, the M2 GeNW seems to indicate a better stability, in comparison with the M1 morphology, and for concentration greater than 8 Li atoms M1 GeNW shows a better stability, in comparison with M2 morphology. By other side, the average binding energy values for both studied GeNWs diminishes as a function of the concentration until a value around of 2.54 eV. These results open the possibility to incorporate the GeNWs as anodic materials in energy storage devices as rechargeable batteries.

Acknowledgements: This work was supported by IPN projects 2020-2091, 2020-2193, 2020-2106, and PAPIIT-DGAPA-UNAM IN109320. The supercomputing resources were given through LANCAD-UNAM-DGTIC-180 and 381 projects and Laboratorio Nacional de Supercómputo del Sureste de México of the BUAP through project No. 201903082 N.



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**[NSN-137] Fabrication of superhydrophobic cotton base on silica
nanospheres with different sizes**

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Superhydrophobic cotton fabrics were prepared by the incorporation of silica nanoparticles with different sizes and sub-sequent hydrophobization with hexadecyltrimethoxysilane. Silica nanospheres with different diameters were synthesized using the Stöber method. Simultaneously addition of tetraethyl orthosilicate to different ammonium hydroxide solution varying in concentration produced silica nanospheres with sizes ranging between 22 and 230 nm. The nanotextile was prepared by simple immersion in a silica nanospheres colloidal solution. The wettability of cotton textiles was evaluated by the water contact angle (WCA) measurements. The results showed that the treated cotton simple displayed remarkable water repellency with a WCA of 169.9° for a 8 mL water droplet, increasing with the decrease in the diameter of the nanospheres. Transmission electron microscopy, scanning electron microscopy and FT-IR spectroscopy were used to characterize the size and morphology of silica nanospheres and nanotextile.



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[NSN-144] AuAg bimetallic nanoparticles: effect of their finely tuned surface composition in the catalytic reduction of nitroaromatics

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Bimetallic nanoparticles have been characterized by the improvement of their catalytic properties, when compared to monometallic ones, due to the synergistic effect between the metals that formed. In this work, the gold nanoparticles (AuNPs) surface partial modification by Ag traces was proposed (AuAgX %, where X represent the surface coverage percent). The obtained colloidal nanoparticles were characterized by TEM, UV-Vis spectroscopy, ICP, XPS. It was revealed that the incorporation of Ag traces did not affect the average size of the AuNPs (~17nm) used as seeds nor the position of the Au surface plasmon resonance crest (~521nm). The effect of the incorporation of Ag traces in the AuNPs surface were studied in the catalytic reduction of the 2-, 3- and 4-nitrophenol isomers (2-NP, 3-NP and 4-NP). It was found that the reaction rate depends on the Au surface coverage % with Ag, as well as on the nature of the molecule to be reduced. Colloidal Au-Ag nanoparticles stabilized in PVP were catalytically more active than those reported in the literature with similar compositions, reaching TOF values up to 72 $\mu\text{mol}^{-1}\text{s}^{-1}$ for the colloid AuAg 30 % in the 4-NP isomer transformation, 103 $\mu\text{mol}^{-1}\text{s}^{-1}$ for the AuAg 50 % colloid in the 2-NP isomer and 234 $\mu\text{mol}^{-1}\text{s}^{-1}$ for the AuAg 80 % in the 3-NP isomer.



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**[NSN-145] Effect of temperature on the growth diameter of carbon
spheres synthesized from rosin**

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The different geometric shapes of carbon at nanometer dimensions such as nanotubes, spheres (CSs) and others possess exceptional electrical, mechanical and chemical properties, which can be exploited in different technological and scientific fields. However, such properties are affected by different parameters such as growth diameter, chemical composition and graphitization, which could be attributed to different factors such as reaction time, reaction temperature, carbon source, etc. The objective of this research was to evaluate the effect of temperature on the growth diameter of CSs synthesized from rosin by Chemical vapor Deposition (CVD). Rosin was used as carbon source, argon as carrier gas and stainless steel core as catalyst. Three reaction temperatures were carried out: 750, 800, 850 °C for 60 minutes. The samples obtained by this method were analyzed by scanning electron microscopy (SEM) and Raman spectroscopy. The variable used to determine the effect of temperature was the diameter of the CSs measured with ImageJ software. The SEM micrographs showed solid CSs where some of them tended to form agglomerates by coalescence. CSs presented diameters between 520 and 735 nm at 750 °C; at 800 °C diameters around 550-830 nm were recorded; and at 850 °C diameters ranging between 600 and 900 nm were shown, respectively. Raman spectra at the three temperatures showed the main bands (D and G) characteristic of CSs. The tendency of the diameter of these particles is related to the temperature, since although at the lower temperature (750 °C) the values of diameter were lower, there were fractured spherical bodies and irregular points, which can be attributed to concentric layers of grafene that start from the nucleus and are united by Van der Walls forces until they form agglomerates by nucleation and



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growth processes for the formation of more stable spherical structures. It can be concluded that temperature is a primordial and determinant parameter for the growth of CSs with different diameters. Acknowledgements to the Scientific Research Coordination of UMSNH and CONACyT México for the financial support.



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**[NSN-147] The promotional effect of Cu traces in the catalytic
performance of NiCu bimetallic nanoparticles**

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In this work, the decoration of Ni nanoparticles with Cu traces at different Cu loadings was carried out to study their catalytic performance in the reduction of model nitroaromatics molecules. The catalysts were synthesized by the colloidal approach and characterized by ICP, TEM, XRD and XPS. It was found that Cu deposition promoted the hydrolysis of the initial Ni nanoparticles. The catalysts were characterized with hierarchical morphologies firstly obtained for the NiCu bimetallic nanoparticles, with a high metal dispersion. The synergetic effect between Ni and Cu metals, independently on the Cu content, in the reaction rate was revealed. The bimetallic NiCu nanoparticles were characterized with higher activity in the catalytic reduction of the 2- 3- and 4-nitrophenol isomers than the monometallic Ni or Cu nanoparticles. To the best of our knowledge, the catalytic activity of NiCu bimetallic nanoparticles, presently prepared, exceed the catalytic activity of those reported in the literature studying the same reaction.

Keywords: Bimetallic catalysts, nitroaromatics, nickel, copper, reduction.



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[NSN-148] Synthesis and study of the nonlinear refractive index of CuO nanoparticles by laser ablation

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Synthesis and study of the non-linear refractive index of copper oxide nanoparticles as a function of ablation time were studied using the Z-scan technique. An excitation diode laser with a wavelength of 534 nm and a power of 40 mW was modulated by a chopper with a frequency of 14 Hz. A 10 cm lens, the excitation laser was focused, making it move around the focus. From the excitation laser, the transmittance was obtained as a function of the position of the sample. The synthesis of the copper nanoparticles was obtained through different ablation times between 1 to 6 minutes in a copper disk, immersed in a liquid or solvent medium, such as acetone. For the ablation process, an Nd: YAG laser was used with emission of wavelength of 1064 nm at a frequency of 15 Hz and with a pulse energy of 47 mJ and pulses of 7 to 2 ns. The copper nanoparticles showed high non-linear refractive indices between 0.61 to 3.73×10^{-8} cm²/W, in which a non-linear increase in the non-linear refractive index was observed as a function of ablation time. The colloidal solutions were analyzed with UV-visible spectroscopy and the shape and size of the nanoparticles were obtained by transmission electron microscopy (TEM). The utility of this work has potential applications in the study of nanomaterials for high power compact solid state laser gain amplifier systems.



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**[NSN-149] Characterization by SEM and X-ray diffraction of solid carbon
nanospheres synthesized from rubber**

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Synthesis of carbon nanomaterials had caused great interest in the scientific and technological fields due to the great advances and new applications of these materials. It is natural that all the progress in this branch is directed towards the production of new materials, products and technologies. In this study, carbon nanospheres were synthesized from natural rubber as a carbon source precursor by Chemical Vapor Deposition (CVD) method to later be characterized by Scanning Electron Microscope (SEM) and X-Ray Diffraction (XRD). The synthesis was realized at 850 °C in a quartz tube reactor for 15 minutes using a steel core bar as catalyst. The micrographs from SEM analysis showed solid carbon spheres. The spheres diameters were between 600-1200 nm and no other structures were present. Through Energy Dispersive Spectroscopy (EDS) it was possible to obtain the chemical composition of the spheres, percentages of carbon above 92% and oxygen below 8 % were observed. On the other hand, by X-Ray Diffraction analysis it was possible to analyze the behavior of the structures, it was possible to analyze two slightly widened peaks, one around 25° (002) that can be assigned to the graphitic carbon of the sample, and the peak around 45° that can be easily assigned to graphene diffraction (100) indicating a hexagonal graphite network. The presence of strong and broad bands in the samples suggests a low graphitization degree and the possible presence of amorphous carbon, and also the presence of crystalline graphitic carbon in the carbon spheres. The solid carbon spheres from natural rubber were synthesized by CVD and characterized by SEM and X-Ray Diffraction. We acknowledge the Scientific Research Coordination of UMSNH and CONACyT México for the financial support.



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**[NSN-150] Photocatalytic Bleaching of Rhodamine 6G on Titanium Dioxide
Nanoparticles Monitored by Thermal Lens Spectroscopy**

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In this work, the TiO₂ synthesis of nanoparticles using a modified sol-gel method and titanium tetrabutoxide as a molecular precursor is reported. The photocatalytic activity of TiO₂ nanoparticles was evaluated on bleaching of rhodamine 6G (R6G) by thermal lens spectroscopy (TL). This is a nondestructive and highly sensible photothermal technique. It is widely used to study the thermo-optical properties of nanofluids containing metallic and semiconductor nanostructures. The TL experimental array included two mismatched laser beams: Ar⁺Xe laser as excite beam and He-Ne laser as probe beam. Thermal diffusivity variation as a function of TiO₂ concentration into nanofluid was investigated by fitting TL experimental data to a theoretical model. This study will provide the viability to use nanostructured materials in liquid heat transfer optimization applied in catalytic sewage water pollutants bleaching.



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**[NSN-151] Chemical synthesis and photothermal characterization of
monodisperse silica nanospheres of compact and porous structure for
markers and controlled drug transport-release**

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Mesoporous silica nanoparticles (MSN) have attracted great attention to develop efficient drug delivery systems, mainly due to their high porosity and biocompatibility. This work presents the synthesis of mesoporous silica nanospheres with a diameter of 212 nm using the modified Ströber method. It was determined that by controlling the reaction by neutralizing the pH, monodisperse silica spheres of different particle diameters are obtained. For structural characterization, complementary techniques such as TEM and FTIR spectroscopy will be used to determine the size and chemical composition of SiO₂ respectively. The enrichment of the thermal properties of nanofluids will be obtained by thermal diffusivity by means of the thermal wave resonant cavity (TWRC) and thermal lens (TL) techniques of water-based nanoparticles of smooth and porous SiO₂. The accuracy and precision of the two photothermic techniques were established by comparing the two techniques of distilled water for values reported in the literature. Very similar values of thermal diffusivity were found for the TWRC and TL techniques, which shows that these two techniques are useful tools in the thermal characterization of nanoliquids.



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**[NSN-153] Evaluation of PdRu@SiO₂ nanoreactors in the catalytic
reduction of 4-nitrophenol to 4-aminophenol**

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In this work, the one-pot synthesis of core-shell nanoreactors based on Pd, Ru and PdRu nanoparticles as nuclei and mesoporous silica spheres as shell (@mSiO₂) is presented. The obtained samples were characterized by XRD, TEM, N₂ Physisorption and XPS. The results confirm the confinement of the mono- and bi-metallic nuclei inside the amorphous and mesoporous silica structures (pore size ~3 nm). The catalytic efficiency of the nanoreactors was evaluated in the model reaction of 4-nitrophenol reduction to 4-aminophenol, further compared with their reference supported catalysts (Pd/SiO₂, Ru/SiO₂ and PdRu/SiO₂). The TOF estimation revealed the following trend in activity PdRu@mSiO₂ > Pd@mSiO₂ > Ru@mSiO₂ with 400, 271 and 215 min⁻¹ μmol of metal⁻¹ values, respectively. The highest activity of the PdRu@mSiO₂ bimetallic nanoreactor is attributed to the synergetic effect between metals due to the electrons transfer from Pd to Ru, and the low agglomeration of nanoparticles because of the presence of the shell. The catalytic stability test showed that the nanoreactors remained active even after 4 consecutive runs, in contrast to the reference supported catalysts. The optimized synthesis methodology made it possible to prepare nanoreactors with a uniform structure, independent of the nature of the nucleus.



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**[NSN-154] Comparative statistical analysis of carbon concentration in
cvd-synthesized nanomaterials for samples obtained from catalyst and
quartz tube surfaces**

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In recent decades, carbon nanomaterials have stood out thanks to their unique properties, which can be applied in different areas of research. Of the wide variety of carbon structures that can be found, carbon nanospheres attract attention due to their unique properties that enhance numerous applications such as: coating material for electrodes, hydrogen storage, drug vehicles, reinforcement material in composites, to name a few. The synthesis of the nanostructures was carried out with the chemical vapor deposition (CVD) technique, since it has advantages over other synthesis methods, such as the variety of structures that can be obtained, synthesis at atmospheric pressure and applying the principles of green chemistry, making it a more environmentally friendly process. In this work we propose a statistical analysis using Taguchi's design of experiments (DOE), where we will measure the percentage carbon content of the nanospheres synthesized by CVD at different temperatures (800 and 900 °C), at different times (60 and 90 minutes); finding the best synthesis conditions to obtain higher carbon concentrations in the samples. The samples were obtained from the surfaces of AISI 304 catalyst and quartz tube respectively using expanded polystyrene (EPS) as carbon precursor. The Taguchi DOE was analyzed with the software Minitab 19, reducing the time and correct application of the equations. The synthesized samples were characterized by scanning electron microscopy (SEM) finding the morphology of carbon nanospheres in their majority, presenting diameters from 110 to 1200 nm of the samples obtained from the catalyst surface and from 120 to 2800 nm for the samples collected from the quartz tube surface, the energy dispersive spectroscopy (EDS) showed high carbon contents higher than 93 %. The Raman spectra showed the



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characteristic G and D bands, presenting the overtone of the G' band in some cases. FTIR spectroscopy of the carbon spheres showed mainly the OH, CH_x, C=O and C=C bands. We acknowledge the Scientific Research Coordination of UMSNH and CONACyT México for the financial support.



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**[NSN-163] Optical and electrical characterization of III-N-V quantum well
heterostructures embedded in GaAs photovoltaic device**

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The development of molecular beam epitaxy (MBE) allowed the synthesis of heterostructures that are currently applied to the photovoltaic technology *i.e.*, quantum wells (QW) and dots are employed to overcome the theoretical maximum efficiency of single junction photovoltaic devices, being usually embedded in a semiconductor material with an optimum band gap energy between 1.4 and 1.6 eV which optimizes the relationship between open-circuit voltage and short-circuit current. In this work, photovoltaic structures where the 1.42 eV bandgap via GaAs and a lower energy gap obtained by GaNAs are applied to QW photovoltaic system to increase the absorption of lower 1.4 eV photon energies. Technology computer-aided design is employed to compare the performance of (a) GaAs/GaNAs/GaAs (b) AlGaAs/GaAs/GaNAs/GaAs/AlGaAs, and (c) AlAs/GaAs/GaNAs/GaAs/AlAs layer sequences of QW where the band behavior in conjunction with the confined energy levels improves the photon absorption. A numerical model to predict the strain distribution was used indicating that even though the thickness of a single QW is below the critical thickness of GaNAs at nitrogen concentration of 1.5 % stacking of such wells will finally generate defects that can be reduced by controlling the GaNAs layer thickness lower than 10nm. Ten sequences of the designed QW were grown by MBE, exhibiting a good grown process, according to reflection high-energy electron diffraction pattern, and being embedded in a p-i-n GaAs structure. High-resolution X-ray diffraction indicated a lattice mismatch around 0.3 % in the grown heterostructure which produces a tensile stress of 2.5×10^{-3} as it was stated by LO-phonon shift of Raman spectra. The *p-i-n* host semiconductor system was evaluated by photoreflectance where two contributions can be distinguished: the third-derivative lineshape exhibited by the bandgaps of the material employed and Franz-Keldish oscillations associated to the *p-i-n* electric field distribution of $\sim 2 \times 10^7$ V/m. Electrical characterization was obtained by current-voltage curves under illumination at AM1.5, showing a short-circuit density of 2.5 mA/cm² for (a) structure and being degrading by the insertion of Al-based layer in the (b) and (c) sequences. With this study the authors developed a numerical simulation process to design a QW structure to be included



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into a GaAs-based *p-i-n* solar cell and the grown process protocol to allow the crystallinity of the whole heterostructure.

ACKNOWLEDGMENTS: The authors acknowledge the financial support of FRC-UASLP and CONACYT-Mexico through grants: INFR-2015-01-255489, CB 2015- 257358, PNCNP2014-01-248071 and the Catedras CONACYT.



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**[NSN-167] Adsorbed molecules in AuNPs / InAs Quantum Dots studied by
SERS**

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Nanotechnology is the area of research that studies, designs, and manufactures materials at the nanoscale and gives them some practical application, for example biosensors. The most used and henceforth as well synthesized nanomaterials are possibly the gold (AuNP) and silver (AgNP) nanoparticles because they offer a great possibilities of being functionalized. Likewise, since the Bovine serum albumin (BSA) analyte is a quite similar to human serum albumin (HSA), it is widely used as a substitute for the former in applicable purposes. Besides, the BSA is also a well characterized analyte whose reported spectra is well known offering significant advantages when any application is required. In this work, we study the electromagnetic interactions of the Au NPs with the properties of the InAs/GaAs quantum dots (QDs) that could modify the SERS amplification factor in the BSA molecule. The QDs were self- assembled by molecular beam epitaxy under different growth parameters in order to propitiate a variety of morphologies for que further adsorption of the AuNP. Once removed from the ultra-high vacuum environment the QDs templates were characterized ex-situ by atomic force microscopy to obtain information on their morphology and distribution prior- and post to the AuNPs deposition. It is found that the SERS enhancement is caused by combinations of several types of resonances in the combined system, surface, exciton, charge-transfer, and molecular resonances. Furthermore, by considering the involved contributions to the SERS enhancement, we studied mechanisms for adjust the interaction between the nanoparticles, semiconductor nanostructures and BSA. the findings of this study open the possibility to design, evaluate and synthesize efficient SERS substrates for the use of biomarkers.



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**[NSN-172] Optical characterization of molecular beam epitaxial grown
(Al)GaAs/InAs (quantum dots)/(Al)GaAs heterostructures**

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The study of InAs quantum dots (QDs) has been of great interest due to their unique physical properties and huge potential for optoelectronic applications [1, 2]. For practical applications, the encapsulation of the zero-dimensional nanostructures is mandatory, and thereby, interesting challenges like segregation, intermixing, strain, among others, are added to the already complicated self-assembling process. In this work, the optical properties of (Al)GaAs/InAs-QDs/(Al)GaAs heterostructures were investigated. Characterization techniques such as Raman (RS), photoreflectance (PR) and ellipsometry spectroscopy were employed. The intensity reduction of the L- frequency mode located close to 270 cm^{-1} for the Raman spectra suggest changes of the QDs sizes with GaAs capping layers due to In/Ga intermixing effects in comparison with InAs/AlGaAs interfaces. Further, the InAs/AlGaAs sample showed phonon resonances around 255 cm^{-1} , associated to TO InAs QDs signal, while this signature is not observed in the InAs/GaAs sample spectra. PR spectroscopy showed clear differences between the built-in electric fields intensity associated to the QDs interfaces, which depended on their type of encapsulation environment. The strain provokes PR line-shape broadening (from 18 to 9 meV) as well as blueshifts corroborated with the second derivative of the pseudo-dielectric function obtained from ellipsometry spectra for the GaAs/InAs/AlGaAs sample in comparison with AlGaAs/InAs/GaAs. Numerical simulations were employed to support the strain field effects with the experimental heterostructures.

[1] Tomah Sogabe, Qing Shen, Koichi Yamaguchi, "Recent progress on quantum dot solar cells: a review," J. Photon. Energy 6(4), 040901 (2016).

[2] Rakhlin, M.V., Belyaev, K.G., Klimko, G.V. *et al.* *Sci Rep* 8, 5299, (2018).



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**[NSN-174] Periodical corrugation control via in situ monitoring and W-
Rheed feedback**

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Since the advent of molecular beam epitaxy (MBE) several experiments have been done over high index crystallographic orientations (HICO) concerning the construction of complex heterostructures that contain periodic corrugated interfaces. The advantages of including periodical corrugation into multi-quantum well (MQW) and superlattice (SL) heterostructures have been widely extended in previous group work publications and from other authors. Nevertheless the growth processes over HICO are far from being fully understood, although it is well known their surfaces are generally speaking unstable and tend to break up into energetically stable faceting. We can assert that until now there has been scarce or nonexistent *in situ* characterization that could bring us to grasp the real display of the real-time growth process performed over HICOs. This work is a first step in the quest to achieve this goal and it does so by merging the main in situ characterization device of a MBE ultra-high vacuum (UHV) chamber with a powerful method that allows access to large areas of the reciprocal space forecasted by the HICO named Weissenberg RHEED (W-RHEED). A 360° mapping of the reciprocal space have been successfully retrieved from the GaAs (631) high-index high anisotropy substrate during growth and at stand-by. From this mapping we were able to obtain Patterson maps that unveil the atomic arrangements or positions in this complex growth scenario. Finally by analyzing our results we are able to elaborate technical guidelines that allow us to characterize the real-time state of the periodic mesoscopic corrugation (MPC) that is characteristic of this substrate.



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**[NSN-181] Functionalized graphene oxide nanoparticles for the study of
in vitro antitumor activity on cervical cancer cells**

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Progress in fighting cervical cancer has been very slow, due to the time required to evaluate new therapies. The World Health Organization estimates that this is the fourth most common cancer in the female gender, and the seventh worldwide. In Mexico between 2000 and 2010, there were 82,090 new cases and 42,308 deaths. Within the various antitumor therapeutic strategies, have been tested various nanoparticles and nanostructured materials in the field of nanotechnology for diagnostic and therapeutic purposes. We are working in this direction and we present some previous results.



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**[NSN-189] Effect of lanthanide ions (Eu + 3 and Tm + 3) on the
luminescence of ZnO nanoparticles.**

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Zinc oxide (ZnO) is one of the most popular semiconductor materials in the new nanometric technologies development, formed by elements of II-VI groups, with a wide band gap of 3.37 eV at room temperature, in addition to other physical properties that have generated great interest in the possible optoelectronic applications development. The optical properties in ZnO nanoparticles can be modulated by doping with lanthanide ions. In this work, we report the preparation of ZnO pure and doped with Europium (ZnO: Eu+ 3) and Thulium (ZnO: Tm+ 3) using the hydrothermal method. We studied the influence of concentration these lanthanide ion from 3 at% to 17 at%. In the synthesis, we used aqueous solutions of zinc acetate with two concentrations 0.5M and 1M to vary the size of the particles and can to determined their influence on the luminescence properties, where we expect observe the emissions in the red and blue for doping Eu+ 3 and Tm+ 3 respectively. The synthesis was carried out under a 3 Mp of pressure and 200 ° C for 2 hours. The characterization was carried out by X-ray diffraction where it was verified that all the nanoparticles obtained without doping and doped showed the Wurtzite phase (hexagonal). Additionally, we determined the particle size of varies from 18 nm to 30 nm and from 35 nm to 50 nm for concentrations of 0.5M and 1.0M respectively. Using UV-VIS we determine the E_g value is around 3.2 eV and 2.9 for the samples Eu and Tm doped. The photoluminescence emission bands on the nanoparticles was measured in the range of 300 to 1100 nm were analyzed using an excitation wavelength of 285 nm showing the typical transitions for Eu + 3 and Tm + 3 ions.



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[NSN-190] Electronic properties of [001]-Ge nanowires with superficial

Na: a DFT study

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In this work, we present a theoretical study of the electronic properties of Hydrogen passivated Germanium nanowires (GeNWs), grown along the crystallographic direction [001], considering five different diameters. The model considers the systematic substitution of H atoms for Sodium (Na) ones. The study is developed using the Density Functional Theory (DFT), within the local density approximation (LDA) incorporated in the SIESTA code. The results indicate that the nanowires present the known effect of quantum confinement, where the energy band gap decreases as a function of the diameter of the nanowire. A semiconductor character is also observed where the energy band gap decreases as a function of the concentration of Na atoms for all studied systems. The formation energy results, indicate an energetic stability as a function of the concentration of Na atoms. On the other hand, the binding energy results indicate a value around 2.5 eV as the necessary energy to extract one Na atom from the system. These results help us to understand the effects of Na atoms on the electronic properties and structure of the GeNWs, and open the possibility of incorporate them as anodic materials for the development of a new generation of rechargeable Na batteries.

Acknowledgements

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**[NSN-191] Statistical tools for the improvement and optimization of
electrochemical sensors**

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The response of electrochemical sensors for substance detection critically depends on the sensing potential, the value of which is often selected by the visual inspection of the sensor's response, as given by, for example, electrochemical methods like cyclic voltammetry (CV). Using experimental data from CV, we show how the selection of the sensing potential can affect the sensitivity and linear range of the measurements. Whenever the magnitude of the sensor's response is crucial, it can be better to optimize the sensor for its sensitivity; however, if the testing conditions involve a variable range of concentrations, with putative very small or high concentrations, a reliable response can be obtained if the sensor is optimized for the linear range.



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**[NSN-196] Optical properties of thin films and nanostructured
conducting polymeric hybrid arrays**

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In the past recent years, the conductive polymers PEDOT:PSS and Poly-pyrrol have reemerge as relevant building blocks in field of organic opto-electronics. Despite its key role in that field, a complete and deep comprehension of its optical properties in the visible regime (refractive and dielectric functions) is still missing. For this reason, in this contribution, the optical properties of a wide variety of conductive polymers PEDOT:PSS and Polypyrrol thin films, were measured and analyzed by using means of spectroscopic ellipsometry. To this aim, samples were synthesized onto ITO and silicon substrates by using an electrodeposition system. A wide variety of thin films of PEDOT:PSS were synthesized with different Ethyleneglycol (wt%) levels of dosages, ranging from 2 % to 50 %. On the one hand, the morphology and roughness of the samples were characterized by using scanning electron and atomic force microscopies. On the other hand, the optical properties of these materials were characterized via spectroscopic ellipsometry. The pseudo-dielectric function and reflectance were obtained directly from the ellipsometry measurement of the samples. Different theoretical dispersion models were used to fit in a proper manner the complex refractive index and the complex dielectric function of each of the conductive polymers. With the extinction coefficient obtained it was possible to calculate the absorption coefficient and develop the respective Tauc plots for each structure to determine the bandgap (and the modulation of it by introducing the dopant agent in the case of PEDOT:PSS) and the type of transition allowed for each case and structure. The optical conductivity was calculated using the relationship between refractive index and the absorption coefficient. Moreover, both type of polymers, were synthesized in the form of nanotubes arrays within membranes templates, with the purpose to induce sub-wavelengths optical effects, obtaining well reproducible means field optical models. Finally, using the reflectance measured it was possible to contrast the effect of the nanostructuration, the polymeric interphase phenomena and the repercussion of having an effective medium (roughness and alumina/polymer) of the conductive polymers (polypyrrole and PEDOT) and compare the obtained reflectance (of all samples) with a numerical simulation performed by finite element method via COMSOL Multiphysics via Scattering matrix method using the optical properties fitted.

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**[NSN-199] Gold and Silver nanoparticles synthesized by LASL at low
fluence values**

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The laser ablation of solids in liquids (LASL) technique has shown to be a highly versatile physical method to synthesize nanoparticles. The great variety of materials that can be produced together with its low production of residues and the high quality of obtained nanoparticles, make LASL a promising technique to be used for technological applications.

Gold and silver nanoparticles have demonstrated to be very interesting for surface plasmon applications. In this sense, obtaining high quality, small and stable colloidal nanoparticles is a challenge for nanomaterials research scientists.

Usually high laser fluences (energy density) are used to produce nanoparticles by LASL. This can have the disadvantage of combining processes known as melting and fragmentation during the ablation experiments. The use of low laser fluence values, can allow to decrease the combination of melting and fragmentation, which can help to reduce size dispersion.

In this work, Au and Ag targets were irradiated with ns pulses in water to obtain colloidal nanoparticles. Fluence values were low as compared with reported in literature (below 1 J/cm²). The obtained colloids were post irradiated to induce a fragmentation process and see if there was a considerable effect on size dispersion. Optical absorption of the colloids was studied by UV-Vis spectroscopy. Size and structure was analyzed by means of TEM. Results are discussed as a function of decreasing laser fluence.



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**[NSN-201] Theoretical study of the optical properties of graphene sheets
with different geometries**

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The different allotropic configurations at the nanoscale level of coal have emerged as new platforms in the development of highly luminescent materials. A Graphene sheet loses its electronic band gap energy (E_g) and for this reason it does not present photoluminescence, therefore emergent methods to design both wide and narrow E_g 's have currently been used as a strategy to produce photoluminescence in carbon nanostructures. In this work computational theoretical calculations will be made considering finite graphene sheets tailored with square, rectangular, hexagonal and triangular geometries; in each geometry the molecular weight of each of the structures will be increased to analyze their optical properties, it is worth mentioning that their optical properties are characterized by the distribution and arrangement of the atoms at the edge, finding mixed edges, that is, the zig-zag and armchair type, thereby it is expected that there will also be different behaviors in the optical properties of graphene sheets with different geometries, in addition to finite widths combined with periphery effects also provide peculiar optical properties. The graphene sheets are functionalized with hydrogen atoms. For the study and analysis of our obtained photoluminescence spectra we will use the computational tool "GAUSSIAN"; which contains in its package, calculation methods ab initio DFT that allows us to estimate the multielectronic function of the N electron system. In this research we use the bases functions Split-valence 3-21G and 6-31-G* and we calculate the UV / VIS spectra of the tailored graphene sheets.



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**[NSN-203] Relevance of bond force constants in carbon nanomaterials on
technology application**

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Carbon nanostructures have boosted developments in nanoscience and nanotechnology over the past 30 years in the fields of physics. Graphene has become a very promising material due to its extraordinary physical properties including mechanical, thermal, and electrical. Since the graphene structure is the basis of several other important carbon materials such as fullerenes, carbon nanotubes (CNTs) and polycrystalline carbon fibers, it shares many of its extraordinary properties with other molecules. Also, it has been reported that carbon atomic chain structures might be extremely stiff against strain, however these nanostructures might also allow bending deformation without influencing their properties. Bond force constants estimations in nanoscale systems have been mostly based on theoretical predictions due to the experimental difficulties implicit in the manipulation and properties measurement of the nanomaterials. In this regard, the advancement in simulation tools and computer processors have allowed the development of detailed and accurate quantum mechanics simulations oriented to solid states, such as density functional theory (DFT).

The potential technological applications of known bond force constants based on carbon nanostructures render a strong motivation to investigate their mechanical properties in the fields of electronics, optics, nanodevices, energy generation and storage, mechanics, biology, and medicine. It provides important information about their high resistance when composite materials are synthesized with carbon nanomaterials.



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**[NSN-211] A experimental study of δ -doping layers in a GaAs/AlGaAs
nanowire system**

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Semiconductor nanowires (NWRs) are exciting components to study unique one-dimensional physics such as the Coulomb-interaction-strength-dependent electronic charge fractionalization, the quantized conductance in units of $2e^2/h$, or the formation of a perfect periodic charge distributions along the wires, known as a Wigner crystal, first predicted by E. Wigner in 1934 and recently observed experimentally. In addition to be remarkable systems for basic research, NWRs are also key building blocks at the nanoscale for potential applications in the fabrication of functional electronic and optoelectronic devices. Some NWR-based devices that has been widely explored includes field-effect transistors, diodes, nano-logic gates, and nanoprocessors. However, in the design of electronic and optoelectronic devices as well as to explore basic 1D physics, an extrinsic carrier doping must be incorporated in order to modulate the electrical and optical properties. Because the direct doping in the wires imply crystalline defects, it is convenient to explore the alternative incorporation of extrinsic carriers by means of δ -doping layers outside the wires. In this contribution, we explore the effects of two Si δ -doping layers in a structure of GaAs wires inside an AlGaAs barrier (where the δ -doping layers were deposited). Electrical characterization along with photoreflectance and photoluminescence measurements, showing the effects of the δ -doping layers, are reported.



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**[NSN-212] Quantum tunneling between parallel semiconductor
nanowires**

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Parallel arrays of nanowires are a natural and common configuration in the self-assembly by a number of epitaxial techniques. Such configuration can be convenient and must be considered in the design of electronic and optoelectronic devices along with its extrinsic doping, which is needed to modulate the electrical and optical properties. In addition, as the wires could be close enough to allow quantum tunneling between them, it must be considered. Even when it is clear that all these factors could be able to modify the electronic distribution in the wires, due to the difficulty to theoretically model the many-body interaction in realistic wires, such redistribution remains largely unknown. In this contribution, we report the electronic distribution in two parallel GaAs nanowires separated by an AlGaAs barrier, where the collective nature of electrons is calculated by using an effective potential based on a Yukawa-like electron-electron interaction. We focus in the regimen of diluted electronic densities, where a configuration of localized electronic states can be induced along the wires. We show that under appropriate conditions the tunneling can take place only between adjacent localized states, which in turn creates a periodical 3D tunneling distribution. We highlight the practical importance of such finding as an alternative to establish a tree-dimensional superlattice made from an array on many parallel nanowires and some consequences in the design of new FET architectures.



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[NSN-220] Self-assembled InGaN nanostructures on Si substrates

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In_xGa_{1-x}N thin films are widely used in tandem solar cells and light-emitting devices. This material makes it easier to tune bandgap values from infrared to ultraviolet wavelengths changing the concentration of In atoms. However, the synthesis of this ternary alloy maintains some controversial issues because In incorporation above 22% induces spinodal decomposition which causes compositional inhomogeneities, bandgap variations, potential fluctuations, and compositional-dependent morphologies. This phenomenon is originated from the lattice mismatch between GaN and InN, as well as the different diffusion lengths of In and Ga adatoms during the growth process. This work describes diverse growth kinetics observed during the synthesis of In_xGa_{1-x}N thin films grown on Si (111) substrates by plasma-assisted molecular beam epitaxy. Five samples were grown where In nominal concentration was varied from 0 (GaN) to 1 (InN) by changing In/Ga flux ratio. In-situ reflection high-energy electron diffraction (RHEED) was applied during the growth process and additional high-resolution X-ray diffraction (HR-XRD), photoluminescence (PL), and scanning electron microscopy were used to analyze the samples. Before the synthesis of InGaN thin films, an AlN transition layer was grown on Si (111) substrate to prevent amorphous Si_xN_{1-x} formation. For the case of the GaN thin film (x=0), a nanocolumnar morphology was obtained with a Poisson-like diameter distribution around 110 nm, a result that was corroborated by SEM micrographs and spotty RHEED diffraction patterns at the final surfaces. InN sample (x = 1) also showed columnar growth kinetics whose nanostructures coalesce on the final surface exposing a final inverted conical nanostructure whose RHEED evolution change from spotty to semilinear patterns. For the samples with x = 0.15, 0.2, and 0.47 RHEED patterns evidence the formation of periodic three-dimensional nanostructures with a relative orientation on the growth plane. In concentration-dependent flake-like nanostructures clearly are defined on measured SEM micrographs. Fast Fourier transform of SEM images shows



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the preferential orientation of superficial nanostructures. These morphologies are explained in terms of differences in the growth kinetics induced by the immiscibility of In adatoms in InGaN thin films, as well as the difference of surface diffusion lengths of In and Ga adatoms, which limits In incorporation on this ternary alloys.

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**[NSN-227] Thermal wave cavity technique for the study of the thermal
properties of resin/graphene nanocomposites.**

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The enrichment of the thermal properties of resin/graphene nanocomposites has a strong influence with respect to their synthesis, particle size, the type of concentration and their agglomeration with time. In this study, changes in the thermal diffusivity of resin-based resin/graphene nanocomposites are explored. The thermal wave resonant cavity (TWRC) technique was used for small amounts of sample, the measurement being carried out by a pyroelectric detector with a sweep of the length in the resonant cavity. The accuracy and precision of this technique was established by comparing the thermal diffusivity of distilled water. Different concentrations of graphene nanoparticle nanocomposites from 0.1 to 0.5 wt.% were used, increasing the thermal diffusivity of the nanocomposite. The results showed the high sensitivity of the TWRC technique, which is a powerful tool for measuring the optical/thermal properties of nanofluids. This technique can be applied to thermally thick and non-transparent samples that cannot be measured with other traditional techniques.



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**[NSN-247] Effect of Ag additions on the mechanical properties of Zn-Al
alloys manufactured by mechanical alloying**

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Currently, innovation in light alloys, such as Zn and Al alloys, has opened the door to its possible application in the aircraft and land transport industries. Therefore, it is interesting to study the physical-chemical and mechanical properties of these alloys. The addition between 1 and 4 wt. % of Ag to the eutectoid Zn-Al alloy, improves the superplasticity and mechanical properties of the alloy due to changes in its microstructure. In this work it was studied the effect of Ag additions on the mechanical properties on the Zn-Al eutectoid alloy. The alloy was fabricated by mechanical alloying. From the characterizations performed in the resulting alloys, it was that the particle size of powders after milling stage is minor than 1 micron. XRD analysis confirm the presence of the original metallic phases after the sintering stage. The microstructure of the alloy is homogeneous, showing the presence of Ag at intergranular zones. With respect to mechanical properties (elastic modulus and hardness) these was improved in the way that Ag contents in the alloy are bigger.



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**[NSN-250] Enhanced structural and optical of CBD-CdS thin films
stimulated by doping with (Cu²⁺, Ag⁺, Au⁺) metallic ions**

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In this work, the modified crystalline structures of the cadmium sulphur nanostructured semiconductor (CdS) stimulated by doping with (Cu²⁺, Ag⁺, Au⁺) metallic ions are studied. Good crystalline quality thin films were obtained by chemical bath deposition and doped in-synthesis without the need for additional steps with controlled thicknesses around 100 nm, which were measured by ellipsometry. The binding energies of the CdS matrix and their interactions with the different metal ions were determined by X-ray photoelectron spectroscopy (XPS). The quality and crystalline phase of the materials were studied by X-ray diffraction (XRD), which were confirmed by Raman spectroscopy. A change from monocrystalline structure to polycrystalline structure was observed in the doped CdS thin films by XRD, maintaining the zincblende phase; this behaviour was confirmed by HRTEM micrographs in addition to the different levels of quantum confinement promoted by each incorporated transition metal. The Raman scattering confirmed the zincblende phase and also allowed the analyses of the phononic interactions of the CdS binary compound, where the Raman shifts give structural information and confirm the effects of quantum confinement. The UV-visible optical spectroscopy describes the effect of the crystalline structural modifications with blue shifts in the optical band gap energies of the evaluated samples, related with the different levels of quantum confinement given by the metal dopants.



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[NSN-252] Controlled synthesis of electrospun TiO₂ nanofibers and their photocatalytic application in the decolouration of Remazol Black B azo dye

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The obtaining of monocrystalline TiO₂ nanofibers with high specific surface area synthesized by the electrospinning technique with controlled crystalline structure and morphology is reported. The nanofibers were annealed at 500, 700 and 900 °C in a controlled atmosphere in the presence of air for two hours to achieve crystalline phase transformation. By means of TEM, it was possible to clearly corroborate the presence of solid nanofibers with a well-defined shape, a smooth surface and without the presence of interconnections and defects called beads. The chemical stoichiometry of electrospun TiO₂ nanofibers was estimated by EDS, finding that at low annealing temperatures excess of oxygen was detected and at high temperatures excess of titanium that originates oxygen vacancies. By Raman scattering was found that the TiO₂ nanofibers showed a crystalline phase transformation from pure anatase, mixed anatase-rutile and pure rutile as the annealing temperature is increased, caused by the generation of oxygen vacancies, which was corroborated by X-ray diffraction. The band gap energy (E_g), obtained from optical absorption spectra, decreases as the temperature is increased, which is ranged in $2.42 < E_g < 3.27$ eV, caused by the anatase→rutile crystalline phase transformation. Photoluminescence shows that the radiative bands show a gradual red shift as the temperature increases due to the E_g reduction. In addition, the photocatalytic properties of the annealed TiO₂ nanofibers were evaluated in the decolouration of the Remazol Black B azo dye. Changes in absorption spectra were noticeable as the measurement time increases. Absorbance spectra showed a decrease in the intensity of the main absorption band at 589 nm, which gradually decreases until it completely disappears, indicating that the decomposition of the organic compound is complete, while physically there is an absence of colour from the solution. The anatase crystalline phase was the one with the highest specific surface area and the highest photocatalytic activity.



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**[NSN-261] Synthesis and Raman characterization of graphene
nanoribbons**

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This study focuses on the manufacture of graphene nanoribbons (GNRs) by high energy mechanical milling, using graphite rods recovered from spent Zn-C cells as a carbon source. The forces of impact, shear and friction caused deformations in the crystalline structure of carbon, as well as delamination of its layers. The topology and high quality of the GNRs is confirmed by Raman spectroscopy. In the Raman spectra of the RG-6H and RG-12H samples, the radial-breathing-like-mode (RBLM) are presented in 311 cm^{-1} , this band confirms the formation of nanoribbons 9 and 7 atoms wide. The low intensities of the D and D' bands indicate the few defects at the edges of the GNRs. The deconvolution of the 2D band of the specimens makes it possible to know exactly the number of layers of the graphene nanoribbons. The ratio of intensities of I_D / I_G increases from 0.21 to 0.32 with increasing milling time, this is associated with the reduction of the width of the nano-tape. The Raman fingerprint favors the identification of narrow graphene nanoribbons, suitable for implementation in electronics.



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[NSN-270] Deep eutectic mediated synthesis of TiO₂ nanostructures:

Effect of co-solvent on microstructural and optical properties

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Herein, we reported the fabrication of TiO₂ nanoparticles (NPs) by solvothermal method using reline as deep eutectic solvent (Choline chloride:urea=1:2; DES) and 2-propanol as co-solvent. Different wt% of propanol was used in this work: 0 (pure reline), 5, 10, 20, 50 % and 100 %. The solvothermal temperature and time was set at 180 °C for 15 h. The obtained product was subjected to thermal treatment in a muffle furnace at 450 °C for 3h to promote the crystallinity. Different techniques were implemented to study their structural, optical and morphological properties. X-ray diffraction (XRD) and Raman scattering analysis revealed the exclusive formation of anatase phase. Raman spectra of unannealed TiO₂ suggests the commencement of crystallinity in the samples obtained by ≤ 20 wt% of propanol. Diffuse reflectance spectra of TiO₂ NPs show a slight red shift in absorption edge by increasing wt% of propanol. The estimated optical band gap (indirect transition) for TiO₂ varied from 3.15 eV for 0 wt% propanol up to ~ 3 eV when 50 wt% of propanol was used. TEM results manifest a gradual increase in particle size by increasing the wt% of propanol. A possible reaction mechanism has been put forward to explain the observed changes in physical properties. ACKNOWLEDGMENTS. Andrés Guzmán Cruz (CVU # 862151) is thankful to CONACYT-PNPC for extending doctoral scholarship. Financial support received through the project VIEP-BUAP-2021 (grant no. 100468355-VIEP2021) is acknowledged.



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**[NSN-277] Photocatalytic effect of Ni, Fe-Ni, Magnetite doped TiO₂
catalysts synthesized by the microwave-assisted sol-gel process**

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Pollution by the textile industry has a very limited regulation of environmental hazards. The colorants, designed to be highly resistant, even with microbial degradation, highly toxic, prevent the penetration of light, inhibiting biological processes. These effluents only remove 50 % of the colorants in the wastewater. TiO₂ is an ideal semiconductor for photocatalysis, it has been modified by doping it with metals, non-metals, sensitization with dyes, under visible light and UV light. In this work we use the microwave-assisted sol-gel process to synthesize catalysts and evaluate the photocatalytic degradation of Acid Blue 9 dye (AA9 at 20 ppm) for percentages of Ni (0.05, 0.25 and 1 %) obtaining: at 0.05 % -Ni without heat treatment 90 % degradation in 75 min, similar with heat treatment at 600 ° C. Those of TiO₂ doped with iron-nickel (0.05, 0.10 and 1.4245 %) and (0.05, 0.25 and 1.00 %) respectively, show for 0.25 % of nickel (TiO₂ 0.25-NI-0) without heat treatment a 62% degradation in 90 min, similar to that of TiO₂-Fe-0.1-Ni-0.25 at 600 ° C in 100 min with 60% degradation. TiO₂ - magnetite (DT-M-Min 0.025 %) at 600 ° C showed 95 % in 80 min. Unlike those treated at 400, 500 °C which was 120 min. Concluding that the doping element contributes to the degradation rate of the dye (AA9).

Key Words: Photocatalyst, doping, photodegradation.



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**[NSN-279] Synteshesis of TiO₂ nanotubes by the electrochemical
anodization method**

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Titanium oxide nanotubes (TiNTs) have excelled in various applications thanks to the excellent physical and chemical properties conferred by the nano-scale. In electrocatalysis their hollow cylindrical morphology in the anatase crystalline phase positions them better than other morphologies due to their greater surface area. Its performance can be optimized by the electrochemical anodization synthesis method, since this allows the ordered growth of nanotubes parallel to each other and perpendicular to the substrate, facilitating the transfer of charges and a less recombination of holes-electrons.

The objective of this work is to synthesize TiNTs for future electrocatalytic applications, for this, three electrochemical anodizing treatments were tested in a conventional cell of two electrodes suspended in an electrolyte consisting of ethylene glycol, deionized water and F⁻ ions, evaluating the effect of the water content and the presence of hydrochloric acid (HCl) under conditions of room temperature and constant potential of 30 V for 45 minutes, followed by calcination at 500 °C for 2 h. The morphology, composition and structure were analyzed by scanning electron microscopy, X-ray diffraction and RAMAN spectroscopy techniques.

The X-ray diffractograms and the RAMAN spectra confirmed the formation of titanium oxide in the anatase phase in the three treatments, while the micrographs illustrated the morphological effects of the percentage of water and HCl, verified the nanometric range and showed the treatment with which the desired characteristics of the TiNTs were achieved.



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**[NSN-35] Multiferroic Lithium Niobate (LiNbO₃) nanoparticles and its
potential application in magnetic refrigeration**

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The LiNbO₃ crystal is a multi-functional material with favorable piezoelectric, nonlinear optical and electro-optic properties. However, there are few reports concerning the ferromagnetic properties of this material. In this work LiNbO₃ nanoparticles were produced by, using high purity lithium carbonate (Li₂CO₃) and niobium oxide (Nb₂O₅) as precursors. The milling was process followed by a calcination heat treatment at 650 °C in in air atmosphere to obtain stoichiometric LiNbO₃ nanoparticles, in the size range of 40 – 60 nm.

After obtained LiNbO₃ nanoparticles a second reduction heat treatment process were performed at 650 °C and 900 °C in a 5 % H₂-Ar atmosphere to induce oxygen vacancies at the nanoparticle surfaces. The thickness of the particle surface layer, in which the oxygen vacancies are located, was characterized by ultra-high transmission electron microscopy and high resolution X-ray photoelectron spectroscopy analysis.

It is found that previous to the reduction process, the particles have the typical ferroelectric response, whereas, after that treatment, the particles present both a ferroelectric and ferromagnetic response (multiferroic nanoparticles). During the presentation experimental evidence as well as computational quantum mechanical modelling based on the density-functional theory (DFT), will show that the oxygen vacancies, located at specific lattice sites, are responsible for the multiferroic behavior of the nanoparticles.



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**[NSN-260] Electrochemical study of Ni-based nanocrystalline alloys
prepared by high-energy ball milling**

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Ni-based nanocrystalline materials exhibit superior properties, compared to the conventional coarse grain alloys. These alloys have been also studied over the years due to their great anti-corrosion properties and applications in abrasive environments. These materials can be processed by different techniques including mechanical alloying (MA). MA process offers several advantages during the synthesis of materials, however, the properties and characteristics of mechanical milled alloys are affected by the milling parameters. In this regard, limited investigations concerning the influence of milling parameters on the corrosion resistance of Ni-based nanocrystalline alloys has been studied. Therefore, the aim of this investigation is to analyze the influence of the milling time on the corrosion resistance of nickel-based alloys with different compositions. Ni, NiCr, NiCoCrAlY and NiCoCrAlHfYSi were prepared by high-energy mechanical alloying using two different milling times (8 and 12 h) and its effect was evaluated on the corrosion resistance of the alloys using electrochemical techniques via linear voltammetry in a NaCl solution. The results show that longer milling times, as well as the addition of new components such as Cr and Co, considerably improve the electrochemical properties of the Ni-based alloys.



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PLASMA AND VACUUM

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Plasma and vacuum science and technology, are widely used in a great variety of synthesis and characterization processes used in materials science, as well as in many industrial developments.

Plasmas are quasineutral distributions of particles (ions, electrons, neutral molecules and atoms), which exhibit collective effects; such as, Debye shielding, plasma oscillations, acoustic waves and sheath formation. Plasmas occur more commonly than usually considered; more than 99% of the known universe consists of plasmas. Plasma research has led, not only to a better understanding of the universe, but to many practical uses: new manufacturing techniques and consumer products.

The term "Vacuum" describes pressure conditions below standard atmospheric pressure. Vacuum technology is applied to all processes and physical measurement carried out under vacuum conditions.

A large variety of deposition and characterization techniques work under vacuum conditions and many of them make use of plasmas

- Sputtering
- Pulsed Laser Deposition
- Plasma Enhanced CVD
- Plasma Assisted MBE
- Atomic Layer Deposition
- Plasma Polymerization
- Plasma Etching
- Closed Space Sublimation
- and any other PVD techniques
- Inductively Coupled Plasma
- Laser Induced Breakdown Spectroscopy
- Mass Spectroscopies
- Scanning Probe Microscopies (SEM)
- X-ray Photoelectron Spectroscopy
- etc.



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Furthermore, plasmas can occur within liquids, either during Cavitation phenomena or by laser ablation, the later allowing for the synthesis of Nanoparticles.

Although plasma and vacuum science and technology are often considered to be mature fields, with little new developments; in fact, arc processes, nanotechnology and biomaterials continue to provide and demand new research in this field.

We invite you to present in this symposium your latest research, observations and developments in this very important basic area of study.



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**[PLV-86] A Pulsed-DC Magnetron Sputtering source: plasma spectroscopy
studies in the presence of reactive gases**

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Magnetron sputtering is a thin film deposition process where energetic ions from a plasma impinge a target located at the discharge cathode and, as a result of a collisions cascade, atoms (M) are sputtered out from the target to be condensed afterward at the substrate. If a reactive gas R ($R = N_2, O_2$, etc) is introduced to the deposition chamber during the sputtering process, a compound (MR_x) deposition can be achieved. The compound stoichiometry, i.e. the x value, depends on several experimental parameters such as the R concentration in the gas mixture, the system pressure, as well as the plasma properties. Besides, the presence of R within the chamber makes the atoms at the target surface react producing the so-called *target poisoning*, which changes the deposition rate and affects the film composition [1]. The target poisoning also depends on the employed power supply, whether it is Direct Current, Pulsed-DC, HiPIMS, or RF [2].

In this work, comprehensive studies of a Pulsed-DC power supply via plasma emission spectroscopy are performed when Ar and N_2 or O_2 are introduced into the chamber. The aim is to analyze the behavior of the different species within the plasma when different deposition parameters are varied. Such parameters are pulse frequency, duty cycle, the concentration of reactive gas within the chamber, system pressure; where the power supply was set to be controlled by power or current. A discussion of which deposition parameters are more important to achieve an optimal deposition outcome will be provided.

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[2] Anders A 2017 Tutorial: Reactive high power impulse magnetron sputtering (R-HiPIMS) *J. Appl. Phys.* **121** 171101



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**[PLV-104] AlN thin films deposited by ECR microwave assisted laser
ablation**

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The main aim of the present work is to report on the study of the combination of continuous plasma, formed by a microwave electron cyclotron resonance (ECR) discharge and the plasma obtained from the laser ablation of a solid target. In this configuration the formation of materials in the form of thin films making use of the relatively high densities of the microwave discharge and the wide range of ion energies produced in the pulsed laser ablation plasmas is studied. With this arrangement it is possible to introduce into the microwave discharge elements which at room temperature are solids, without the use of corrosive and pollutant substances, as the required element is obtained from a pure solid target. The laser ablation process was carried out at low pressures in the range of 10^{-4} Torr, where the microwave discharge works stable. The presence of the microwave plasma allows carrying out the ablation process with an enhanced formation of excited species in comparison with the low interaction of the laser ablation plasma with the neutral gas in the range of pressures used. For the purpose of the present paper a nitrogen microwave ECR discharge was combined with the plasma created during the ablation of an aluminum target, in order to deposit AlN thin films. The obtained films were characterized by XPS, and showed a significant reduction of oxygen in the films and the formation of stoichiometric AlN compound. Plasma parameters were measured by a Langmuir probe, and the chemical species contained in the plasma were analyzed by optical emission spectroscopy (OES).



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**[PLV-138] Characterization of hybrid plasma generated by combining
microwave nitrogen plasma with laser ablation plasma of a molybdenum
target**

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The use of plasmas for the modification of the properties of different materials is a topic that has been known for several decades and has attracted the attention of specialists because, through the exposure to plasmas of different materials, it is possible to modify mechanical, electrical and magnetic properties. In the literature there are very few works on experimental designs that allow studying the plasma parameters resulting from the combination of a continuous plasma, formed by a microwave discharge and a pulsed laser ablation plasma.

In the present work a nitrogen microwave ECR (electron cyclotron resonance) discharge was combined with the plasma created during the ablation of a molybdenum target, in order to deposit MoN thin films. Plasma parameters were measured by a Langmuir probe. The chemical species contained in the plasma were analyzed by optical emission spectroscopy (OES). The structure and chemical composition of the molybdenum nitride films results are reported.



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**[PLV-198] Influence of plasma parameters in the Pulsed Laser Deposition
of boron thin films**

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Boron thin films were deposited by Pulsed Laser Deposition in vacuum on silicon wafers at room temperature. The plasma of the deposition process was analyzed by a planar Langmuir probe to mainly diagnose ion density and ion mean kinetic energy of the plasma, in this sense, boron thin films were deposited with an ion density almost constant and different ion mean kinetic energies. The boron thin films were characterized by Raman spectroscopy, X-ray diffraction, four-points tests for electrical properties and atomic force acoustic microscopy. The results shown structural and morphological variations with the increment of the kinetic energy on the boron thin films. Atomic force acoustic microscopy characterization revealed significant roughness changes from the boron thin films. These differences on the films were related with the ion mean kinetic energy variations of the B plasma during the Pulsed Laser Deposition experiments.



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**[PLV-13] Photocatalytic degradation performance of Lignin using
Nitrogen plasma doped-CdS/GO compounds**

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N-doping of semiconductors has been carried out using a variety of nitrogen precursors. Doping is considered a promising method to achieve the reduction of the energy bandgap (E_g) interval to shift its absorption spectrum to a lower energy level and also improving the separation of the photogenerated charge. These doped semiconductors tested as photocatalysts, offer great potential for the degradation of organic pollutants dissolved in water. Typical procedures to induce nitrogen doping are based on chemical methods that use precursors which generate some residues from the synthesis processes, which in many cases are potentially polluting.

An interesting alternative to induce doping is through the use of N_2 plasma. The production of plasma from N_2 gas is a novel, simple, and reliable technique. In the present work, CdS-N/GO compound was synthesized. The synthesis of CdS was carried out in a reactor heated by microwave radiation. A discharge system has been used to produce a nitrogen plasma to achieve the N-doping in CdS structure. For the GO synthesis, the modified Hummers method was used. The structures were tested in a photocatalytic process to study the degradation of lignin molecule. Furthermore, the structural, morphological, and photochemical properties of samples were determined by X-ray diffraction (XRD), UV-Vis spectroscopy, energy dispersion spectroscopy (EDS), and scanning electron microscopy (SEM). In addition, X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy analyzes were achieved. Photocatalytic degradation studies confirm the improved efficiency of CdS-N/GO systems compared to CdS. The maximum percentage of MB degradation under UV energy irradiation using CdS-N/GO was 100 % in 30 min. In the case of lignin, the degradation was 91 % in 90 min for CdS-N/GO. Those results are promising regarding the methodology to achieve nitrogen doping and also in terms of photocatalytic performance.

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**[PLV-81] LaCuOS: Fabrication of target by two-step solid-state
reaction/sulfurization process and p-type TSO films by PLD technique**

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LaCuOS has a potential to be used as *p*-type transparent semiconductor oxides (TSO), due its wide and direct band gap of 3.1 eV and its conductivity. The application of *p*-type TSO films to electrodes in solar cells is very attractive for suppressing the electron-hole recombination at the interfase region between the TSO and the *p*-type layer. There are many techniques for the synthesis of semiconductor materials, in this work we proposed a two-step SSR (solid state reaction)/ sulfurization method to prepare LaCuOS ceramic target. First the synthesis of CuLaO₂ by SSR, later the sulfurization of the ternary compound, to finally the manufacture of a LaCuOS target. We prepared CuLaO₂ and LaCuOS films on glass substrates by pulsed laser deposition (PLD). The X-ray diffraction analysis shows that polycrystalline structure for the CuLaO₂ target, and the Raman spectroscopy indicates the presence of vibrational modes characteristic of the CuLaO₂, E_g and A_{1g}. For the LaCuOS, the X-ray diffraction analysis shows that polycrystalline and pure structure for the target was obtained, the Raman spectroscopy show the presence of modes vibrational associated of certain phases of sulfur, that indicates the insertion of sulfur into the CuLaO₂ structure. Analysis of reflectance spectrum by Kubelka Munk method show a E_g of 3.1 eV for the LaCuOS target. Spectroscopy UV-VIS indicates that the optical transmission of the LaCuOS films is greater than 70 percent. The effect hall measurements indicate a *p*-type conductivity for the films with a bulk concentration of 1.2×10¹⁶ cm⁻³, mobility of 1.1×10² cm²/Vs and resistivity of 6.6 cm.

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**[PLV-82] Effect of Growth Temperature on the Structural and Optical
Properties of CdTe Films Grown by Pulsed Laser Deposition**

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The cadmium telluride is a p-type semiconductor compound considered one of the most promising photovoltaic materials for having a direct band gap of 1.45 eV at room temperature. CdTe films have been used in the photovoltaic system CdS/CdTe because of their crystalline compatibility, both can crystallize either in cubic and hexagonal phase, reaching theoretical efficiencies of almost 30 %. One of the most important methods of semiconductor deposition is the PLD technique having the possibility of controlling growth parameters such as growth temperature and avoiding the compositional change of CdTe while the deposition occurs. It is known that the phase in which CdTe crystallizes can change with the rising of temperature. In this work, the CdTe compound is deposited by PLD technique on previously prepared CdS substrates grown by Chemical Bath Deposition varying the thiourea composition (0.075 M and 0.1 M), CdTe films were deposited at different temperatures: room temperature, 100 °C, 200 °C, 300 °C and 400 °C. Raman spectroscopy for the CdS films presented modes at 300 and 600 cm⁻¹ associated to the 1LO and 2LO of the CdS, respectively. For the CdTe films show the presence of vibrational modes associated to Te at 122 and 137 cm⁻¹, and the 1LO of CdTe at 164 cm⁻¹. Spectroscopy UV-VIS indicates that the optical transmission of the CdS films is greater than 80 percent, the E_g values for the films are to 2.4 eV, for the CdTe films the E_g values for the films are close to 1.45 eV.

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**[PLV-83] Effect of Flourine Impurification on the Optoelectronic
Properties of Chemical Bath CdS Films**

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The cadmium sulfide is a II-VI semiconductor compound considered of great importance due to its optoelectronic properties, in particular, for photovoltaic applications. CdS thin films have been used as window and n-type semiconductor in CdS/CdTe. CdS films prepared by CBD usually present high resistivity (106-1012 Ωcm), in order to overcome this, CdS films have been doped with several elements: Zn, Cr, F, Al, Sn and In among others. In this work, semiconductor films of CdS impurified whit fluoride were produced using the chemical bath technique on commercial glass/SnO₂:F substrates using thiourea, cadmium acetate and ammonium fluoride as sulfur, cadmium, and fluorine sources, respectively. CdS:F films were deposited varying the concentration of ammonium fluoride to explore the effect of the F nominal concentration on optoelectronic properties of CdS films. Undoped and F-doped CdS films were characterized by Raman spectroscopy, UV-VIS spectroscopy, and Hall Effect measurements. To determine whether the fluorine impurified films are suitable for use for photovoltaic devices, a CdTe film was deposited by close space sublimation technique to form the SnO₂:F/CdS:F/CdTe heterostructure which was characterized with a solar simulation by current versus voltage measurements. Results showed, the presence of vibrational modes characteristic of CdS:F in the Raman spectroscopy. Spectroscopy UV-VIS indicates that the optical transmission of CdS and CdS:F is above 90 percent and the E_g values were around 2.3 - 2.4 eV. On Hall Effect, the electrical properties such as the mobility are 7.043 - 95.34 cm^2/Vs , a resistivity of 269.78 $\Omega\text{ cm}$ and a conductivity of 0.01697 $1/\Omega\text{ cm}$. The highest efficiency of the solar simulator was 7.47%.

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**[PLV-193] Pulsed laser deposition of TiO₂/Au composites by combining Ti
and Au plasmas**

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In this work, thin films of TiO₂/Au composites were grown by pulsed laser deposition. Mean kinetic ion energy and density were used as control parameters by choosing fixed values of both mean kinetic energy and density for Ti plasma while varying ion density of Gold in order to change the atomic content incorporated into the TiO₂ matrix. Deposition pressure was kept constant at 20 mTorr using air as oxidizing atmosphere. A film of pure TiO₂ was grown in order to use it as control sample.

Films were structurally characterized by Raman spectroscopy and X-ray diffraction. Chemical composition and oxidation state of the films were studied by X-ray photoelectron spectroscopy. Thickness was measured by means of profilometry. Optical properties were determined by UV-Vis spectroscopy. Results are discussed as a function of Au plasma density.



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[PLV-284] Plasma Diagnostics with a Langmuir Probe

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A Langmuir probe of stainless steel with copper tip was used to study the signal from a plasma that results from laser ablation of metallic targets of Cu, Ag and Au in a vacuum chamber with 3.5×10^{-5} Torr of pressure. With an oscilloscope, the plasma signals were registered and the flight time and kinetic energy E_k of ions and the plasma density ρ were calculated. The ablation was made with a Nd:YAG laser with emission on the third harmonic $\lambda=355$ nm, a 10 Hz of frequency, and laser pulses of 5 ns width and energies of 20, 86 y 123 mJ per pulse. The atomic weight of ablation target turned out to be one more factor to consider during the ablation process. Despite the fact that Au was the element that presented ions with the highest kinetic energy, which implied a greater amount of absorbed energy, using heavy metals reduces the number of ions expelled in the plasma during laser ablation. Monitoring ablation plasma with a Langmuir probe is helpful in achieving experimental reproducibility. Parameters of the signals of a Langmuir probe, such as its intensity, can be used as a reference to adjust experimental variables in order to obtain similar plasmas.



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RENEWABLE ENERGY: MATERIALS AND DEVICES

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The symposium Renewable Energy: Materials and Devices, has the aim to provide a forum to present and discuss the research relating to the science and technology of energy generation, storage, and managements. An important theme is the research concerning to first generation solar cells, based on mono and poly-crystalline silicon; second generation cells, including CdTe, CIGS, CZTS, amorphous silicon, micro-crystalline and polymorphous silicon; third generation cells, based on the use of quantum dots, nanowires, carbon nanotubes, photo-electrochemical cells, polymer solar cells, nano-crystalline cells, dye-sensitized cells, perovskite solar cells, etc. Moreover, the symposium cover othertopics in renewable energies, emphasizing but not limited to:

- Biomass Conversion
- Solar Thermal Applications
- Wind Energy Technology
- Water Treatment
- Solar and Low Energy Architecture
- Geothermal Technology
- Wave, Tide and Ocean Thermal Energies
- Hydrogen Production Technology and Fuel Cells

The symposium covers the synthesis of new materials, characterization and applications incatalytic process, energy storage and energy production devices. Oral and posters sessions are designed to promote the exchange of the advances in these fields by the participants



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**[RWE-36] Photodetectors with Schottky diode structure based on CdS
doped by the different elements**

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We studied Schottky diodes with structure TCO/CdS(M)/C where TCO is transparent conducting oxide (ITO in this case), M - atoms of different metals, and C - graphite electrode. Thin films of pure CdS and CdS doped with Al, Sn or Eu were obtained by Chemical Bath Deposition (CBD) and characterized using XRD, SEM, EDS, XPS, UV-Vis spectroscopy, I-V curve, and photoresponse estimation. The dark characteristics of the diodes show high rectification (up to six orders of magnitude); at illumination, the best diodes present photoresponse of $1 \times 10^{-1} \text{ A} \cdot \text{W}^{-1}$ that is comparable to the parameters of industrial photodiodes. CdS films in all cases were polycrystalline with crystallite size ranging from 10 to 30 nm, the smallest one in Eu-doped samples. The optical absorption spectra show the blue-shift in Sn- and Al-doped samples (this is due to quantum confinement effect similar to that described earlier [1, 2]) and red-shift in case of Eu doping; these effects influence the photosensitivity spectra. It must be also mentioned that sample with Eu exhibit the smallest stress and dislocation density that also has effect upon optical properties. The data of refractive index and extinction coefficient indicate the presence of porosity that is typical for CBD-made material and is essential for quantum confinement observation. Another cause of the quantum confinement effects is the presence of near-interface quantum wells in CdS films which are the consequence of the non-stoichiometry of the corresponding parts of a film. The illumination dependence of the photoresponse is linear, the inertiality is in the millisecond range, so the devices developed are quite acceptable for light sensing applications.

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**[RWE-43] Photoactive layer for semitransparent organic solar cells
obtained by Spray coating deposition in air**

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Organic solar cells (OSCs) stand as one of the most promising technologies in the field of renewable energy production. Some of the most attractive characteristics of the OSCs are that they can be low-weight, low-cost, semitransparent, and solution-processed. In this context, semitransparent OSCs have been proposed as an attractive way to harvest energy from windows and buildings using readily available surfaces while being aesthetically appealing. To achieve this kind of application deposition methods that are simple, scalable, and low-cost are required. Spray coating is a method that fulfills these requirements and can be used for the deposition of the multiple layers that conforms the OSCs. However, the obtention of films with large homogeneous areas and obtaining the desired morphology remains a challenge in which both process and materials selection play a major role. In this study, spray coating technique approach is used to obtain thin films of a photoactive layer based on P3HT and 2D materials (selectively oxidized graphene and molybdenum disulfide) using a non-halogenated solvent and performing the deposition under ambient conditions in air. It has been found that the thickness can be controlled showing a linear increment with the number of spray passes while maintaining the other parameters constant. The roughness, radiation, absorption, and haze parameter of the different films are discussed, as well as the impact of the different 2D materials with the polymer matrix as a ternary blend. The results show promising potential for the use of spray coating technique to obtain thin films of P3HT and 2D materials.



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**[RWE-45] Use of Reduced Graphene Oxide Quantum Dots is a Sensitized
Solar Cell**

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In this research, we have synthesized and characterized materials for the manufacture of a sensitized solar cell using the protoporphyrin IX dye. Titanium dioxide nanoparticles, reduced graphene oxide, graphene oxide quantum dots were synthesized and protoporphyrin IX was used as a dye. The titanium dioxide nanoparticles used for the photoelectrode were synthesized using the Sol-Gel technique, the graphene oxide quantum dots were synthesized by the microwave-assisted cutting technique and these two compounds were mixed with protoporphyrin IX in order to increase light absorption. For the counter electrode, we used reduced graphene oxide, which was obtained through two steps: 1) synthesizing graphite-based graphene oxide using the modified Hummers technique and 2) reducing the graphite oxide using a sonication method. The materials were characterized by UV-Visible and Raman spectroscopy. The quantum dots showed a size of 0.7 nm which was obtained by the Dynamic Light Scattering technique. We have found evidence of molecular interactions between the quantum dots of graphene oxide reduced with titanium dioxide and protoporphyrin IX shown by some changes in the wavenumbers of some bands in Raman spectroscopy, we confirmed this information by ultraviolet spectroscopy. In the electrical characterization, the photosensitive behavior was observed as well as an increase in the conversion efficiency, from 0.09% for TiO₂ to 6.09% for the TiO₂ + RGOQD + PIX compound.



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[RWE-47] Intelligent controller for solar tracker motorization to provide additional assisted natural cleaning of photovoltaic modules surface

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One of the problems with photovoltaic energy installations is the cleanliness of the solar module's surface. Soiling, shading, among other causes, are known to decrease energy production up to 70 % in some severe cases. Traditional solutions involve manual or robotic cleaning which lead to notable resources waste, especially on big installations, frequently equipped with solar tracking devices. There is an overlooked potential in using the embedded motorization of such installations to provide additional assisted natural washing, drying of the surface with weather phenomena such as rain, dew, and wind. We performed a controlled environment study involving soiling, shading, and different types of stain formations on the module's surface within a laboratory weather simulator. Particle size, haze and overall shading of the surface, as an effect of soiling and stains formation, were analyzed. A solution is proposed, based on intelligent internet-connected solar tracking controller, to increase the module's overall cleanliness. Algorithms of passive and active assisted natural cleaning were developed that use internet weather servers for forecasting and local meteorological station for climate variables monitoring in order to perform assisted natural washing and drying of the module's surface. Experimental prototype showed promising results in controlled environment and is being prepared for relevant environment testing.

Keywords: photovoltaic surface cleaning, solar tracking, soiling, intelligent control, weather station



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**[RWE-56] Efficient Photoelectrochemical Water splitting on
NiCo₂O₄/CoS_x composite**

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The development of a highly active catalyst for energy conversion in the water-splitting process is challenging work. Here, the NiCo₂O₄/CoS_x composite was fabricated by a simple hydrothermal – annealing – wet impregnation route, and the effect of cobalt sulfide loading onto NiCo₂O₄ spinel for photoelectrochemical water splitting was also investigated. The results showed that the CoS_x loading positively affected the electrochemical water splitting performance of the NiCo₂O₄ spinel allowing lower onset potential, low charge transfer resistance, more active sites, and faster kinetics for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in alkaline media. In addition, a remarkable enhancement was exhibited using solar light irradiation on the NiCo₂O₄/CoS_x composite, reducing the energy to drive HER and OER around 150 mV compared to the NiCo₂O₄ spinel, attributed to an efficient photogenerated charge carrier transport due to the synergistic effect of the heterojunction synthesized.



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**[RWE-69] Study and evaluation of thin films by chemical deposition for
the design of a semitransparent photovoltaic device**

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Semiconductor materials using for the build-up of thin films is one of the globally studied topics, due to the various uses that these materials can provide. The production of photovoltaic cells from metallic sulfides has taken a great boom since 2011¹ due to the present abundance of the compounds and their low toxicity. The main problem related with the use of these materials comes from the diverse methods of elaboration of a thin film². In the following work, the S.I.L.A.R method is used to obtain thin films of tin oxide, cadmium sulfide, and zinc sulfide. Where it is intended to deposit such materials in a single thin film for the formation of semitransparent photovoltaic device. It is worth mentioning that the chemical deposit technique used in this project handles different cycle times that are important to establish: the rinsing, draining, and submerging time varies between each material to be deposited and favors the absorption reaction in the substrate and the growth of the semitransparent thin film. A reaction mechanism is proposed for the first layer between glass and SnCl₂ to explain the reaction that takes place in it. Six samples deposited with two different methods were analyzed, in both methods, the products were annealed at different temperatures and with variation in the processing time. The absorbance data obtained from the analysis of the films in a visible light spectrophotometer gives a wide panorama of information about the deposit that was made on the substrate. In both methods, the characteristic absorbance values of the deposited materials are found (glass = 320 nm, SnO₂ = 350 nm, ZnS = 333.33 and CdS = 500 nm). These films were analyzed by the four-point Kelvin method in various regions of the film to specify the electrical resistance for the two deposition methods the values are 25 Ω and 0.1 Ω respectively. Such characterizations in principle give a positive idea of the deposit made on the substrate and give rise to new characterization methods that will be carried out later.



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**[RWE-92] Tuning the properties of the photovoltaic material CsSnI₃ by
the partial metal substitution of Sn by EA, with EA = Mg or Ca**

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Perovskite solar cell (PSC) technology is about to break into the photovoltaic market this year or the next one, nevertheless, the toxicity of the perovskite's constituent-species hinders the deployment of this technology. Inorganic tin halide perovskite, CsSnI₃, arises as a good option to substitute the perovskites with lead content in a PSC; notwithstanding, there is another big problem: the more stable oxidation of Sn(II) into Sn(IV) is apparently impossible to eradicate and it is responsible of the unstoppable internal degradation of this absorber material. In order to address this problem, the partial metal substitution of tin by earth-alkaline (EA) species could be an option. Driven by the above-mentioned, a first principles study based upon Density Functional Theory was performed on the perovskite material CsSn_{0.75}EA_{0.25}I₃ with EA = Mg or Ca. It was proven by formation energy calculations that both perovskites CsSn_{0.75}Mg_{0.25}I₃ and CsSn_{0.75}Ca_{0.25}I₃ could be obtained in laboratory. Besides, by means of a COHP analysis it was found that there is a more ionic nature on the EA-tin halide bonds within CsSn_{0.75}Ca_{0.25}I₃ than within CsSn_{0.75}Mg_{0.25}I₃, furthermore, owing to the ICOHP analysis there were a slightly strengthening on CsSnI₃ perovskite by the partial metal substitution of Sn by Mg. As a consequence of these results, CsSn_{0.75}Mg_{0.25}I₃ obtained the greatest bulk modulus (B_0) among the three structures with $B_0 = 19.967$ GPa, followed by the one for CsSnI₃ ($B_0 = 19.403$ GPa) and, last but not least, the one for CsSn_{0.75}Ca_{0.25}I₃ ($B_0 = 18.891$ GPa). Finally, it was calculated the bandgap of the three perovskites by means of the HCTH/407 functional, the values obtained were: 1.11 eV, 1.32 eV, and 1.55 eV for CsSnI₃, CsSn_{0.75}Mg_{0.25}I₃ and CsSn_{0.75}Ca_{0.25}I₃, respectively; however, indirect transitions were found on the perovskite with Mg content. The present theoretical findings could contribute to the field of perovskite photovoltaics as it could serve as a starting point for further investigations.



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**[RWE-95] Revisiting the charge transport properties of high performance
tandem solar cells to improve their characterization**

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The charge transport properties of solar cells even those of outstanding performance are rarely fully characterized, strongly limiting the information on the device physic properties. Often providing just a current-voltage curve under illumination and the corresponding data that qualifies its performance: open circuit voltage (V_{OC}), short circuit current (J_{SC}), fill factor (FF) and efficiency. However, parameters as saturation currents at dark (J_0), ideality factor (n), parasitic series resistance (R_s), which are extremely important to better understand and assess the quality and behavior of the device and its associated technology, are neglected. Worse than that, such way of presenting the results might leave some readers with the impression that the last mentioned parameters are neither necessary to understand the solar cell physics nor to improve its performance.

In this work it is shown that the general $J(V)$ of a tandem solar cell is straightforwardly obtained from the PN junction model of Shockley, whichever the number of junctions in the cell. Then, using it with the solely reported data of: J_{SC} , V_{OC} , and fill factor, the above-mentioned information that is not provided by the corresponding authors can be obtained. Such data constitute valuable feedback to reshape the cell design, its technology, and processes if necessary. The procedure developed here to recover those physic parameters has been applied to data of some of the most efficient solar cells reported, reveling their main issues and several other interesting things as well. One of which is the PN junction ideality factor frequently quite far from its theoretical value, strongly decreasing the cell's efficiency, and that under high concentration levels the cell's parasitic series resistance is not constant, etc.



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**[RWE-113] Microwave-Assisted Synthesis of BiVO₄ Microstructures
Decorated with Au Nanoparticles for Potential Pollutants
Photodegradation**

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Bismuth vanadate (BiVO₄) is a material that has carried great interest in recent years due to its photocatalytic activity and great chemical stability. The BiVO₄ has a low bandgap energy (~2.41 eV), which promotes the photocatalytic reactions for decomposition of pollutants and water splitting in the visible range of the electromagnetic spectrum [1, 2]. Nevertheless, the recombination rates of the photogenerated charges in this material restrict its applicability [3]. Therefore, a heterojunction with metals, such as Au nanoparticles (AuNPs) can overcome this issue. In addition, AuNPs can work as a trap for photo-induced electrons and absorb visible light due to localized surface plasmon resonance [4].

In this work, the BiVO₄ powders were prepared using microwave-assisted hydrothermal synthesis. To find optimal crystalline phase, the reaction time was explored from 30 s to 10 min. In comparison with the conventional hydrothermal method, the time needed for BiVO₄ obtention was dramatically reduced. Afterward, the BiVO₄ powders were characterized by X-ray and Raman spectroscopy. Optimal reaction conditions allowed the monoclinic BiVO₄ to be synthesized successfully in just 30 seconds.

On the other hand, the AuNPs were synthesized by a modified seed method, which allows incorporation of BiVO₄ powders and control on size and shape of nanoparticles. First, a cetyltrimethylammonium bromide (CTAB) solution was prepared and then BiVO₄ powder was added. Chloroauric acid (HAuCl₄) and sodium borohydride (NaBH₄) were added to obtain gold seeds on the surface of BiVO₄ microstructures, which were then deposited in a solution with Au ions. Due to surfactant, Au seeds were growing to form nanorods. UV-vis spectra show two principal bands, which may confirm Au nanorods.

Photodegradation experiments are currently in development to determine potential organic molecule degradation performance in the polluted water of the synthesized photocatalysts. The influence of synthesis parameters and the role of heterojunction on the physical properties of the samples are discussed.

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[RWE-165] Analysis of the surface states effect on built-in electric field of multi-layered GaAs-based solar cell structure by optical spectroscopy

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Self-assembly of quantum wells and dots, and highly mismatched alloy such as III-N-V materials are applied to photovoltaic structures where the multi-wavelength absorption process is looked, being usually embedded in a GaAs-based photovoltaic by their promising properties of this semiconductor binary compound. Nevertheless, surface recombination is still a key challenge in the development of solar cells and detectors specially for nanostructured devices where surface atoms make up a considerable part of this, being surface characteristics an important factor for their functioning and performance. In this work, the effect of surface states (Nss) on the built-in electric field distribution in GaAs-based solar cell is investigated. We grew two set of samples by molecular beam epitaxy: (a) simple p-n junction device and (b) multilayered system where the FSF and BSF (Front Surface Field and Base Surface Field) layers were designed and inserted with the aim to reduce the effect of the SRH recombination. The Nss in samples were modulated by chemical passivation with ammonium sulfide. We determined the depletion region and their modification with the passivation by Raman spectroscopy which have strong modification with passivation in (a) structures. Franz-Keldish oscillations (FKO) in photorefectance spectrum were employed to evaluate the built-in electric field. We found that the total built-in electric field diminishes around 10% and 4% with the passivation process for the (a) and (b) structures, respectively. To determine the contribution of each electric field of the photovoltaic structure on FKO and their modification by the chemical treatment both the laser excitation wavelength and power in the photorefectance measurement was varied, obtaining changes in the FKO lineshape and period as indicative of their modulation and origin. Fast Fourier transform (FFT) was employed to find the contribution of electric fields to FKO, where two frequencies associated to depletion zone and surface dominate the frequency spectrum. We found that the (b) structure is less sensitive to Nss by the insertion of FSF layer. Additionally, changes in Nss density are translate into a redistribution of carriers, producing modification in the built-in electric fields distributions along the whole (a) and (b) structures according to FFT. Current density is strongly affected, rising 15% with reduction of Nss for the treated sample in contrast with the as-grown case, according to current-voltage under AM1.5. All our experimental results are contrasted with



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numerical process. With this study we demonstrate that in nanostructured solar cells surface have a strong impact on the device performance.

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**[RWE-209] High energy transport shifting performance of a thermal
switch based on surface instability phenomena of magnetoactive
nanofluids**

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A proposed thermomagnetic switch that takes advantage of the surface instability of paramagnetic nanofluids was developed in this research. Direct measurement of the variation of heat flux passing through a ferrofluid as a function of the temperature gradient and the incident magnetic field was performed. The presence of an external magnetic field produces a spike-like instability surface that allows to obtain a thermal switch whose heat flux is relatively constant. When comparing the active and inactive state of the device there is a significant difference in the amount of heat flow. The variation of the angle of incidence of the external magnetic field outside the vertical symmetry axis produces a decrease in the heat transfer capacity of the device. This research shows an alternative for the use of magnetic fields and magnetoactive nanofluids in thermal management.



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**[RWE-229] Biodiesel production, characterization and prediction of its
physicochemical properties.**

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Biodiesel is an alternative energy source that can be a substitute of conventional diesel obtained from petroleum. It is produced from renewable biomass, is biodegradable, sulphur free and a renewable biofuel. The production of biodiesel worldwide and the use of mixtures (diesel/biodiesel) in diesel engines has increased because presents economically and ecologically advantages [1]. In this work the biodiesel production through direct transesterification using a bismuth-based catalyst [2], the characterizations and the evaluation of mixtures (diesel/biodiesel) in diesel engine are presented. Additionally, the residual biomass obtained as by-product from direct transesterifications was mixed with different acrylic and polymeric resins to modify its rheological properties and obtained coatings for various applications, finally its presented a prediction of biodiesel physicochemical properties using the software *Biodiesel Analyzer* based on the results obtained from GC-MS[4].

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**[RWE-267] CO₂ separation properties of deep eutectic solvents-based
supported liquid membranes**

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Deep eutectic solvents (DES) have been proposed in the last years as viable and more sustainable solvents in a myriad of applications. CO₂ capture or adsorption is one of those possible applications where DES can act as an alternative to the amine-based solvents currently being used in carbon capture and storage processes. In this work, different choline chloride-based DES were prepared, and CO₂ gas transport coefficients were measured. Two DESs were prepared by mixing and heating the hydrogen bond acceptor (choline chloride) with either urea and D-glucose as hydrogen bond donors. The Fourier transform infrared spectroscopy confirmed the hydrogen bond interactions in the resulting DES. The DES-based supported liquid membranes were investigated systematically to determine the permeability and selectivity for CO₂ at both room temperature and elevated temperatures. The DES were immobilized in TiO₂-rutile macroporous support, and the pure gas permeability of N₂, CO₂, and CH₄ was assessed to establish liquid membrane's ideal selectivity.

The results showed that Choline Chloride-urea, Choline Chloride-D-glucose-based membranes exhibited CO₂ permeability of 272.1 and 166.36 Barrer respectively at 25°C while ideal selectivity of these membranes was found 5.78 and 2.99 for CO₂/N₂, respectively. Therefore, the studied membranes showed excellent selectivity of CO₂ 4.01 and 1.27 for CO₂/CH₄. This high selectivity of CO₂ over CH₄ and N₂ can be attributed to the physisorption of CO₂ with DES as well as the high basic features of the DES. The effect of operating temperature on membrane performance was also investigated, evidentiating an appropriate alternative to the conventional ILs.



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[RWE-274] PEDOT:PSS nanofibers used for supercapacitor applications

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Electrospun poly(3,4-ethylene dioxythiophene) polystyrene sulfonate (PEDOT: PSS) nanofibers were deposited onto flexible polyethylene terephthalate (PET) substrates to obtain electrodes for flexible and all solid-state supercapacitors (SCs). The nanofibers improved considerably their conductivity when they were immersed in ethylene glycol (EG), producing a removal of the excess of PEO around the nanofibers, which causes that the PEDOT:PSS nanofibers became more conductive, then improving their electrochemical performance. The removal of PEO was observed by scanning electron microscopy (SEM) and corroborated by energy-dispersive X-ray spectroscopy (EDS). The PEDOT:PSS electrodes were used in supercapacitors, with poly (vinyl alcohol)/phosphoric acid (PVA/H₃PO₄) gel polyelectrolyte, forming an all solid-state SC. The SCs reach an areal capacitance of 1.8 mF/cm² and a gravimetric capacitance of 3.6 F/g at a discharging current of 5 μA/cm² by galvanostatic charge discharge technique (GCD). The capacitances of the SCs were also calculated by cyclic voltammetry showing very similar results than GCD. These results using PEDOT:PSS nanofibers as electrodes showed better performance in comparison with doped PEDOT:PSS films with the same gel polyelectrolyte. The devices showed very good stability since they were charged and discharged at 20 μA/cm² by 1000 cycles maintaining ~92 % of the initial capacitance. These results open the possibility of fabricating wearable and 3-D interconnected electrodes for energy-storage devices that could be implemented on clothes and on any non-flat surface.



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[RWE-283] Inorganic membrane reactor for CO₂-O₂ separation and H₂ production

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The aim of this work is to fabricate a membrane reactor for the selective separation of CO₂-O₂ and subsequent syngas production (H₂ and CO) at high temperatures through the oxidative reforming of the methane process. Firstly, a dense inorganic membrane was prepared by fabricating a porous support material in disk shape comprised of cermet powders (LiAlO₂-Ag 50:50 vol %) and then incipient densified by an infiltration process with a ternary mixture of molten salts (42.5/ 32.5/25 mol % of Li₂CO₃, Na₂CO₃, and K₂CO₃). Next, the membrane was assembled in a permeation setup, and a good reforming catalyst of Ni/CeO₂ was placed just underneath the membrane. A gas mixture of CO₂, O₂, and N₂ was fed into the system for simultaneous permeation measurements, and a CH₄ stream was supplied into the permeated species side for the syngas production in a temperature range of 750-850 °C. Structural characterization of the membrane was carried out by X-ray diffraction (XRD) technique; Archimedes method was used to determine the membrane's pore volume fraction before infiltrating with the molten salts. Moreover, scanning electron microscopy and unsteady state He permeation analysis was used to characterizing the morphology characteristics of the sample and demonstrate its complete densification with molten salts. Results show that inorganic membrane reactor shows high simultaneous permeation of CO₂ and O₂, reaching a total flux of 0.82 and 0.44 mL·min⁻¹·cm⁻² at 850 °C, and showing stable rates of H₂ and CO production for long term (>100 h).



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**[RWE-286] Conjugated materials for photocatalytic carbon dioxide
reduction**

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Photocatalytic carbon dioxide reduction is a research area of immense interest due to its potential in converting a greenhouse gas into useful chemical building blocks using the energy of the sun. Most of the studied photocatalysts are inorganic and organic materials have been far less studied, with the exception of carbon nitride materials. Here, I will present our work on the application of conjugated polymers¹ and covalent organic frameworks^{2,3} to photocatalytic carbon dioxide reduction. These materials can be made at low temperatures and using a wide range of monomers allowing to systematic tuning of materials' properties. A particular focus will be on comparing polymeric to molecular photocatalysts³ and the metal-catalysts as these are important to obtain high yields and selectivity for carbon dioxide reduction.⁴

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**[RWE-19] THE COPPER BACK CONTACT INFLUENCE ON THE CdTe-BASED
SOLAR CELLS EFFICIENCY**

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Cadmium telluride (CdTe) is one of the leading and most promising materials for thin-film solar cells. It has a direct optical band gap between 1.44 - 1.50 eV, which is close to the optimum value for photo-conversion. Additionally, it has a large optical absorption coefficient ($>10^5 \text{ cm}^{-1}$), which means that a layer thickness of a few micrometers is enough to absorb 90% of incident photons. Cadmium sulfide (CdS) is commonly paired with CdTe to create a high-quality n-p heterojunction solar cell due to it is the only material among all semiconductors that exhibits the lowest lattice misalliance with CdTe along with its potential as window layer, meaning that a thickness of $<100 \text{ nm}$ is enough to transmit a high short-wavelengths light fraction ($<520 \text{ nm}$). A key concern and one of the greatest challenges for CdTe photovoltaic technology is the successful formation of a stable ohmic back contact. The utilization of copper (Cu) plays an important role in the formation of a good ohmic contact by acting as a substitutional acceptor for Cd, thus increasing the doping concentration near the surface of p-type CdTe. In this work, CdS and CdTe films were obtained by sputtering and close space sublimation (CSS), respectively. Sputtering is a widely used deposition technique mainly due to its capability of growing high-purity thin films and extremely high adhesion, whereas the CSS is a leading method for CdTe thin film deposition because of the ease of use and cost-effectivity. CdS films were grown onto commercial $\text{SnO}_2:\text{F}$ substrates at a 300°C substrate temperature and 30 W of power. CdTe films were obtained at low vacuum (10^{-1} Torr), followed by an activation treatment in a chlorine atmosphere at 410°C . The metallic back contact Cu/Au was deposited by sputtering on CdTe films, varying the growth time of Cu metallic film. The final stacks were annealed at 150°C and then characterized in a solar simulator under a 1.5AM illumination. The variation in the Cu growth time showed that increments in the Cu deposition time results in better ohmic contact, improving electrical parameters but an excess tends to lower the performance of the solar cells (roll-over effects), which can be interpreted through the J-V curves. The best device reached an efficiency of 10 %.



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**[RWE-32] Synthesis of materials by green chemistry for future
photovoltaic cell applications**

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In the world of technology, researchers are searching for new protocols for the nanoparticles synthesis without hazardous and toxic chemicals in order to reduce environmental impact. Green chemistry is defined as the design of chemical products and processes to reduce or eliminate the use and generation of hazardous substances. Phytochemicals from plant extracts are important for the development of green synthesis of nanoparticles such as titanium dioxide TiO₂. The phytochemicals extracted from plants acted as surfactants, modifying the growth mechanism and stabilizing high quality, small, nearly spherical, non-aggregated TiO₂ nanoparticles. TiO₂ nanoparticles have several applications as components in photocatalytic, pharmaceutical, cosmetic products, and photovoltaic cells as electron transporting material (ETM). In this research work, the development of the synthesis of TiO₂ nanoparticles using phytochemicals from plant extracts such as clove, green tea and horsetail, the SEM, XRD, FTIR, UV-vis results confirming their obtaining will be presented. The development of new syntheses for obtaining nanomaterials allows the development of photovoltaic devices in an economical and environmentally friendly way.



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**[RWE-66] Theoretical and experimental study of thermoelectric response
of cadmium telluride doped with bismuth**

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Cadmium telluride (CdTe) is a semiconductor compound considered a candidate for thermoelectric materials due to its low thermal conductivity. To enhance its performance doping with bismuth can be an alternative because this semimetal exhibits high electron mobility. In this research, a theoretical and experimental study of CdTe doped with Bi has been studied for its potential use as a thermoelectric material. Nanofilms were obtained according to SILAR synthesis process. The nanofilms were characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive x-ray spectroscopy (EDS) and ultraviolet-visible spectroscopy (UV-vis). For nanofilms nanostructures an important position at 28° (2θ) was associated to (111) in F43M space group. The bandgap energy was obtained using the Kubelka-Munk function, showing a direct band gap between 1.6-1.8eV. DFT based wave plane pseudo potential as is present in CASTEP was used to investigate the structural, optical, and electronic properties of CdTe with Bi as doping concentration. The comparison between the obtained theoretical results agrees with the experimental.



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[RWE-79] Implementation of NAPC-TCNQ for Flexible Organic Solar Cells

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This work is related to the progress on the implementation of sodium phthalocyanine for flexible organic solar cells. A NaPc/TCNQ structure was deposited on TCO/PET for the solar device and silver contacts were used to determine the photovoltaic properties. HV Thermal evaporation of small molecules and spin coating processes were used for device deposition. The Characterization of the solar cell was conducted using FTIR, AFM, UV-Vis, and IV characteristics for structural, morphological, opto-electrical properties. FTIR measurements confirm an efficient transfer for the device to the PET flexible substrate with a smooth and homogeneous surface topography. A direct transition bandgap of 2.5 and 2 eV were obtained for different the NaPc deposited thicknesses. Diode type characteristics were obtained with threshold voltages of ~1.5 V and ~15 microAmpers current across the device at 6 V. IV characteristics were measured with different incident led light colors showing a variation of the curves. Further analysis was conducted by measuring EQE on the NaPc-TCNQ flexible device which gives evidence of the device and interfaces quality for solar cell applications. This work is related to the progress on the implementation of sodium phthalocyanine for flexible organic solar cells. A NaPc/TCNQ structure was deposited on TCO/PET for the solar device and silver contacts were used to determine the photovoltaic properties. HV Thermal evaporation of small molecules and spin coating processes were used for device deposition. The Characterization of the solar cell was conducted using FTIR, AFM, UV-Vis, IV characteristics and EQE for chemical, structural, morphological, opto-electrical properties. FTIR measurements confirm an efficient transfer for the device to the PET flexible substrate with a smooth and homogeneous surface topography. A direct transition bandgap of 2.5 and 2 eV were obtained for different the NaPc deposited thicknesses. Diode type characteristics were obtained with threshold voltages of ~1.5 V and ~15 microAmpers current across the device at 6 V. IV characteristics were measured with different incident led light colors showing a variation of the curves. Further analysis was conducted by measuring EQE on the NaPc-TCNQ flexible device which gives evidence of the device and interfaces quality for solar cell applications.



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**[RWE-87] Effects of the manufacturing process on the P3HT:PCBM
absorber layer properties**

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In recent years, great emphasis has been placed on promoting renewable energies, which has allowed the development of different kinds of photovoltaic solar cells (PSCs), among which are the polymeric-based PSCs. Besides many polymeric absorber layers, the poly-3-hexylthiophene (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM) blend is a promising material, and conversion efficiencies of around 5.4% have been obtained. It has been reported that the properties of the P3HT:PCBM blend are directly related to the performance of PSCs, therefore, the material optimization is a necessary step in order to improve the efficiency. A key factor for obtaining high quality P3HT:PCBM absorber layers is the processing of the precursor solution, since it is the starting point for obtaining the layers.

Therefore, in this work we carried out a study on the effects that solution process and annealing-temperature produces on the absorber layer properties. The P3HT:PCBM blend was prepared with 1:1 ratio and diluted in chlorobenzene. The time and temperature of the stirring solution were varied from 4 to 18 h and 27 to 80 °C, respectively. Thin films were deposited onto glass substrates by using the spin coating technique. Then, an annealing process was carried out at a temperature from 0 to 150 °C. Samples were characterized by optical techniques. Preliminary results indicate that, at low stirring time and temperature, the annealing produces a shift of the absorbance spectrum towards higher wavelengths and promotes a better definition of the characteristic shoulders of the absorption edges (550 and 602 nm), which indicate a greater structural ordering of the films. However, as the stirring time increase, the annealing temperature produces an unfavorable effect, causing an increase in the structural disorder of the polymer blend; indicating that long stirring times could induce degradation of the material. Solar cell devices with glass/ITO/P3HT:PCBM/Al structure are being explored using these variables, first results indicate a bulk heterojunction (BHJ) formation; however, optimization process is being carried out.

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[RWE-171] Electrochemical characterization of Ni-20Cr catalyst

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Fuel cells represent a good alternative for energy generation and storage technique and also provide a highly efficient and environmentally friendly technology. As a result of their good performance, alkaline fuel cells (AFC) were the first fuel cell technology to be implemented for the generation of electricity from hydrogen. Fuel cells depend greatly on noble metal catalysts, mainly platinum (Pt), moreover, the oxidation kinetics of H₂ on Pt in alkaline media is slower than in acidic media. Therefore, new and more active H₂ oxidation electrocatalysts must be developed allowing a higher efficiency in AFC. Thereby, the aim of this work is study the electrochemical properties of a catalyst based on Ni-20Cr alloy to be used as an anode in AFC. The catalyst was prepared by mechanical alloying using different milling times. Then, the alloy was prepared to perform electrochemical tests including open circuit potential, linear voltammetry, cyclic voltammetry and rotating disk electrode in a KOH solution, to obtain the catalytic properties of the material. The results of the electrocatalytic properties of Ni-20Cr alloy show that as the milling time increases the hydrogen oxidation reaction kinetics improved. The characteristic signals of hydrogen adsorption/desorption process were not observed. However, the alloy can be used as a substrate to deposit Pt or Pd films because presents good stability when subjected to different oxidation and reduction cycles at a potential range near 1V.



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**[RWE-234] Synthesis and electrochemical characterization of
nanostructured cerium oxide thin film**

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Hydrogen is considered an important energy vector, that is, it is capable of storing or transporting energy. However, the energy efficiency of hydrogen production using water is still modest, which makes it necessary to develop electrocatalysts and photocatalysts with better performances. In this work, nanostructured cerium oxide thin films were prepared on FTO substrates by ultrasonic spray pyrolysis, using cerium acetylacetonate as a metallo-organic precursor dissolved in anhydrous methanol. The substrate temperature was set at 475 °C, the deposition time was 30 min, the carrier and director gas flows, air in both cases, were set at 1.0 L/min and 1.5 L/min respectively. The morphological, structural, optical and vibrational properties were studied by X-ray diffraction, scanning electron microscopy, Raman spectroscopy and UV-Vis. Homogeneous thin films with fluorite structure of ceria are obtained in all cases. The calculated band gap was 3.2 eV. Electrochemical measurements showed that the films can be used in the water reduction process, applying a potential of -1.5V vs Ag/AgCl, as the potential increases the current density increases, and when it reaches -2.0V vs Ag/AgCl the film suffers an excessive loss of oxygen, due to this the CeO₂ loses crystalline. Using the Mott-Schottky charts, the position of the valence and conduction bands was calculated with respect to the Ag/AgCl electrode. The position of the valence and conduction bands in all cases indicate that the films are suitable for use as catalyst in the photoelectrocatalytic water reduction process.

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**[RWE-235] Nanostructured gadolinium doped cerium oxide thin films
obtained by ultrasonic spray pyrolysis for solid oxide fuel cells**

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Cerium dioxide presents great interest for application in solid oxide fuel cells and catalysis. In this work, gadolinium doped cerium oxide thin films were prepared by Ultrasonic Spray Pyrolysis. The influence of deposition conditions on the morphology, optical and electrical properties of the films was studied. In particular, gadolinium concentrations of 10, 15 and 20 %, substrate temperatures of 425, 450 and 475 °C and flow rates of 0.5 and 1.0 L / min, 1.0 and 1.5 L / min and 1.5 and 2.0 L / min for carrier and director gases respectively were evaluated. The films obtained were characterized by X-ray diffraction, UV-vis spectroscopy, scanning electron microscopy, and impedance spectroscopy. Variations in temperature and air flows modify the morphology, grain size and texture of the films. Increasing the temperature of the substrate produces an increase in the band gap of materials, but does not substantially modify the activation energy, except for samples grown at 10% Gd. The activation energy for ion conduction increases considerably when using low flows (0.5 and 1.0 L / min for the carrier and director gases respectively). The better conditions for obtaining homogeneous and fracture-free films with low conductivity activation energies are substrate temperatures of 450 ° C and flow rates of 1.0 and 1.5 L / min flows for carrier and director gases respectively.

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**[RWE-238] Sb₂Se₃ film growth by close space sublimation for thin film
solar cell processing**

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The antimony-based chalcogenide compound Sb₂Se₃ has emerged as a potential candidate to replace some of the existing materials in thin-film solar cell technology, because according to its properties and characteristics, it manages to overcome the disadvantages of some compounds made up of elements toxic or scarce on the planet, such is the case of the CdTe and the CIGS. Sb₂Se₃ is a promising absorber material for photovoltaic cells because of its optimum band gap, strong optical absorption, simple phase and composition, and earth-abundant and nontoxic constituents. The rationale to choose close space sublimation for Sb₂Se₃ film deposition was first discussed, followed by detailed characterization of Sb₂Se₃ film deposited onto FTO with different substrate temperatures. Prototypes were developed to test the quality of thin films deposited using this technique, so the FTO/CdS/Sb₂Se₃/Au photovoltaic device was built, achieving an encouraging solar conversion efficiency. Our results indicate that this close space sublimation technique is a promising approach for antimony chalcogenide solar cells.



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**[RWE-241] Ammonia plasma treatment as an effective passivation
scheme in black silicon solar cells**

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The surface treatments in crystalline silicon solar cells are very important and have a great impact on the final efficiency of the devices. In particular, in Black silicon solar cells, the passivation scheme on the surface are very necessary to passivate the dangling bonds and to form stable final terminations on the surface of the device. In this work, black silicon solar cells were prepared after different alkaline and MACE treatments so as to form porous pyramidal structures on the surface of device to increase the absorption processes. Furthermore, the final device structures were finally passivated in the presence of ammonia plasma environment in a PECVD system. Finally, short circuit current and open circuit voltage were measured using an Abet AAA solar simulator and the results were compared with the measurements obtained from Sinton Suns- Voc equipment.



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**[RWE-245] Synthesis and Study by DFT of Mn₃O₄ as a Possible Cathode in
Aqueous Aluminum Ion Batteries**

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Currently the rapid expansion of the electrification of transport vehicles and the storage of renewable energy sources, has created a demand for electrochemical energy storage systems. Due to the high cost of current lithium-based systems and their deficiency of safety, new electrochemical energy storage systems based on multivalent ions are being investigated. In order to develop a new electrochemical storage system based on more abundant elements and that is safer, particles of approximately 500nm in diameter were synthesized by annealing of waste Zn-C batteries at 900°C in open atmosphere, they were characterized by XRD, SEM, EDS and Raman Spectroscopy and indexed to the Hausmanite phase of Mn₃O₄, and proposed to be used as cathode in an electrochemical energy storage system based on the aluminum ion in an aqueous electrolyte. An *ab initio* analysis of the insertion thermodynamics of the Al ion was carried out on this material by means of DFT, in which the octahedral sites of the spinel structure were obtained as a preferential site for a phase transformation from spinel to layered compound and insertion of aluminum afterwards. Experimentally AlCl₃ * 6H₂O was used as a Water in Salt electrolyte, in which it was confirmed that it is possible to intercalate aluminum in Mn₃O₄ to give way to a layered phase of Al_xMn₂O₄ by XRD analysis. Finally, an experimental open circuit voltage of 1.6 V was obtained from the assembled electrochemical cell against the 2.89 V calculated by theory.



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**[RWE-246] A new Passivation Scheme for the Performance Enhancement
of Black Silicon Solar Cells**

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Several works prove how the silicon is capable to reduce the front reflection and to improve light trapping due superficial micro and nano texturizations, enhancing on solar cells to increase such efficiency. The last is very important and have a great technological relevance in the final efficiency of the devices. Black silicon solar cells refers to crystalline silicon solar cells with complex grades of surfaces texturization schemes. Metal-assisted chemical etching (MACE) method is one of them, which form nanopillar, porous silicon and different pyramidal structures on the substrate surface. These structures have low surface reflectance and appear dark (black) and therefore referred to as 'black silicon'. On the other hand, the increase in the surface area, intensifies the recombination velocity and respectively increases the saturation current density " J_0 ". For that reason, it is very important to implement different passivation surface schemes. Surface plasma annealing combined with different thin films as antireflection coatings are some alternatives to this.

In this work, we prepared silicon solar cells with diverse grade of chemical surface treatment and plasma annealing (ammonia) with silicon-rich silicon nitride as antireflection and shift conversion coatings. Spectral response, surface reflectance, I-V curves in dark and under illumination were measured.



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**[RWE-249] Analysis of HTL and ETL layers to improve the efficiency of Sb₂
(Se_{1-x}S_x)₃ solar cells**

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Nowadays, the best efficiency reported in antimony chalcogenide compounds corresponds to the structure FTO/CdS/Sb₂(Se_{1-x}S_x)₃/spiro-OMeTAD/Au with 10.5%. In this work, a comparative study was carried out by changing the spiro-OMeTAD as HTL (hole transport layer) and the CdS as ETL (electron transport layer). The performance of the compound Sb₂(Se_{1-x}S_x)₃ in the solar cell was also analyzed, varying parameters such as its composition, band gap, thickness, etc. This with the objective of studying the influence of each layer on the electrical parameters of the solar cell and at the same time evaluating the synthesis method of each layer that guarantees the real transfer on an industrial scale of these devices. The main photovoltaic parameters such as short circuit current density, open-circuit voltage, fill factor, energy conversion efficiency, and external quantum efficiency of devices in nip heterojunction structures are analyzed using SCAPS software. 1-D. The variation of ETL, HTL and absorber thicknesses, as well as the influence of the density of apparent defects in Sb₂(Se_{1-x}S_x)₃, the density of defects of the interfaces and the influence of the electrical properties of HTL and ETL in the final efficiency of the device was investigated. After the optimization of the previous physical parameters, the efficiency improves reaching 16% with the FTO / ETL / Sb₂(Se_{1-x}S_x)₃ / HTL / Au proposed structure.



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**[RWE-269] Designing Cu₂ZnSn_{1-x}Ge_xS₄-based thin films solar cells for
indoor photovoltaic applications: A simulation study**

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Indoor photovoltaics (IPVs) are gaining significant interest for the possible power source in future, recycling the photons of the artificial light sources installed in the indoor environment. In this work, a numerical simulation model is used to explore the potential of low-cost single-junction kesterite solar cells in IPV devices. With the help of Shockley-Queisser (SQ) model, we have calculated the efficiency limit of Cu₂ZnSn_{1-x}Ge_xS₄ (CZTGS) solar cells ($0 \leq x \leq 1$; $x = [\text{Ge}]/[\text{Sn}+\text{Ge}]$) using two different artificial light sources, namely compact fluorescent (CFL) and light emitting diode (LED) bulbs with different color temperature. It has been found that a high SQ-limited efficiency between 51.4 to 54.7% can be obtained for an absorber layer with a band gap of 1.73 to 1.94 eV. Our simulations reveal that a high power conversion efficiency of 23.8% can be obtained using a particular CZTGS stoichiometry ($x = 0.75$) with a band gap of $E_g = 1.79$ eV and eco-friendly ZnS as n-type buffer layer.

Keywords: Cu₂ZnSn_{1-x}Ge_xS₄ solar cells, Numerical simulation, Wide band gap semiconductors, Indoor photovoltaics (IPVs), Limit of power conversion efficiency.

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[RWE-271] Improvement of power conversion efficiency in CuSbS₂-based thin film solar cell by optimizing the device structure: A computational analysis

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In spite of the adequate optical and electronic properties of orthorhombic CuSbS₂ (CAS) as absorber material, the maximum power conversion efficiency (PCE) of solution-processed CAS-based solar cells has been stagnant at 3.22 %, which is far lower than that of Cu(In,Ga)(S,Se)₂ (23.5%) and Cu₂ZnSn(S,Se)₄ (12.6%). One of the major challenges affecting the performance of CAS-based solar cells is the sub-optimized cliff-like conduction band offset at the CAS/CdS interface, leading to enhanced carrier recombination at trap states near the interface. Besides, the Schottky-type Mo back contact contributes largely to rear surface recombination, lowering further the device efficiency. With the aim of improving the PCE of CAS solar cell, we have designed a new device structure (Glass/MoO_x/CuSbS₂/ ZnO_{0.3}S_{0.7}/ZnO:Al/Al), where CdS is replaced by eco-friendly ZnOS buffer and Mo is substituted by ohmic MoO_x electrode. Using the numerical simulation through SCAPS-1D software, we have studied the effect of these two modifications on the photovoltaic parameters of the device. To validate our theoretical model, initial benchmarking of an experimental solar cell (glass/Mo/CuSbS₂/CdS/Al) has been performed by incorporating a suitable defect model to match the simulation results with experimentally obtained values. The maximum efficiency is estimated to be 6.35% including all possible recombination pathways such as Schokley-Read-Hall and radiative recombination. Further progress in PCE involving the optimization of physical properties of bulk CAS is under progress.

Keywords: CuSbS₂, band offset, buffer layer, back contact, SCAPS.

Acknowledgment: Edgar Puente Lopez (CVU: 928399) is thankful to CONACYT for extending his doctoral scholarship in Materials Science. Financial support received through the project VIEP-BUAP-2021 (grant no. 100468355-VIEP2021) is acknowledged. The authors are grateful to Prof. Marc Burgelman and his research group at the University of Gent for providing the facility of SCAPS-1D for our use.



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**[RWE-273] An algorithm to generate the donor / acceptor
interpenetrating network of organic solar cell morphology**

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Organic solar cells represent an alternative to conventional devices in the use of solar energy due to their attractive promising characteristics: flexibility, semi-transparency, low cost, and diversity of organic semiconductors. However, the complexity, the physical mechanisms that occur within the active layer are not yet fully understood. In this work, we present an algorithm that generates two-dimensional disorder morphologies using a simple and fast method to grow donor / acceptor phases. Domain size, mixing ratio, and resolution are the morphological parameters that can be controlled by the algorithm. This tool will allow in future works the analysis of the distribution of the electric field within the active layer, some results of the numerical device simulation considering the two phases of donor and acceptor materials in the active layer are presented.



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**[RWE-282] Silicates as basic catalysts in the heterogeneous
transesterification reaction to produce biodiesel**

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Energy demand and the finite nature of fossil fuel reserves have motivated the search for more sustainable energy sources. A promising approach to mitigating energy and environmental problems is the use of clean biofuels. In this sense, biodiesel can provide a significant contribution since it is a sustainable, renewable, non-toxic, biodegradable and offers a reduction in CO₂ emissions. Biodiesel is a mixture of fatty acid alkyl esters derived from renewable feedstock such as vegetable oils or animal fats.

In this work, the influence of the catalytic properties of sodium and lithium silicate as heterogeneous catalysts are evaluated in the transesterification reaction to produce biodiesel. The synthesis of the catalysts was carried out by solid state. Silicates were characterized structurally and microstructurally. The transesterification reactions were carried out with varied catalyst content between 1 and 5 wt. Also, the catalytic stability of the silicates was determined. The maximum yield obtained from biodiesel was ~ 99 % and the reuse capacity was greater than 5 successive reactions with a yield of ~ 95 %, using Na₂SiO₃ without a previous treatment.

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Una labor completa en investigación científica se cumple cuando se complementa con actividades de divulgación de la ciencia. La divulgación de la ciencia tiene como finalidad proporcionar un panorama general a toda la sociedad sobre los diferentes desarrollos científicos y tecnológicos que se realizan en el país. Para los investigadores, es una herramienta útil para promover sus investigaciones y alentar, principalmente a los jóvenes, a interesarse por el quehacer científico. Es por ello que, a partir del 2005, la SMCTSM se propuso fomentar las actividades de divulgación de la ciencia a través del simposio de Divulgación de la Ciencia que tiene lugar dentro del marco del congreso anual de esta sociedad.



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[SCD-108] Electrónica Flexible Reciclable: Una Alternativa

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Recientemente, el cambio climático se ha convertido en un tema que causa preocupación no solo a la comunidad científica, sino a la gente en general. Por esta razón, los sistemas y dispositivos electrónicos que puedan ser fabricados en sustratos reciclables están siendo muy atractivos para solventar este problema. Aplicaciones como pantallas enrollables, sensores, parches médicos y circuitería electrónica flexible sobre sustratos de papel de oficina se encuentran actualmente en desarrollo. En este trabajo, se presenta el desarrollo de dispositivos semiconductores y circuitos electrónicos usando sustratos flexibles de papel bond. Para que el papel sea funcional se utiliza una película de ftalocianina de cobre, de esta forma se pueden fabricar pistas de aluminio que soporten un stress mecánico de hasta 1,000 ciclos [1]. Esta tecnología puede ser una alternativa a las tarjetas de circuito impreso y abrir un campo en el desarrollo de dispositivos electrónicos sobre sustratos reciclables.

Referencias

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**[SCD-182] Depósito en Baño Químico, una técnica de síntesis de
materiales semiconductores para Tecnologías más sostenibles.**

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La base de la fabricación de los aparatos electrónicos que hoy en día definen nuestro estilo de vida como los teléfonos celulares, ordenadores, reproductores de audio y video, televisores entre otros, son los materiales semiconductores. Estos materiales son la materia prima en el ensamble de estructuras de elementos electrónicos fundamentales para las telecomunicaciones y el aprovechamiento y transformación de la energía, tales como transistores, diodos, resistores, detectores y filtros de radiación. Las tecnologías de semiconductores monocristalinos, como las de silicio (Si), aleaciones de germanio y silicio (SiGe) y arseniuro de galio (GaAs) son las más utilizadas por su eficiencia en la industria electrónica y fotovoltaica, pero también son las más costosas y sofisticadas. Las llamadas tecnologías de capa fina representan una innovación en esta materia, constituyendo una alternativa más versátil que las tecnologías convencionales de erosión catódica, depósito en fase de vapor (CVD) y el crecimiento epitaxial molecular (MBE), estas son algunos ejemplos de tecnologías de fabricación para materiales de película delgada de alta pureza pero que requieren condiciones de control altamente sofisticadas. El depósito en baño químico (CBD) es una técnica de crecimiento de películas delgadas de semiconductores, que ha tenido gran interés por sus bajos requerimientos de infraestructura y energía, así como por el control relativamente simple de los parámetros de la síntesis y la versatilidad de las propiedades que se pueden conseguir en los materiales obtenidos. De una forma simple y económica por CBD se pueden obtener materiales con enormes potenciales de aplicación en diversos tipos de dispositivos electrónicos y optoelectrónicos.



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[SCD-183] Polímeros eco-amigables

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La demanda de plásticos derivados del petróleo ha ido aumentando a través de los años y por consiguiente las preocupaciones ambientales. Los esfuerzos están dirigidos a encontrar una solución para sustituir los materiales sintéticos con una creciente variedad de materiales naturales. En los últimos años, ha aumentado la conciencia sobre disminuir la explotación de los recursos fósiles limitados y el deseo de una mayor prevención del daño hacia el medio ambiente e impulso de una tecnología sustentable. Por lo tanto, las investigaciones científicas han dirigido su interés hacia un tipo especial de materiales: los polímeros eco-amigables. Estos se presentan como un complemento y, en parte, como una alternativa a los polímeros comunes, un paso lógico y necesario hacia una industria de plásticos moderna y orientada al futuro. La fabricación de un producto utilizando un 100% de recursos renovables es un área con un gran futuro y la tendencia por utilizar una mayor proporción de los recursos renovables disponibles es cada vez más trascendente. Los polímeros eco-amigables son de materias primas renovables naturales y presentan un amplio espectro de aplicación tales como bolsas para composta agrícola, láminas, hortícolas, productos infantiles, juguetes, fibras, textiles, etc. Actualmente, se obtienen este tipo de materiales de diferentes hidratos de carbono como son: azúcar, almidón, proteína, celulosa, lignina, biograsas o aceites.



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**[SCD-221] Piezoelectricidad como la base las comunicaciones
inalámbricas modernas**

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La cotidianidad de muchos dispositivos electrónicos como los “smart-phones” y las “lap-tops” han mantenido a la gran mayoría de los usuarios alejados del entendimiento de su funcionamiento por décadas. En México, prevalece la urgencia de aumentar nuestra capacidad de desarrollar tecnología de vanguardia, pero ¿cómo podemos conseguir este objetivo?, ¿qué hacemos los mexicanos en la actualidad para contribuir a alcanzar esta meta? En esta charla, además de intentar plantear un panorama para resolver estas preguntas, se mostrarán los esfuerzos del grupo de investigación “Diseño y Optimización de Recubrimientos Avanzados (DORA-Lab)” por establecer una línea de investigación enfocada en el desarrollo de películas delgadas piezoeléctricas de nitruro de aluminio mediante depósito por capas atómicas. Abordando este caso desde el punto de vista fundamental, es decir, controlando el ordenamiento de los átomos de nitrógeno y de aluminio durante la síntesis de las películas piezoeléctricas, para que tengan una interacción adecuada con el espectro de radio frecuencias, estas investigaciones buscan una potencial aplicación en la industria de las comunicaciones inalámbricas que son fundamentales en el funcionamiento de estos dispositivos móviles.



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**[SCD-222] Inteligencia Artificial y su uso en la Caracterización de
Materiales**

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En años recientes, nuestras sociedades han observado la llegada de términos como algoritmos inteligentes, big data, machine learning e inteligencia artificial. Este tipo de metodologías han surgido como herramientas de gran utilidad que conjuntan por lo menos tres áreas: el conocimiento específico del problema a resolver, el manejo adecuado de la teoría de los métodos, y la capacidad de implementar computacionalmente los procesos de cálculo requeridos. Para el caso de ciencias de los materiales, hay grandes oportunidades del uso de este tipo de métodos en la caracterización de algunas propiedades físicas de los mismos. Por ejemplo, pueden utilizarse para predecir propiedades de una nueva aleación en la que realizar pruebas experimentales sea muy costoso o bien para pronosticar las propiedades de un material que aún no existe sin la necesidad de haberlo fabricado. En esta charla se dará una explicación accesible sobre cómo están diseñados los métodos de inteligencia artificial y se darán algunos ejemplos de uso de estas ideas.



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**[SCD-223] Nano-Tecnología y Nano-Electrónica: Física, Química, fisiología,
átomos y electrones que se manipulan en el laboratorio**

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Las ciencias físicas y químicas que dan soporte a las nano-ciencias, son en conjunto la plataforma fundamental para el desarrollo de las nano-tecnologías. Entendiendo estos temas como un conjunto de avances tecnológicos sustentados en el estudio y ensamble de los elementos químicos, de los materiales a nivel molecular y de la materia viva a nivel de componentes de las células.

A partir de esta concepción general de las nano-tecnologías, es posible visualizarlas cuando se entiende que con ellas se logra el desarrollo de los modernos sistemas electrónicos, cuyas aplicaciones de manera cotidiana las ubicamos en el hogar, en nuestras actividades diarias de comunicación con nuestro entorno. Pero también se intuye lo complejo que pueden ser estos avances cuando se aplican en el control de procesos industriales, en las modernas telecomunicaciones a base de satélites y también en lo que ahora se llama internet de las cosas. En otro contexto resulta interesante conocer otros aspectos, más allá de las complejas teorías que sustentan estos desarrollos, en concreto se hace referencia a los instrumentos científicos y los principios en que basan su funcionamiento. Es decir, escudriñar en los laboratorios de investigación y los de innovación, donde se manipulan de manera precisa los nano-objetos (átomos y moléculas en principio), para lograr obtener los modernos materiales que dan forma a los chips, a las celdas solares o a los complejos sensores que se utilizan para analizar y tratar problemas de salud.

En esta charla se abordarán los conceptos y las herramientas tecnológicas para el desarrollo de las nano-tecnologías, un enfoque desde las Nano- y Micro-tecnologías que se desarrollan en nuestro país (Tecnología PolyMEMS INAOE).

Al final se abordará el desarrollo de las modernas pantallas ultra-delgadas tipo “papel electrónico”, para visualizar imágenes en ambiente de luz solar directa.

Esta charla será la primera parte de una segunda conferencia enfocada en los desarrollos de nuestra tecnología nacional aplicada en Ingeniería Biomédica (CD-MEMS INAOE).



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**[SCD-224] Sobre la importancia de las Micro-Tecnologías y la fabricación
de circuitos con aplicaciones en el sector Salud**

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De manera gradual pero consistente, en algunas entidades del país se han ido estableciendo laboratorios (cuartos limpios) con el objetivo de desarrollar tecnologías para la innovación en diversos prototipos de sensores. En este contexto es relevante mencionar la existencia de una creciente infraestructura nacional para el desarrollo de Micro-tecnologías, para la experimentación en la fabricación de circuitos integrados, sensores y actuadores.

Es también pertinente el preguntar la importancia de este tipo de tecnologías para el desarrollo del país. Por lo anterior es relevante revisar los fundamentos de las micro-tecnologías y abordar los aspectos relativos a las disciplinas involucradas cuando se trata de conocer de manera concreta sobre el papel de los especialistas involucrados en este tipo de actividades.

En el contexto de desarrollo de micro-tecnologías para el sector salud, se presenta una infraestructura nacional para la innovación en Microelectrónica y Sistemas MicroElectroMecánicos (MEMS, BioMEMS), conocida como CD-MEMS INAOE, establecida en Puebla. Utilizando polímeros y metales bio-compatibles, se presenta el desarrollo de circuitos integrados de silicio y algunos dispositivos sensores y actuadores. Un proyecto particular es el uso de una novedosa técnica conocida como "Micromaquinado Superficial", para la fabricación de sensores con características de flexibilidad mecánica (Electrónica flexible), para adaptarse a diversos ambientes biológicos. En colaboración con médicos y fisiólogos, algunos experimentos tienen el propósito de consolidar las posibilidades de implante en tejido vivo o en contacto directo con algunas membranas como la córnea.

Esta infraestructura con capacidades de fabricación de Biosensores y BioMEMS, se presenta como una alternativa viable con características de innovación para aplicaciones en el sector Salud.



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[SCD-226] Cosecha de lluvia, ¿estrategia viable?

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El agua cubre aproximadamente el 70% de la superficie del planeta. Sin embargo, el 97% de ella es salada y solo el 2.5% es agua dulce, de la cual poco más del 5% puede aprovecharse para el consumo humano. Además, el uso de este líquido se ha incrementado 1% anual a partir de los años 80's debido al crecimiento poblacional y al incremento de productos que se han desarrollado para mejorar la calidad de vida. Cabe señalar que estos productos generan contaminantes emergentes, en los cuerpos de agua, que pueden generar problemas ambientales y de salud pública. En este sentido, el programa de cosecha de lluvia puede considerarse como una alternativa inmediata. Por lo tanto, esta charla versará sobre los trabajos desarrollados en la UPIITA del IPN en relación con la captación y tratamiento de agua. Se agradece al proyecto SECTEI 289/2019.

[SCD-230] La sustancia más extraordinaria

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Ante esta pregunta, se espera una sustancia poco común. Pero seguramente muchos se sorprenderán de saber que esta plática se refiere al agua, lo cual no lleva a que sabemos poco de este líquido con increíbles propiedades, las cuales permiten desde la existencia de nuestra vida hasta la del planeta tal cual lo conocemos. En esta plática se comentarán preguntas poco comunes como cuantos tipos de agua hay y como una sustancia tan sencilla y común tiene propiedades tan increíbles. Se comentarán algunas propiedades termodinámicas del agua que explican, por ejemplo, por qué los hielos flotan y el impacto que esto tiene en el planeta. Presentaremos las diferencias entre el agua de mar, de los ríos y de lluvia, y qué características tiene el agua potable. Y por supuesto, comentaremos la importancia del cuidado del agua y de contar con un agua de calidad para tener una buena calidad de vida.

Agradecimientos:

Se agradece el apoyo del Instituto Politécnico Nacional a través del proyecto SIP 20210716 y a SECTEI con el proyecto CM 059/2021.



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**[SCD-237] La ciencia de materiales como coadyuvante en la problemática
del calentamiento global**

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Actualmente se presenta una discusión en la comunidad científica mexicana debido a planteamientos relacionados con una posible orientación en la asignación de los recursos financieros para la investigación científica que aporta el gobierno.

La ciencia de materiales es una aplicación especializada de la física básica y aporta herramientas para entender principios fundamentales de la naturaleza así como para aportar soluciones que podrían contribuir a la mejora en la calidad de vida de la humanidad y en particular de la población mexicana.

En la platica comentaremos brevemente acerca de la importancia, para estudiantes interesados en la ciencia, de contar con recursos humanos de alto nivel para aportar soluciones a la problemática ambiental.

Se presentara una discusión general del estado de aplicación de la ciencia de materiales en la mitigación de problemas que contribuyen al calentamiento global.

Se describirá trabajo realizado en mis laboratorios relacionados con la síntesis de materiales semiconductores en forma de película delgada y su aplicación potencial en el desarrollo de materiales fotovoltaicos y fotocatalisis. También se discutirá sistemas pasivos para aprovechar la energía térmica solar empleando compositos electrohilados.

*: trabajo apoyado parcialmente por CONACyT



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**[SCD-242] Las celdas solares: El efecto fotovoltaico para generar Energía
Eléctrica**

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Los paneles solares son dispositivos que captan la radiación solar y la convierten en algún modo de energía. En esta charla se abordará en su concepción más simple el llamado efecto fotovoltaico, el cual se desarrolla cuando la radiación solar incide sobre una placa o sustrato de silicio semiconductor. El efecto fotovoltaico se aprovecha de manera óptima cuando el silicio se acondiciona con una serie de materiales y circuitos electrónicos, que al final posibilitan que la energía eléctrica generada sea utilizada de manera convencional. Los materiales necesarios para fabricar celdas fotovoltaicas, las etapas de colección y reconversión de la energía eléctrica generada, serán discutidas para su comprensión general.

En particular, se aborda un proyecto de investigación sobre celdas fotovoltaicas Grätzel, también conocidas como celdas solares sensibilizadas con colorante (DSSC), pertenecen a la tercera generación de celdas fotovoltaicas. Estudios recientes se enfocan en el aumento de su eficiencia por diversos métodos y diseños ya que es una de las tecnologías más prometedoras por su bajo costo de producción, Estas tecnologías usan metales como colorantes sensibilizadores del efecto fotovoltaico, lo que aumenta el costo de las celdas y contaminan el medioambiente. Por lo anterior, en nuestro proyecto se propone emplear colorantes orgánicos provenientes de frutas, plantas, hojas, etc., en lugar de colorantes sintéticos, como una alternativa ecológica, de menor costo y mayor eficiencia de conversión.

A partir de las ventajas planteadas y considerando los laboratorios de investigación involucrados, se pondrá en discusión por qué en México no se producen sistemas fotovoltaicos comerciales para generación de energía eléctrica.



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**[SCD-243] Los Dispositivos electrónicos en el desarrollo de los sistemas
automotrices**

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Las tendencias en el desarrollo del automóvil se centran en temas tales como materiales ligeros, miniaturización de los componentes electrónicos, inteligencia computacional, movilidad, energía y sustentabilidad. Tales tendencias han dado lugar a que los sistemas electrónicos tomen una gran importancia.

La evolución de la electrónica de consumo ha cubierto los requisitos más exigentes para las comunicaciones y las funciones de seguridad en los vehículos. Actualmente, el 30 por ciento del costo de producción de un vehículo está relacionado con los dispositivos semiconductores. Más aún, 90 por ciento de las innovaciones en los automóviles modernos son o están relacionadas con algún tipo de sistema electrónico y comunicaciones.

En esta conferencia se presenta un panorama de los sistemas electrónicos, los dispositivos semiconductores y las redes de comunicación, que se utilizan entre las diferentes unidades de control electrónico en los automóviles.



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**[SCD-244] Aplicaciones industriales de las nanoTecnologías en México en
el horizonte 2021.**

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La nanotecnología contiene un grupo de disciplinas y técnicas, encaminadas a la síntesis y caracterización de materiales a escala nanométrica, es decir, a escala de átomos, moléculas y estructuras moleculares. A dicha escala, los límites entre la química, la física y la biología se traslapan y modifican. Por lo tanto, las innovaciones basadas en la nanotecnología explican una cantidad de problemas y necesidades en la sociedad, que representan un reto para las actividades industriales y económicas, hasta el punto de que se considera como una pieza clave para la siguiente revolución industrial. Considerando un estudio del CONACYT se puede señalar, que en el mundo se gastó en el 2015 alrededor de 34.3 MMD, tomando en cuenta un conjunto de proyectos en los que se utilizó la nanotecnología, mientras que para el 2021, se proyecta un gasto en éste sentido del 90.5 MMD. El presente estudio, se pretende mostrar algunos campos importantes de aplicación de la nanotecnología, los cuales se han abordado en el grupo de trabajo del proponente, para identificar algunas necesidades actuales en México, y así, proporcionar información de utilidad para alentar a las nuevas generaciones, de involucrarse en el emprendimiento que sirva para elaborar estrategias, que promuevan el desarrollo y aplicación de la nanotecnología en nuestro país. Para su realización, se han consultado al menos siete líneas de investigación entre nuestros actuales colaboradores, todos ellos expertos investigadores laborando en centros de investigación, con la industria y en la universidad.



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[SCD-276] Biosensores basados en micro-trampolines

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En la actualidad, los biosensores han emergido como una herramienta útil en la detección biológica que puede ser aplicada a importantes sectores como: detección oportuna y control de enfermedades, contaminación ambiental, industria de alimentos y plataformas *lab-on a chip* para un sensado inteligente y autónomo de diversos parámetros de interés.

Un biosensor se puede definir como un dispositivo compuesto por dos elementos: un receptor biológico (elemento de reconocimiento) preparado para detectar específicamente una molécula, virus o sustancia; y un transductor capaz de interpretar la reacción de reconocimiento biológico y traducirla en una señal cuantificable. Para cubrir las necesidades de todas estas aplicaciones, los biosensores deben poseer dos características importantes: selectividad y sensibilidad. La selectividad es una particularidad que recae principalmente en el receptor biológico, y establece su capacidad de reconocer de manera precisa una especie química y diferenciarlo de aquellos que lo rodean, es decir su afinidad biológica. Mientras que la sensibilidad es una propiedad que debe alcanzarse a través del mecanismo de transducción del sensor. En este aspecto, los biosensores mecánicos basados en micro-trampolines, que son estructuras suspendidas y micromaquinadas a base de silicio y otras alternativas de materiales poliméricos, permiten adaptarse a esquemas de transducción en modo dinámico y estático, e incluso a instrumentaciones ópticas para la cuantificación de las señales de reconocimiento, lo que permite establecer una plataforma de detección atractiva.

Actualmente, en el Centro de Ingeniería y Desarrollo Industrial en colaboración con el Instituto Nacional de Astrofísica, Óptica y Electrónica, la Universidad Politécnica de Valencia y el Centro de Investigaciones en Óptica, se está desarrollando una plataforma de detección simultánea de diversos pesticidas basada en biosensores mecánicos con instrumentaciones eléctricas y ópticas. Los resultados experimentales derivados de la instrumentación óptica han demostrado una resolución para detectar deflexiones mecánicas de 1nm, lo cual incrementa la sensibilidad del biosensor y conduce a detección de niveles de concentración por debajo de 20ug/uL.



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SEMICONDUCTORS

Chairmen:

Dr. Salvador Gallardo Hernández (CINVESTAV-DF), sgallardo@fis.cinvestav.mx

Dr. Joaquín Alvarado Pulido (BUAP),

Research on semiconductors has been an extremely important research field for most of the past century and will continue to have a central role worldwide during the twenty first century. Current technology would not exist if silicon-based electronics had not been developed. This impressive progress has been extended to other semiconductors such as gallium arsenide, group-three nitrides and related materials. The pace at which technology advances is a direct consequence of the research efforts in growth, characterization, control of properties, development of novel devices, performance improvement, new materials such as alloys and solid solutions, theoretical approaches to predict and understand semiconductor properties, and so on. The Mexican Society for Science and Technology of Surfaces and Materials (SMCTSM) has had, since its beginnings, an important tradition among its members in pursuing research in the important field of semiconductors. This Symposium has been an important forum, for many years, for the generation, discussion and exchange of ideas where stimulating and fruitful collaborations have arisen among the participants. The themes covered in the symposium include:

- Growth: chemical and physical methods
- Single crystals
- Thin films: epitaxial and polycrystalline
- Surfaces
- Structural characterization
- Electronic properties: optical, thermal and electrical
- Lattice dynamics and phonon properties
- Homo and heterojunctions
- Devices
- Novel semiconductors: compounds, alloys and solid solutions
- Nanoscaled semiconductors
- Carbon: nanotubes, graphene, and fullerenes



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- Theoretical models and calculations of semiconductor properties
- Novel characterization techniques
- Other (it is such a wide and beautiful area!)

We look forward to your participation in the Symposium of Semiconductors, whose success and high impact is guaranteed by the contribution of the SMCTSM members.



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**[SEM-52] PHOTOCATALYTIC STUDY OF Z / ZnO AND Z / CeO₂ COMPOUNDS
(Z = NATURAL AND SYNTHETIC ZEOLITE)**

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The photocatalytic activity of composite materials of Z / ZnO and Z / CeO₂ was evaluated from aqueous solutions of organic dyes at initial concentrations of 10 mg / L. The ZnO and CeO₂ compounds supported by natural (clinoptilolite) and synthetic (NaA type) zeolite were obtained by the physical milling method, while the oxides were previously synthesized by the sol-gel method. The structural, morphological and topological characteristics of the photocatalysts were studied using characterization techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), N₂ physisorption and UV-Vis spectrophotometry. The structural analysis of the samples confirmed the obtaining of nanoscale compounds, with a crystallite size range between 20-30 nm. While the morphological analysis shows a more homogeneous distribution and with respect to the surface area, this increases with respect to the pure oxides. The performance of nanocomposites for the removal of synthetic dyes under UV radiation increases by around 50% compared to zeolites without oxides. In conclusion, photocatalytic degradation using zeolite-supported oxide nanocomposites could result in an efficient treatment process in reducing pollutants present in wastewater.



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**[SEM-60] Synthesis and characterization of ZnO / CNT compounds doped
with silver and chromium (Ag and Cr) with photocatalytic applications.**

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In the present work, ZnO photocatalysts, ZnO / NTC at 0.5% and 1% of CNT, ZnO /CNT / Ag at 1% Ag and 0.5% and 1% of CNT and a ZnO / CNT / Cr photocatalyst were synthesized. 1% CNT and 1% Cr, by means of the microwave-assisted synthesis method at a power of 400 W and at temperatures between 207-214 ° C. The materials obtained were characterized in their structural, optical and morphological properties by X-ray diffraction (XRD), scanning and transmission electron microscopy (SEM and TEM) and by UV-Vis spectroscopy. The results show that the crystalline phase of the ZnO obtained was wurtzite, the cubic phase of the Ag and a peak associated with the structure of the CNTs were identified. For ZnO / CNT and ZnO / CNT / Ag, a trend of increase in the crystallite size is observed, calculated from the Debye-Scherrer equation with respect to the crystallite size of pure ZnO. The bandgap (E_g) decreases for ZnO / CNT and ZnO / CNT / Ag with respect to pure ZnO. The evaluation of the photocatalytic activity using synthetic dyes shows a greater effect on materials with CNT and metals, with degradation of 98%.



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**[SEM-105] Solution processed NiO (p type) /FTO (n type) thin film
rectifying junction as a highly responsive Ultraviolet Photodetector**

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Recently, the solution-processed fabrication of semiconductor devices has been highly researched because of its economical, easy, and large area synthesis. This report demonstrates the simple solution process for the synthesis of p-type Nickel Oxide (NiO) semiconductor on n-type FTO by sol-gel route for the fabrication of rectifying diode. The delocalizing of the hole charge carriers by adjusting the pH value and thermal annealing leads to crystalline P-type NiO semiconductors. The crystallinity and the chemical composition of the synthesized NiO were confirmed by XRD and XPS characterization respectively. Uniformity of the spin-coated NiO thin film confirmed by a FESEM characterization. The device's current-voltage features (I-V) have been examined under different light and dark intensities. The photocurrent generated by Ti /n-FTO/ p-NiO interfaces has been shown to vary on the intensity of light. The responsivity of the fabricated device under UV light illumination was calculated to be 9 mA/W. Upon UV light illumination, photogenerated excitons are generated in NiO and due to the built-in electrical field at the heterojunction, there is an effective separation of photogenerated carriers leading to the efficacious collection of carriers at the metal. The successful demonstration of the NiO/FTO rectifying junction is a major step ahead in the low-cost, uniform solution-processed fabrication which finds potential applications in transistors, sensors, and optoelectronics, etc.



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**[SEM-164] Structural properties of compositionally hyperbolic-tangent
graded In_{1-x}Ga_xAs layers**

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The generation of dislocations due to the lattice mismatch between InAs, InGaAs and GaAs heterostructures is a problem for the development of new devices that require well crystalline quality. Particular importance on these material compounds arises for instance from the growing interest in THz technology, where a wide variety of devices like THz sensors, emitters, transistors and photomixers have been developed and yet, great research efforts are still under process to reach improved characteristics. For the growth of these mismatched systems the use of linear gradual layers has proven to confine the dislocations below a critical thickness z_c [1]. Furthermore, graded layer engineering has shown that the use and optimization of non-linear graded layers are able to further absorb and extend the defect-free zone above z_c . In this work, we study the structural properties of hyperbolic tangent In concentration profiles composition in InGaAs/GaAs structures. All along the molecular beam epitaxy process the growth temperature was adjusted according to the In content of the alloy. The samples were characterized by high resolution x-ray diffraction (HRXRD) and Raman spectroscopy (RS). The HRXRD rocking curves show clear InAs and GaAs diffraction peaks corresponding to the initial and final portion of the gradients, and between these peaks a wide plateau distinctive of gradual concentration layers is observed. The rearrangement of the structure after annealing is revealed as a more defined plateau. The Tersoff model [2] has been applied in order to calculate the thickness z_c for the hyperbolic tan profiles, indicating that z_c is larger (shorter) than the value for linear graded samples in samples starting (ending) with In (Ga) -rich films. The material reorganization provoked by the samples annealing is also accounted by RS, where the LO phonon resonances redshift approximately 3.6 cm^{-1} for both gradients. This shift involves a strain relieve of $2.83 \times 10^{11} \text{ dyn} \cdot \text{cm}^{-2}$. On the other hand, the TO/LO GaAs intensity ratio is increased for the sample that goes from InAs to GaAs, while the mirror sample (from GaAs to InAs) a severe change in the RS lineshape was perceived, presumable related with the deterioration of sample due to In segregation. Finally, preliminary THz emission experiments shows an increment in the THz emission from the sample that goes from InAs to GaAs.

[1] H. Choi, Y. Jeong, J. Cho, M.H. Jeon, J. Cryst. Growth. 311 (2009) 1091–1095.

[2] J. Tersoff, Appl. Phys. Lett. 62 (1993) 693–695.



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**[SEM-219] InGaAsSb quaternary alloys grown on GaSb(100) substrates: A
study of the physical and chemical properties**

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Antimonide family-based compounds have demonstrated, throughout different studies, to be important alloys for the development of new generation infrared semiconductor devices. They share some common properties, among some, all of them display a zinc blende structure under certain conditions; however, one of the properties which make it possible for these materials to be applied into infrared semiconductor devices is a direct band gap energy that may cover a large part of the solar spectrum, moving through the near-infrared (1.7 μm) up to the mid-infrared (3.5 μm) at room temperature. All these properties allow us to engineer different devices as photodetectors, light emitting diodes and laser diodes. An important compound that belongs to this family InGaAsSb quaternary alloy. This material permits the tailoring of its band gap as a function of the content of the precursor elements that were employed at the growth time. For this work, an analysis of a series of $\text{In}_{0.145}\text{Ga}_{0.855}\text{As}_y\text{Sb}_{1-y}$ films was performed using energy-dispersive spectroscopy (EDS), High-Resolution X-ray Diffraction (HR-XRD), Transmission Electron Microscopy (TEM), and photoluminescence spectroscopy (PL) to determine their chemical, structural, and optical properties. The films were grown by Liquid Phase Epitaxy (LPE) on GaSb substrates, with a variation of the As(y) content. Using TEM, we obtained the thickness of grown films. Likewise, applying fast Fourier transform (FFT) to an image of an amplified area of the transversal cut of the film, we were able to observe the reciprocal lattice of the formed crystal. The indexing of the points revealed the type of structure of the grown samples (zinc blende) and, the interplanar spacing was observable (1.53 Å). This result corroborates the obtained by HR-XRD. We determined with EDS the atomic content of each element (In, Ga, and Sb) in the quaternary alloys, and the As content (y) for the different alloy, according to Vegard's Law was obtained. The emissions of the $\text{In}_{0.145}\text{Ga}_{0.855}\text{As}_y\text{Sb}_{1-y}$ alloys were also measured by PL. The alloys presented two optical transitions, the first one attributed to bound-exciton states, and the second one to donor-acceptor pairs. With all the collected information, a computational simulation was developed using MATLAB computational package. The simulation provides the lattice constant for different element content, the bond length, and the cohesive energy for the quaternary.



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**[SEM-239] Effects of nitrogen incorporation on CdTe nanoparticles
embedded within a silicon dioxide matrix ****

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CdTe has become a very important material to produce photovoltaic devices and recently it has been observed that nitrogen incorporation produce improvements in its performance.

In this work we report the synthesis of self-assembled systems produced via a sequential deposition process of SiO₂/CdTe/SiO₂ layers using the RF reactive sputtering technique and its optical, electrical and structural characterization. The results are contrasted with samples produced incorporating nitrogen in the deposition atmosphere

The samples were prepared on silicon (111) p-type substrates and commercial glass. The spatial distribution and CdTe particle size were controlled by the reactive atmosphere composition employed in the production of the first SiO₂ layer.

The images of transmission electron microscopy shown distributed nanoparticles with sizes between 10 and 15 nm. The results of X-ray diffraction confirm the presence of CdTe nanoparticles. The results of the transmittance, photoluminescence and Raman spectroscopies are discussed in terms of nanoparticles size. Transport properties are discussed in terms of the presence of CdTe-SiO_{1-x}N_x core-shell structures

*: on sabbatical leave from Departamento de Ciencias Basicas, UAM-Azcapotzalco

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**[SEM-6] Processing and characterization of indium sulfide thin films
processed by RF-sputtering.**

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In₂S₃ thin films were deposited by RF-Sputtering onto glass substrate at room temperature. These thin films were analyzed by RXD, SEM, UV-Vis spectroscopy and electrical resistance. The thin films showed a cubic phase as principal phase. The average grain size is around 32 nm. The optical band gap was estimated using the optical transmittance measurements obtained values of 2.3-2.6 eV. The electrical resistance is the order of $\times 10^3$ Ohm.

**[SEM-25] Alternative synthesis of CdSe films using chemical bath
deposition and ionic exchange.**

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In this work, an alternative method is proposed to synthesize CdSe films using chemical bath deposition and ion exchange techniques. A CdCO₃ film was performed and used as precursor film, then it was immersed in a Se ion solution; the CdCO₃ film change from white to dark brown color immediately. The synthesized film was characterized by DRX, UV-Vis, SEM & EDS. The results showed that CdCO₃ film was effectively converted to CdSe; DRX displayed a preferential plane (200) and hexagonal crystalline structure, the bandgap resulted in 1.66 eV, the morphology change considerably from CdCO₃ to CdSe and EDS showed a good stoichiometry relationship between cadmium and selenium.



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**[SEM-31] Photodetectors with Schottky diode structure based on CdS
doped by the different elements.**

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We studied Schottky diodes with structure TCO/CdS(M)/C where TCO is a transparent conducting oxide (ITO in this case), M - atoms of different metals, and C - graphite electrode. Thin films of pure CdS and CdS doped with Al, Sn, and Eu were obtained by Chemical Bath Deposition (CBD) and characterized using XRD, SEM, EDS, XPS, UV-Vis spectroscopy, I-V curve, and photoresponse estimation. The dark characteristics of the diodes show high rectification (up to six orders of magnitude); at illumination, the best diodes present a photoresponse of $1 \times 10^{-1} \text{ AW}^{-1}$ that is comparable to the parameters of industrial photodiodes. CdS films in all cases were polycrystalline with crystallite size ranging from 10 to 30 nm, the smallest in Eu-doped samples. Their optical characteristics show the blue-shift in Sn- and Al-doped samples (this is due to quantum confinement effect like that described earlier [1, 2]) and red-shift in case of Eu doping; these effects influence the photosensitivity spectra. It must be also mentioned that samples with Eu exhibit the smallest stress and dislocation density that also affects optical properties. The data of refractive index and extinction coefficient indicate the presence of porosity that is typical for CBD-made material and essential for quantum confinement observation. Another cause of the quantum confinement effects is the presence of near-interface quantum wells in CdS films which are the consequence of the non-stoichiometry of the corresponding parts of a film. The illumination dependence of the photoresponse is linear, the inertial is in the millisecond range, so the devices developed are quite acceptable for light-sensing applications.

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**[SEM-33] THEORETICAL STUDY OF THE INTERACTIONS BETWEEN ORGANIC ADDITIVES
AND HYBRID PEROVSKITES FOR THE STABILIZATION OF SOLAR CELLS**

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Hybrid halide perovskites are considered as emerging semiconductor materials, since in the last decade there has been a great advance in high performance photovoltaic energy due to the fact that in the last 10 years the efficiency of perovskite-based solar cells (PSC) has steadily increased from 3.8% to a certified efficiency of more than 25%.

Despite the growing interest in hybrid perovskite solar cells, their commercialization is hampered by serious stability problems, which limit the useful life of the devices. Many attempts have been made to obtain high quality perovskite films that mitigate these challenges. An effective approach to modifying the surface of halide perovskite is through the use of additives with several specific functional groups that can interact with perovskite to passivate the material and thus improve the photovoltaic performance of PSCs.

Here we use density functional theory (DFT) calculations to explore the interaction of organic additives (theophylline, theobromine, and caffeine) with the pseudocubic (001) -PbI₂ surface of MAPbI₃.



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[SEM-57] GaSb passivation by sulphide compound.

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Gallium Antimonide (GaSb) based alloys are promising semiconductors to develop infrared (IR) devices, such as light-emitting diodes (LEDs), thermo-voltaic cells, and IR detectors. A very serious issue of these alloys is their high reactivity. Atmospheric oxygen reacts with GaSb surface; In consequence, a series of oxides forming reactions occur. Those surface states negatively impact the performance of the devices. Fortunately, surface passivation techniques are developed to remove the oxides and improve the surface and performance of devices. This work presents the surface passivation of the binary GaSb alloy with Na₂S·9H₂O (sodium sulfide). We studied the influence of immersion time and substance temperature on the surface recombination velocity (SRV) and photoluminescence (PL), then we obtained an interesting behavior and inverse relation of the SRV and radiative recombinations.



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**[SEM-89] Effect of the Zn-doped on the structural and optical properties
of $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$ alloys.**

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The antimonide-based compound semiconductors are a potential family belong to III-V group alloys. Among their main features are the lattice parameter of ~ 6.1 Å, the zinc-blende structure, and that they can be synthesized in complex heterostructures for creating devices able to work in the infrared spectrum. One of the most promising is $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$ because its band gap energy can be tuned in a wide range from near infrared to mid infrared. This alloy is doped to achieve p-n junctions; normally, Zinc (Zn) and Tellurium (Te) are used to p- and n-doped, respectively. Using Raman Spectroscopy, we analyzed vibrational modes of six different Zn-doped $\text{In}_{0.13}\text{Ga}_{0.87}\text{As}_{0.13}\text{Sb}_{0.87}$ films. These samples were grown on GaSb (100) substrates by liquid phase epitaxy (LPE) varying the Zn content. The obtained spectra were deconvoluted using 3 Lorentzian curves centered 217, 227, and 246 cm^{-1} , which are attributed to the InAs TO mode, the contribution of both (InAs-GaSb)-like TO mode and LO-phonon-plasmon coupling, and the (InAs-GaSb)-like LO mode, respectively. Normalized intensity and full width at half maximum (FWHM) were analyzed in function of Zn content. It was found that the peak intensity [YC1] of the (InAs-GaSb)-like LO mode decrease quickly with the decrease of the Zn content. On the other hand, the FWHM of the (InAs-GaSb)-like LO mode decrease [YC2] s until approx. 2.4×10^{-4} of Zn molar fraction (medium doping) from which starts to increase. The Zn content enhances crystalline quality from low to medium doping and decreases it from medium to high doping.



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**[SEM-114] Meta-stable orthorhombic-phase together with stable cubic-
phases in GaAs deposited by CSVT**

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Today, GaAs is one of the most useful materials present in the integrated circuits of many devices. The effects associated with its impurities or defects can expose changes in its properties that can be beneficial for the development of new technologies or the improvement of existing ones.

CSVT (close space vapor transport) is a low cost-effective technique to deposit successfully epitaxial GaAs, regardless of the simple operation at atmospheric pressures and moderate temperatures this technique is barely explored. With the use of this technique, GaAs is deposited on different substrates (high and low resistivity silicon, fused quartz) finding in the same sample a growth direction (120) belonging to the orthorhombic metastable phase in conjunction with other stable growth directions. cubic, this only for one type of substrate. Numerous experiments associate the phase transition to deposits at high pressures (16GPa) of this material (J. Nayak 2004), finding the response of this phase transition in deposits to atmospheric pressures due to tensions in the lattice.

In this study we analyze the difference in the crystalline structure that exists due to each substrate. In addition to an analysis of structural stresses and the possible lattice pressure, which can be related to the morphological analyzes included in this.

The importance of the structural study relating it to other studies in this work, is due to the scope that this material may have due to the existence of this atypical phase. And it is that, once this phase transition is reached, the annealing process cannot change the crystalline structure of these GaAs deposits, then this GaAs with (120) is a good candidate for devices with high temperature operations.



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**[SEM-119] Glass formation area of the CdO-CuCl₂-V₂O₅ ternary system:
optical properties as a function of CuCl₂ content**

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Within the compositions triangle of the ternary system CdO-CuCl₂-V₂O₅ a batch of 25 glasses were fabricated. In the corner of high CdO content the glass formation area (GFA), was found. For each group, the glass former (V₂O₅) content was constant and, the modifier oxides CdO, CuCl₂ were varied. All the fabricated glasses were analyzed by X-ray diffraction patterns, UV-Vis and Raman spectroscopies. In the border of the GFA all the samples presented the crystalline structure of the compound Cd₂V₂O₇, meanwhile inside of the GFA, the samples contain amorphous Cd₂V₂O₇. Into the GFA the samples were organized in 5 groups. For each group, taking as reference the CuCl₂ content, the optical properties were analyzed. Under this point of view, the maximum of their Raman band associated with their amorphous structure, is being confined between 850 and 820 cm⁻¹, depending on the CuCl₂ content. By optical absorption the E_g values were determined in the 2.42 — 1.66 eV range, depending on the CuCl₂ content. By the same spectroscopy the Urbach energy (E_u) for all the glasses was obtained and resulting to be in the 0.65 - 0.22 eV range. The refractive index for this group of samples, was obtained in the 2.57 - 2.90 range, also depending on the CuCl₂ content. Finally, SEM images show a homogeneous distribution goticular into the amorphous matrix, for samples located in the border of the GFA.



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**[SEM-122] Optical characterization of GaN / Si (111) in hexagonal phase
by photoreflectance and photoluminescence**

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The development and control of semiconductor structures have given rise to the development of technology that has marked our daily lives. Since these technological advances allow us to develop devices, semiconductors are the essential constituents of practically any technological device with which we have contact. This work reports the study of GaN / Si bulk material doped with silicon, using photoluminescence, reflectance and photoreflectance techniques, in this work we focus on characterizing GaN-based materials grown by epitaxy of molecular beams on silicon substrate, where some of these films were doped in order to improve their crystalline quality in these samples, the effect of doping on their optoelectronic properties was observed and to see if it is possible to unify these silicon technologies with GaN, the latter feels very distant more. However, it is something that we are experiencing that the era of silicon is about to end and the use of new semiconductor materials is already a necessity for the technology sector.

**[SEM-124] Optical characterization of InGaN films in cubic phase by
photoluminescence**

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The investigations of semiconductor structures are the basis for the technological development of nano-structured materials and systems, such as light-emitting diodes, lasers and solar cells, they are an essential basis for most of the technological devices that we usually use on a daily basis. This work reports a study of $In_xGa_{1-x}N$ films in cubic phase grown by the epitaxy of molecular beams on a GaAs substrate, varying the temperatures of the substrate and that of Indium, characterizing using photoreflectance, photoluminescence and x-ray diffraction techniques. Obtaining their optoelectronic properties, such as the band gap and in turn an approximation of their different concentrations of indium, this allows us to report which are the optimal growth conditions that allow us the emission in the green, since it seeks to be able to increase the emission efficiency in said region for later works.



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**[SEM-168] Evaluation of lattice mismatch in (Al,Ga)As/Ga(N,As)
heterostructure for intermediate band photovoltaic**

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The addition of an energy level between the conduction band (CB) and the valance band (VB) of semiconductor originates the concept of intermediate band (IB) which allows the absorption of photons with a lower energy than the VB to CB transition in solar cell devices [1]. In the obtention of IB, the GaNAs material has been studied and applied to take advantage of the behavior that its electronic structure of bands acquires with the percentage of nitrogen used in the alloy, %N, being the division of the conduction band into two energy levels called E⁻ and E⁺ which can be used in the concept of IB, the most promising property. Nevertheless, the lattice mismatch between GaAs and GaNAs drawbacks the employment of this III-N-V material in IB solar cells, rising as the %N is incremented. In the present work, both a GaNAs/GaAs epilayer and a (Al,Ga)(As,N) photovoltaic heterostructure grown by molecular beam epitaxy (MBE) are studied with the aim to explore a method to determine the effect of lattice mismatch on the optical characteristic of the device. The diffraction of [004] plane obtained by rocking curve method indicated two peaks intensities who dominates the diffractogram at 33.03° and 33.13° which correspond to GaAs and GaNAs with %N=1.2, respectively. This value of nitrogen implies a lattice mismatch lower than 0.5%. Raman spectroscopy was employed to analyses the composition of the photovoltaic structure where modes related to GaAs, AlGaAs and GaNAs were observed as indicative of the success of the grown process. The LO-phonon mode frequency was employed to estimate the strain of the heterostructure when their frequency is contrasted with those of an unstressed sample, obtaining tensile values of 0.003. The optoelectronic response of a device is defined by their band structure which is also affected by the strain. Particularly, tensile strain induces a reduction of the bandgap in III-N-V materials. Photorefectance spectroscopy was used to determine the effect of tensile strain in the heterostructure where third-derivative lineshapes were found related to E⁻ and GaAs gap. The strain redshifts these critical points around 65 meV.



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Finally, we employed numerical simulations to determine the strain distribution along the mismatched semiconductor system by evaluating the minimization of the total elastic energy via a conjugate gradient method to determinate the equilibrium positions of the atoms, thereby obtaining the local strain tensor where variations from 0 to 0.004 were found. Our numerical results agree with the experimental values. With this study the authors show a strategy to evaluate the effect of residual strain in III-N-V photovoltaic structure.

[1] <https://doi.org/10.1063/1.4709405>

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**[SEM-173] Sn non-amphoteric impurification of GaAs(631) layers grown
by MBE**

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The molecular beam epitaxial (MBE) growth and doping of III-V semiconductor compounds on high-index surfaces opens a vast number of possibilities to investigate new physical properties and to develop potential applications. The natural surface anisotropy of these surfaces under appropriated growth conditions conduce to a natural arrangement of unidimensional nanostructures. Recently, by taking advantage of the formation of 1D GaAs (631) self-assembled surface corrugation on top of multi-quantum well heterostructure interfaces, the modulation of the confined state eigenstates has been achieved, attaining quasi-one-dimensional or fractional dimension eigenstates. On the other hand, further applications in electrical and optoelectronic devices demand of the realization doped layers preserving the 1D order. Although Si is widely used as an n-type dopant for GaAs (100), the growth of Si doped GaAs on (631)A surfaces, results in amphoteric behavior, p-type and n-type conduction depending on the growth parameters. The aim of this work is the investigation of the Sn doping effects on the electronic conduction and optical properties of GaAs layers grown by MBE on (631)A substrates. Under the growth conditions studied we always observe n-type doping, and interestingly the doping level was always very similar to (100) oriented layers grown with comparison purposes. The maximum carrier concentration was 2×10^{19} , which is an order of magnitude higher than previously reported for Si, and it is within the same order of magnitude as compared with the growth of on GaAs(100). The electron mobility was 4×10^3 cm²/Vs (1×10^3 cm²/Vs) for carrier concentration of 1×10^{17} cm⁻³ (1×10^{19} cm⁻³), which is good for many optoelectronic applications. The crystal properties were studied by Raman spectroscopy (RS). For the (100) sample with the highest level of doping, the TO mode completely dominates the spectrum, indicating low crystalline quality. On the other hand, the selection rules for the (631) indicate that the TO mode is allowed, estimating its intensity greater than that of LO, and by increasing doping, we observe that the



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spectra do not change as dramatically as for the direction (100). This indicates that the incorporation of Sn in GaAs for high index crystallographic orientations follows a completely different process, which was also supported by strain and atomic force microscopy measurements on the films.



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**[SEM-187] Optical properties of high-quality single-layers obtained by
liquid-phase exfoliation of transition metal dichalcogenides**

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A two-dimensional (2D) material has the minimal thickness possible: either 1 atom for single-atom materials (such as graphene), or as many atoms as its stoichiometrical composition (3 for MoS₂, for example). An example of the latter are transition metal dichalcogenides (TMDCs), are of great relevance due to their wide range of electronic, optical, and thermal properties. In addition, it should be noted that they are indirect bandgap semiconductor materials when in bulk. However, when they get thinned down to single-layers, there is a transition from indirect to direct bandgap so, optical properties arise. In recent years, the synthesis of 2D materials has focused on the production of single layers on a large scale. Liquid-phase exfoliation (LPE) method is a promising technique that is highly scalable, versatile, and low cost to produce a wide variety of 2D materials compared to other growth techniques. LPE refers to a collection of methods that directly exfoliate materials in single-layers dispersed in a liquid medium. This work focuses on the study of the optical properties such as photoluminescence, absorption and Raman spectroscopies of material in the form of single-layers obtained by a custom-designed liquid exfoliation procedure. We demonstrate that the optical properties of single-layers exfoliated this way are comparable to those obtained by other methods of either exfoliation or direct growth. We also show very high crystalline quality and by means of Transmission Electron Microscopy. These results open the way to liquid-phase exfoliation as a useful alternative method to fabricate optoelectronic devices based on 2D semiconductors.



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**[SEM-207] Facile wet-chemical synthesis of $\text{BiOCl}_{1-x}\text{Br}_x$ solid solutions:
properties and photocatalytic activity**

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Semiconductor photocatalysis is one of the most active areas of research in materials science. Specifically, bismuth oxyhalides BiOX ($X=\text{Cl}, \text{Br}, \text{I}$) semiconductors have great physical and chemical properties in addition to their non-toxicity, stability and photocatalytic activity. However, few report about gap modulation between BiOCl (3.22 eV gap) and BiOBr (2.64 eV gap) have been reported. Furthermore, their preparation usually requires high temperature synthesis methods.

In this work, we have synthesized solid solutions of $\text{BiOCl}_{1-x}\text{Br}_x$ (with nominal values for x of 0, 0.25, 0.5, 0.75 and 1) through facile wet-chemical method at room temperature. Their structural properties were studied by X-ray diffraction and Raman spectroscopy. Morphology properties were studied by electron microscopy and their tunable band gaps were studied by UV-Vis spectroscopy. Nominal concentration is discussed with the results. Finally, we studied the photocatalytic activity degrading methyl orange dye (MO) under visible and UV source excitation.

Acknowledgements

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**[SEM-258] Manufacture and characterization of TiO₂-based composites
doped with Co, Fe or Ni for their use as semiconductors**

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In recent years, semiconductor materials had taken a vital role in solving a number of problems, particularly related to energy generation. Semiconductor oxide such as TiO₂, are widely used in the construction of solar cells of third generation due to its physical and chemical properties. But it suffers from poor photovoltaic efficiency caused by insufficient dye absorption and low energy value in the conduction band. This paper presents the manufacture and characterization of TiO₂-based composites doped with different metals (Co, Fe and Ni) looking for the improvement of the photovoltaic efficiency of the material. The results of the characterization in the resulting materials, show that after high energy mechanical mixing of the precursor powders, the average particle size is less than 1 micron, having a good size distributions of the powders. The final phase present in the composite was determined by XRD analysis. The microstructure of the resulting material is fine and homogeneous. The electrical properties evaluated indicate an improvement on the electrical characteristics of the resulting material, this situation makes promising their application as a semiconductor in the construction of third generation solar cells.



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SURFACES, INTERFACES AND TRIBOLOGY

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Dr. Giovanni Ramirez (Oxford Instruments), Giovanni.ramirez@outlook.com

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Tribology studies the friction and wear behavior of surfaces that are in contact and in relative motion. Materials, Lubricants and Coatings are commonly used to increase the durability and life of components in mechanical systems, as well to reduce the energy consumption through reducing friction.

This Symposium aims to cover the most relevant aspects of tribology by presenting papers focused on:

- Wear and friction studies of surfaces and bulk materials.
- Mechanical properties of coatings and thin films.
- Interaction between lubricants and coatings.
- Modeling of tribological phenomena.
- Industrial applications of coatings and thin films.
- Nanomaterials and nanoformulations for lubrication.
- Novel techniques to study wear and friction.
- Studies of tribochemical reactions (tribofilms).
- Diamond Like Coatings for Lubrication.
- Novel techniques to evaluate friction and wear.



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**[SIT-90] TRIBOLOGICAL PROPERTIES OF NANOLUBRICANTS CONTAINING
HALLOYSITE CLAY NANOTUBES AND CARBON NANOPARTICLES**

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In conditions of intensive production and increasing competition, to ensure the stability of the quality of the manufactured products in all technological operations, it is important to use the lubricant that protects the equipment, guarantees product quality and does not pollute the environment. When adding additives to lubricants, many factors contribute to the improvement of tribological performance, such as: percentage of nanoadditives added, geometry of nanostructures, type of nanoparticles and roughness of the surface in contact. These factors together with the tribological mechanisms generated by nanoparticles (loading effect, valley filling, surface separators and rolling/sliding effect, among others, have shown advances in lubrication performance. This work describes the effects of two inorganic nanoparticles as additives, that is, CNp (carbon nanoparticles) and HcNT (halloysite clay nanotubes), in three different lubricants: oil-based, grease, and water-based. The nano-lubricants were prepared by adding 1 wt.% particles to each type of lubricant. The tribological properties of nano-lubricants were determined and compared under anti-wear (AW) and extreme pressure (EP) conditions. CNp showed a decrease in the coefficient of friction (COF) by 22% when added to the lubricant. In addition, CNp demonstrated an improvement in grip pressure limitation (poz) of 74%, 52% and 1621% for oil-based lubricants, greases and lubricantes rich water-based, respectively. Comparing 1% by weight of added water-based CNp with oil and fat based, the improvements become outstanding in EP conditions.



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[SIT-116] Multilayer Method modification for the quantitative chemical composition analysis on the partial oxidation of nickel

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Peak-fitting of the Ni 2p core-level from metallic nickel and its oxides is challenging due to the high asymmetry of the main peak, the complex multiplet structure, and the intense Shirley-type background. This work presents X-ray photoelectron spectra acquired from a clean metallic Ni film (sublimated on Si [001]). These are analyzed with two approaches that account for the apparent asymmetry of the main photoemission line: one being the use of the double Lorentzian asymmetric line shape; the other, a set of symmetric peaks. Both approaches lead to excellent fits with undistinguishable peak envelopes and backgrounds; however, they lead to different sets of previously unreported low-intensity satellites. The application of the *Block Approach* to the analysis of the partially oxidized Ni spectra allowed for the robust identification of five doublets corresponding to the oxide. It is remarkable that the sum of these oxide peaks closely reproduces the Ni³⁺ spectra, which is consistent with the assessed composition (Ni₂O_{3.1±0.3}). The strong overlap and shape similarity of the Ni⁰ L₃M_{4,5}M_{4,5} Auger structure with that of the Ni³⁺ strongly suggests that the Auger Parameter does not provide conclusive insight into the initial nor final state factors affecting the measured XPS binding energies. The latter in contrast to the claims made elsewhere. The angular dependence of the peak intensities is not consistent with a simple layer oxidation mechanism but with the formation of oxide regions protruding deeper into the film.



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**[SIT-126] SYNTHESIS AND CHARACTERIZATION OF TiO₂ DECORATED WITH
Au NANO-PARTICLES OBTAINED BY LASER ABLATION**

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TiO₂ (titanium dioxide) has been extensively studied by now, since its semiconductor and photocatalytic properties are of great interest. We also know that it is a low-cost and nontoxic component. In this study we focus on the properties of TiO₂ before and after being decorated with Au (gold) nanoparticles as well as how they were measured. The co-precipitation method was opted for its simplicity and low cost for synthesizing TiO₂, and we noticed that this method is simpler than other methods such as sol-gel.

For the synthesis we utilized different solutions such as ethyl alcohol, isopropyl alcohol and deionized water. A TiO₂ powder previously synthesized by hydrothermal treatment was used as control sample. Once the synthesis of our TiO₂ powder was concluded we proceeded to examine it by Raman Spectroscopy and X-Ray Diffraction to observe their structural properties as a first approximation. Then, Au nanoparticles obtained by laser ablation were used to decorate the TiO₂ powder to increase the reaction rate constant, Raman and X-Ray measurements were performed again. We proceeded by comparing with UV-Vis the rate of photodegradation of methylene blue in aqueous solution in the presence of the different powders obtained from different precursors and with or without Au decoration.



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**[SIT-127] "Formation of Hard Layers in Ni-Mo Steel for the Railway
Industry"**

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This study evaluated the kinetics of growth and fracture toughness of layered iron borides Fe₂B, FeB on the surface of AISI 9840. The diffusion coefficient of boron in borided phases was determined by the fundamental solution of Fick's second law and the mass balance equation at the interfaces of growth, whereas the layers boride is due parabolic growth law. Similarly, two models were used under the Palmqvist type crack system for determining the value of the fracture toughness of iron boride. The formation of the phases Fe₂B and FeB held by boride with pulp dried at temperatures of 900, 950 and 1000 ° C with treatment times of 2, 4, 6 and 8 hours for each temperature using boron paste dried over substrate surface. Due to the potential of boron employee and absence of alloying elements such as V, W, biphasic substrate and layers obtained sawn borides FeB and Fe₂B.

The mechanical characterization of the layers boride was conducted in two stages: the first was to determine the influence of experimental parameters (time and temperature of treatment) in the harshness of phase Fe₂B and FeB, the Vickers micro hardness test was performed with loads between 1.9 and 2.9 N micro indentation varying distances on the surface of the layer thickness depending on boride phase and the diagonal size produced. Furthermore, in the second stage, was evaluated in experimental form fracture toughness, using the theory of fracture mechanics indentation for Palmqvist type crack system, boride selecting samples to a time constant of 8 h for each treatment temperatures, varying loads and application to 1.9 and 2.9 N and the indentation distances.

Finally, the results of the fracture toughness in the boride layer obtained by theory constraints of the two models used were analyzed together, in function of different distances and indentation loads, and correlating the value graphically fracture toughness with cracking to obtain the best fit of the models used.



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**[SIT-129] Advanced methods for structure and chemical quantification
using XPS data applied to the study of the oxidation mechanism of some
metals**

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The interest for new and high-performance materials has increased the need for understanding how the bulk, their surfaces and interfaces work. Surfaces are one of the most interesting topics to investigate because they are the point of interaction with the environment and other materials. Understanding the way the materials behave chemically and physically on its surface could lead to the development of desired high-performance materials.

Surface analysis techniques are employed to characterize the chemical composition of surfaces; X-ray photoelectron spectroscopy (XPS) is the most used technique to explore surface chemistry. This technique samples the very top surface (~10 nm) and is used to obtain quantified elemental composition (except H and He).

In this work we show how to characterize surfaces of pure metals and their oxides using advanced tools for fitting XPS data to get surface composition. Fitting process is done with AAnalyzer® employing methods like the *Block Approach*, *Simultaneous Fitting*, and *Active Background*. Structure and chemical modeling are done with the XPSGeometry® software, which employs the *Multilayer Method*.

Although it is believed that all metals oxidize forming a protective oxide layer, this work shows that different oxide structures can form on the surface of pure metals. In some cases, the oxide forms a surface layer, in other cases it generates protrusions, while in others the oxides coexist with the metal at different positions.



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**[SIT-140] BURR THICKNESS OF HOLES MANUFACTURED WITH A
COMMERCIAL TWIST DRILL SUBJECTED TO THERMOCHEMICAL BORIDING
TREATMENT**

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The main objective of this work is to study the influence of the surface hardening of a commercial twist drill on the thickness of the burr on the entrance surface of non-through holes manufactured in a 7075-T6 aluminum alloy. A comparative experimental study was carried out between a commercial twist drill bit subjected to a thermochemical boriding treatment and an untreated drill bit. The parameters of the thermochemical boriding treatment were as follows: a conventional furnace without controlled atmosphere was used, exposure time of 5 hours, at a temperature of 900 °C, the technique used was powder-pack and reused powder. The generated boride layers were analyzed by X-ray diffraction analysis. Twist drills made of AISI M2 steel, 7/32 in diameter, 130° tip angle, 35° helix angle, straight shank, without internal cooling were used. The drilling operations were performed on 7075-T6 aluminum plates in a three-axis Vertical Machining Center (VMC) with computer numerical control (CNC). The machining regime applied was as follows: cutting speed 72.3 m/min, feed rate 0.089 mm/rev, depth of cut 12.5 mm; the flooding method was used to apply the cutting fluid at the drill/workpiece interface. The criterion for stopping hole making was the change in chip shape from fan to ribbon. After 1050 holes manufactured with each of the twist drills, the untreated drill bit began to generate ribbon-like chips.

A Mitutoyo optical microscope was used to measure the thickness of the burr on the entrance surface of the manufactured holes. A Mitutoyo optical microscope was used to measure the thickness of the burr on the entrance surface of the manufactured holes. Burr measurement was performed every 80 holes. Four burr measurements spaced 90° apart were made in each hole. The arithmetic mean of these four measurements gives the burr thickness in a hole. The results show that the application of the thermochemical boriding treatment to a commercial twist drill made of AISI M2 steel has no influence on the thickness of the burr formed on the entrance surface of the manufactured holes.



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**[SIT-146] 2D materials (Graphene and MoS₂) decorated TiO₂ for
photocatalytic applications.**

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This work presents an easy and environmentally friendly method for the synthesis of composite materials based on TiO₂, which is decorated with 2D materials, seeking to achieve its activation under visible light irradiation. A previous exploration work allowed choosing weight relationships between TiO₂ and 2D materials. The synthesized materials were characterized by different techniques including UV-vis spectroscopy, X-ray diffraction, Scattering Electron Microscopy, Raman spectroscopy. In addition, photodegradation tests were carried out to evaluate the photocatalytic activity of the samples on methylene blue solutions under UV radiation and visible light, the percentage of degradation of each sample was compared with the respective percentage of a control sample made of pure TiO₂. Degradation was measured by measuring the absorbance of methylene blue after irradiation periods of 30 minutes over a period of 4 hours. Results are discussed in terms of weight ratios for Graphene and molar for MoS₂.



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[SIT-204] ARXPS study on the early stages of manganese oxidation

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X-ray photoelectron spectroscopy (XPS) is an efficient technique for characterizing the physiochemistry of materials' surfaces. One of the least studied elements is manganese most likely due to the complexity of the Mn core-level spectra. The Mn 2p spectrum, which is the core-level of choice for XPS analysis, shows asymmetry, complex multipeak structure, plasmon peaks, and a very large composed background.

In this work, we show an accurate fitting for the Mn 2p photoemission spectra for the clean metallic case and its early stages of oxidation. This was done by exposing a clean metallic Mn sample to ultraclean oxygen.

The fitting of the peaks was carried out using the AAnalyzer® software, whereas the species quantification and stoichiometry were calculated using the multilayer method. The analysis is based on the *Block Approach* which is an advanced spectra subtraction method that allows robust identification of the emerging oxide peaks.

We identified two different sets of peaks associated with two oxidation states: Mn²⁺ and Mn³⁺. The identification was done by correlating with O 1s peaks, which allowed for the calculation of the composition of the oxides. Finally, the change in the chemical composition of the films as a function of exposure to oxygen was characterized.

To the best of our knowledge, this is the first time such a comprehensive XPS analysis of the Mn in the metallic or oxide state is reported.



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[SIT-8] ANALYSIS OF ABRASIVE WEAR AS A FUNCTION OF ALLOY PURITY

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In this research, the analysis of the coating of steel by welding with high resistance stellite® alloy is presented, this in order to protect the surface of mechanical components. In the metal-mechanical industry, most coatings are performed as part of a corrective operational maintenance and are generally applied in those areas where exposure to severe use is continuous. Severe use conditions are; friction, abrasion, impact, corrosion, high temperature, etc. These types of alloys are classified within the group of high hardness alloys or superalloys. The deposit of this alloy was made by means of electric metal arc welding with a coated electrode (SMAW) and was applied on ASTM A-36 Steel. The applied coating was characterized by electron microscopy, abrasion, impact and hardness tests. It was observed that as the alloy coating is purified, the mechanical properties improve, particularly the resistance to abrasion increases, as well as the surface hardness.



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**[SIT-11] Study on the surface modification at atomic level of gold thin
film on nanoporous alumina toward AuNPs formation for biomarkers
detection by SERS**

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In this work, the synthesis of surface-enhanced Raman scattering (SERS) substrates, constituted by gold nanoparticles (AuNps) on nanoporous aluminum anodized oxide (AAO), was achieved by promoting the surface modification of Au thin film on AAO by an accessible thermal treatment. The AAO was synthesized by anodizing an aluminum foil by using 20 V (vs reference electrode) in a potentiostat and a 3 M oxalic acid solution. Afterward, an Au film was sputtered on the AAO surface, and the samples were thermally treated in a nitrogen atmosphere for 15 min at 450 °C. The thickness of the Au layer on the thin film was explored from 15 nm to 180 nm to understand the effect in the AuNPs formation after the thermal treatment. The size of nanoparticles was determined theoretically by Mie theory based on absorbance recorded from Uv-Vis spectroscopy and experimentally by scanning electron microscopy (SEM). The surface modification during the thermal treatment was analyzed by transmission electron microscopy (TEM) and x-ray photoelectron spectroscopy (XPS). The nitrogen adsorption at low-pressure assay revealed that, after the thermal treatment, Au thin film is reorganized as AuNPs layer with disordered-like porous (isotherm curve type IV-H₃) in all the AuNPs layer. Afterward, the enhancement factor of SERS substrates was computed by measuring rhodamine 6G dilutions, particularly a range from 1×10^{-6} to 1×10^{-12} . The possible use of SERS substrate for biomarkers detection is discussed.



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**[SIT-24] Capacitive sensor made from recycled material to evaluate
engine oil condition.**

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In this work, a capacitive sensor made from recycled material is proposed to evaluate engine oil condition. The capacitive sensor was fabricated from a recycled aluminum heat sink and was used to measure the permittivity of engine oils. The proposed method was correlated with FTIR spectroscopy analysis to evaluate the chemical degradation of the oil, as described in ASTM E-2412 standard practice. The results showed a linear trend in permittivity measurements and degradation parameters as mileage increases. Therefore, a correlation between permittivity and degradation parameters allowed establishing a permittivity value of 2.73 as an indicator suggesting the end of the useful life of the engine oils analyzed.

**[SIT-30] Surface treatment of A36 steel with silica from canary seed husk
for corrosion control**

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Environmental pollution and the corrosion phenomenon are serious problems that affect the health and safety of living beings. In this context, agro-industrial waste is a source of environmental pollution. In the present work, canary seed husk (agro-industrial waste) was used as raw material to obtain silica and apply it in the corrosion control for the A36 carbon steel. The study of this type of silica makes it possible to determine whether it is feasible to replace the toxic and expensive inhibitors (for example, hexavalent chromium) that are used in different industries to control corrosion. Silica was obtained by a thermochemical process and its anticorrosive properties were studied using AC and DC electrochemical techniques: Electrochemical Impedance Spectroscopy, Linear Polarization Resistance, and Potentiodynamic Curves. The silica showed good protection for carbon steel in 0.5M sulfuric acid (H₂SO₄).



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**[SIT-40] Contrast surface morphologies on amorphous soda-lime silica
glass implanted with 1.0 MeV Si + and 1.5 MeV Cu + ions.**

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Commercial amorphous soda-lime silica glass substrates were implanted with 1.0 MeV Si⁺ and 1.5 MeV Cu⁺ ions using the Tandem Pelletron accelerator located at the Instituto de Física. The experiments were performed at 70° incident angle with respect to the surface normal, ion currents range from 200- nA to 1- μA with a total ion fluence ranging from 10¹⁶ cm.⁻² to 5 x 10¹⁷cm.⁻² and all in room temperature conditions. The selected energies correspond to similar ion penetration, calculated at approximately 422 - nm and a width of 182-nm for these experiments. The modified substrates were analyzed using surface techniques including scanning electron microscopy (SEM) and atomic force microscopy (AFM). The morphology and topography analysis revealed surface shapes with notably different forms for the two types of ions. Two characteristic lengths have been observed, (1) at low fluences consistent with a linear Bradley-Harper type growth, and (2) at high fluences associated with a non-linear ion- induced residual- stress growth. Two different types of instabilities; (1) Bradley-Harper type instability and (2) Muñoz-Cuerno-Castro type instability resulting from the continued ion bombardment, both showing anisotropy associated with the incoming beam direction. These substrates have been studied for application in optoelectronics as the recent published literature suggest

Acknowledgements: The authors would like to thank the technical assistance of F. Jaimes, M. Escobar, D. Roman and J.G. Morales at the Instituto de Física, Universidad Nacional Autónoma de México (UNAM). Financial support provided by DGAPA-PAPIIT Project IN-114120. In addition, M.A. García recognizes previous support from CONACYT postdoctoral fellowship.



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**[SIT-96] Effect of the Boron Powder on Surface AISI W2 Steel;
Experiments and Modelling**

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Effect of the Boron Powder on Surface AISI W2 Steel; Experiments and Modelling

Abstract; The effect of boron powder on surface AISI W2 steel and growth kinetic of the boride layer are studied. Boron powder mixture was used in the powder pack boriding, this process was carried out in the temperature range of 1173–1273 K with exposure times ranging from 2 to 8 h. The presence of boride was confirmed by optical microscopy, X-ray diffraction, and the distribution of alloy elements in boride layers with energy-dispersive spectrometry using scanning electron microscopy. A mathematical model of the growth kinetics of the single layer was proposed and boron diffusion coefficient was determined by mass balance equation. The morphology of Fe₂B layer was smooth and boron activation energy in W2 steel was estimated as 187.696 kJmol⁻¹. The kinetic model was validated with two experimental condition, so a contour diagram describing the evolution of Fe₂B layer as a function of time and temperature parameters for industrial application.

Keywords: Fe₂B layer, mathematical model, boron powder; kinetic; X-ray diffraction,



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**[SIT-97] Evaluation of mechanical properties of 3D printing with internal
surface honeycomb panels**

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Biodegradable and low-density polymers are in demand in the manufacturing industry, whose applications are used in the biomedical area for the manufacture of rehabilitation equipment, splints for humans and pets, as well as in physiotherapy devices. In the present work the mechanical properties of the material PLA (biodegradable lactic acid), ABS (acrylonitrile butadiene styrene) and carbon fiber filament are studied. Through tensile test under ASTM D63802a, Compression under ASTM D695 and flexion under ASTM-D790-10, the samples were made by 3D printing with a Prusa I3 Metal printer at a constant extrusion temperature of 230° C, 245° C and 230° C , respectively and speed 40mm / s of material deposition. Under conditions of density 40 %and 80 % with internal hexagonal morphology and 100 % without morphology. The tests were carried out on a Shimadzu Autograph AG-X-100K universal machine with a speed of 5 mm / min. This research also shows the changes in densities with the purpose of developing manufacturing methods using these experimental parameters and optimizing geometries in specific applications.



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**[SIT-98] Reciprocating wear on an AISI 4140 erased machinery grade
multilayer Steel**

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In this work, the wear analysis of a boron powder coating on AISI 4140 steel was carried out through a reciprocating wear test for possible applications in machinery manufacturing. The experimental tests were carried out using a tribometer with the ability to measure wear and friction force, through a reciprocating test of ball-on-plane configuration. The tests were carried out with polished and unpolished samples, with a coating in different temperature conditions at 900 °, 950 ° and 1000°, all temperatures lasting 1 h. The tests were carried out with a duration of 3600 sec at room temperature (28-32 ° C and 25-30% relative humidity) with a displacement amplitude of 10 mm with loads at 10N, 15N and 20N. Furthermore, in the reciprocating tests, the roughness was determined and it was characterized with a scanning electron microscopy (SEM) and light microscopy. The results show the differences in the polished and unpolished surface, where the most important but not so significant variation occurs in the variation of the COF and the wear footprint through the profilometry.



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**[SIT-99] Contact analysis of textured bushings in knee prosthesis
application.**

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The objective of the present investigation is the contact analysis of articulated bushings in a knee prosthesis made of ultra high molecular weight polyethylene (UHMWPE) of type GUR 1020. Surface topography plays an important role in a multitude of physical and tribological phenomena such as contact mechanics, friction, adhesion and lubrication. A texturing proposal was made at 20% density to improve the tribological characteristics, where some authors conclude that a considerable factor in the wear of artificial joints is the surface roughness of the polyethylene insert. Results of stress concentration, contact pressures and fatigue analysis were obtained. The latter to determine the life time of textured bushing in comparison with a commercial bushing without texturing. The result was an increase of 6 years of useful life in the textured bushings.



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**[SIT-110] Photodetection effects of MIS-Like structures with silicon rich
oxide films**

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MIS-type structures made up with silicon-rich oxide (SRO) films deposited by the HFCVD technique show interesting I-V and I-T characteristics under different illumination conditions and give rise to a photogeneration effect. From the electrical measurements, an increase of the illumination current of up to 3 orders of magnitude respect to the dark current was found at a polarization of - 4 V, with the latter at approximately 82 nA, while the photogenerated current reaches values of 25 μ A. The increased photogenerated current is corroborated by I-T measurements. In addition, the MIS structures characterized with Current-Wavelength (I- λ) measurements, presented maximum responsivity values at 254 mA/W, a peak of detectivity at 2.21×10^{11} Jones and an equivalent noise power of 49 pW at a wavelength of 535 nm. The Au/SRO/Si structures exhibit good switching behavior with rise and fall times between 120 and 150 ms, respectively. These rise and decay times account for the generation and recombination of charge carriers as well as the process of capture and release of traps, respectively. We stress that the photodetection effect only occurs in MIS-type structures with SRO films without annealing. These results make the MIS-type structures to be used as photodetectors in the 420 to 590 nm range.



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**[SIT-155] Experimental design of surface treatment of magnesium pieces
through the “Sand-blast” technique**

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Reduction of weight is of great interest in the automotive industry because it reduces fuel consumption, helping with gas regulations and increasing the efficiency of automobiles. Among the materials used for structural support, magnesium is one of the lightest, characterized by its low density and high mechanical strength/weight ratio. However, its widespread use is limited by its low hardness and corrosion resistance. In this work, the results of a composite central design of experiments, applied to study the behavior of the mechanical and chemical properties of magnesium under the action of the sand-blast technique, are reported. Hardness, roughness, and corrosion resistance were analyzed as the response variables. The Sand-blast surface treatment technique was applied on 1" x 1" magnesium sheets. Medium roughness measurements were carried out using the ISO 4287 standard. Corrosion was measured by using a saline solution under the ASTM D1141-98 standard as a corrosive medium, showing significant changes in the magnesium substrates as a function of the experimental parameters. The surface hardness measured in an HV-1000 microhardness equipment, showed an improvement up to 44%.

Key words. Sandblast, surface treatment, magnesium.

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**[SIT-195] Nanosecond laser irradiation of metallic Zn surfaces in air and
water**

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99.99% pure metallic Zn surfaces were irradiated with a Nd:YAG laser emitting at 1064 nm with 10 Hz repetition rate and pulse energy output of 750 mJ. The effect of water as confining medium during the irradiation process and the number of pulses were studied and compared with samples irradiated under the same conditions in air.

Surface morphology of the irradiated samples was observed by scanning electron microscopy. It was found that water has a major effect on the morphology. Formation of spherical nanoparticles can be observed in the surfaces irradiated in water, the density of nanoparticles increased with number of pulses. In general, typical surfaces of porous melted material can be observed for all the samples, however, when using water as confining medium, pore size are decreased and nanoparticles are formed through all the surface. This effect is more noticeable with higher number of pulses.

Raman spectroscopy was used to see if there is surface oxidation on the irradiated zones. Profilometry measurements were carried out to see changes in surface roughness of the samples.



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[SIT-197] Titanium surface oxidation by irradiation with ns laser pulses

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Titanium oxides are of great interest for their use in a wide range of different technological applications, such as paint industry, photocatalysis, semiconductor industry, etc. Oxidation of Ti surfaces can be achieved by a variety of techniques. Pulsed laser irradiation has shown to be of interest due to it can produce high quality and controllable oxides, besides it can be scaled to large area applications by applying scanning processes to irradiate surfaces.

In this work, industrial Ti sheets were immersed in bidistilled water and irradiated with ns pulses of a Nd:YAG laser using a wavelength of 1064 nm. The evolution of the oxidation process was studied by irradiating with increasing number of pulses. Surface changes of the films were observed by SEM, AFM and profilometry. Raman spectroscopy was used to analyze structural changes with increasing number of pulses. In order to see chemical changes with increasing number of pulses, X-ray photoelectron spectroscopy was used.



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**[SIT-254] WEAR RESISTANCE EVALUATION OF TiAlCrSiN NANOCOMPOSITE
COATINGS FOR HIGH SPEED MACHINING OPERATIONS**

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Hard coatings have been developed mainly for cutting tools applications where high stress and wear resistances are inherent, however, the wear phenomena associated with the effect of the silicon addition on the TiAlCrN matrix are not well understood. Therefore, the aim of this work is the production and characterisation of innovative ceramic coating where the influence of silicon addition is determined. Nanocomposite TiAlCrSiN coatings with 3 different Si contents were deposited on K20 tungsten carbide substrates using magnetron co-sputtering technique. Coating's thickness, adhesion and hardness have been measured. Wear behaviour was measured via pin-on-disc experiments and the main wear phenomena were analysed. Morphology, semi quantitative chemical composition, and microstructure were investigated by means of scanning electron microscope (SEM), energy disperse spectroscopy (EDS) and X-ray diffraction (XRD), respectively. Analysis of wear patterns shows brittle failure phenomena attributable to high internal residual stresses in the coating, this is noted by the delamination of the coating with the first loads (less than 5N) and also by the chevron tensile cracks. The data illustrates that increases of silicon content improved wear resistance, which is associated to mechanical properties.



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**[SIT-256] Evaluation of nanoindentation characteristics of cubic InN and
GaN epilayers grown by Molecular Beam Epitaxy**

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The potential of the III-nitride semiconductor materials for modern optoelectronic applications as diodes, transistors, LEDs, and photovoltaics has prompted the mechanical characterization of small volumes as thin films. In this work, the load-displacement curves of cubic indium nitride (c-InN) and cubic gallium nitride (c-GaN) obtained during the nanoindentation with a Berkovich indenter were investigated. The samples were obtained by plasma-assisted molecular beam epitaxy growth on c-GaN/MgO (100). The thickness of the c-GaN buffer layer used in all the films studied was 350 nm to eliminate the substrate's effect on the material studied properties. The reflection high energy electron diffraction and the X-ray diffraction results show that the c-GaN and c-InN grown layers had a high cubic zincblende phase with more than 97%. The mean values of the hardness and Young's modulus of cubic InN are 12.5 ± 0.4 GPa, and 365.6 ± 7 GPa, respectively, with a Poisson's ratio of 0.3. The mean values of the hardness and Young's modulus of cubic GaN are 22 ± 1 GPa, and 293 ± 12 , respectively, with a Poisson's ratio of 0.27.



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THEORY AND SIMULATIONS OF MATERIALS

Chairmen:

Dra. Ariadna Sánchez Castillo (UAEH), ariadna_sanchez@uaeh.edu.mx

Dra. María Teresa Romero de la Cruz (FCFM-UAdeC), teresa.romero.cruz@uadec.edu.mx

Dr. Francisco Sánchez (IF-UNAM), fsanchez@fisica.unam.mx

The aim of this symposium is to bring together experts in the field of surfaces and interfaces to discuss recent developments in electronic and transport properties of bulk materials, surfaces, optical properties, physical properties of clusters, and 2D materials, Density Functional Theory and Time Dependent DFT.

The topics include (but are not limited to)

- Density Functional Theory
- Time-dependent DFT
- plasmonics
- chiral materials
- physical properties of clusters
- transport properties
- mechanical properties at the nanoscale
- 2D materials

Oral and poster presentations are welcome.



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[TSM-22] Ab-initio calculations of the physical properties of Li-doped ITO

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¹ Cinvestav Merida

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Using ab-initio calculations through density functional theory (DFT), we explore the effect of Li interstitial doping on the physical properties of Sn-doped In_2O_3 (ITO). We reckoned band structure, density of states (DOS), optical properties and valence band x-ray photoelectron spectrum (XPS) --the latter was compared with measurements. Our preliminary results indicate that the presence of Li plays the role of electron doping in the system. The DOS is dominated mainly by O 2p states with minor contributions in the conduction band from In 3d states as well as Sn 3d states. Although Li s states have a negligible contribution, Li electrons greatly contribute to conduction, therefore raising the Fermi level to higher energies. With respect to the optical properties we observe that there is an increase in light absorption in the visible region for the Li-doped system compared to the pure system, this seems to be in agreement with electrochromic effects reported for ITO. The agreement between the XPS calculations and experiment is fair showing that the DOS is slightly affected by the presence of Li. These results are of importance for researchers working in solar cells, Li-based batteries and electrochromic devices where Li ions play a major role.



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**[TSM-46] DFT study for the effect of Bi adatom and vacancies in
SrTiO₃(111) for H₂O adsorption**

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Density Functional Theory (DFT) calculations were performed to investigate the effect of bismuth adatom and vacancies in H₂O adsorption on strontium titanate (SrTiO₃) surface (111). Calculations were performed using PWscf code of the quantum ESPRESSO package. Water adsorption is relevant because could promote the OH formation. OH is an active species in water pollutant degradation. Actually, pollution is an important global problem. Studying systems that could help to remove and transform dangerous substances is relevant. The first part of this work focused in the water adsorption and how is modified by Bi adatom and vacancies. Adsorption energy, structural and electronic properties of the selected systems are reported and compared. The next step is the OH formation and desorption in order to interact with the pollutant substances.



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**[TSM-61] Adsorption of CO₂, NO₂ and SO₂ on graphene/molybdenum
disulfide heterostructure doped with Ti and Cu: a DFT study**

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Pollution is a global problem that affects human health and the environment. This motivates several investigations around the world. Therefore, in this study we perform total energy calculations of CO₂, NO₂ and SO₂ adsorption on graphene/molybdenum disulfide heterostructure. Effective adsorption is helpful for removing this pollution molecules. The calculations were performed by computational modeling using the PWscf code of the Quantum ESPRESSO package. This software works within the framework of the Density Functional Theory (DFT). The electronic properties of the most stables configurations were calculated. The graphene/molybdenum disulfide heterostructure doped with Ti and Cu show an improvement in adsorption energy of CO₂, NO₂ and SO₂. The adsorption energies values are in the range of chemisorption, where the NO₂ larger adsorption energy of -2.84 eV, in the other hand for the adsorption of NO₂ on the graphene/molybdenum disulfide heterostructure doped with Ti the adsorption energy has the value of -2.78 eV. This result suggests that the graphene/molybdenum disulfide heterostructure could be used for removing CO₂, NO₂ and SO₂.



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**[TSM-159] Theoretical investigation of the AlN (0001)-(2x2) surface doped
with cobalt: structural, magnetic and electronic properties**

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We have investigated the structural, electronic and magnetic properties of the cobalt adsorption and incorporation on the AlN (0 0 0 1)-(2 × 2). Calculations were performed using the density functional theory as implemented in the PWscf code of the Quantum ESPRESSO package. The exchange–correlation energies are treated within the generalized gradient approximation (GGA). Hubbard corrections (GGA+U) have been included, provided that Co is a transition metal with highly correlated electrons. In this work the value of U=1 eV has been determined and used. The surface is treated according to the supercell approach with a 2x2 surface periodicity. Four high symmetry sites were considered, taking into account different coverage: ¼, ½, ¾ and 1 monolayer (ML). First, we have investigated the Co adsorption. Results show that in the ¼ and ½ of ML coverage the T4 site is the most favorable structure. In the ¾ ML coverage, the trimer formation is the most stable configuration. Finally, in the full ML coverage it is obtained the formation of tetramers. All coverages present a ferromagnetic (FM) behavior. In the Co incorporation with Al as adatom, the T4 is the most favorable site with FM, AFM, AFM and NM behavior corresponding to the ¼, ½, ¾ and full ML, respectively. In the substitution of Al by Co without the formation of adatoms, the ¼ ML coverage surface shows a FM behavior, and at higher coverages the system becomes AFM. Under Al-rich conditions, the surface formation energy (SFE) shows that the cobalt substitution with no adatom formation (1,2 and 4 Co Subs) are the most favorable cases. Under N-rich conditions the clean surface is the most stable structure. The minimum energy pathways of the Co adsorption show activation energies of 1.04 eV. Concerning the incorporation, the minimum energy pathways display activation energies of 0.742 eV. The DOS and PDOS indicate that the 1st ML of the surfaces is metallic and the lower layers are semiconductor. The systems show interesting electronic and magnetic properties useful for spintronic applications.



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**[TSM-169] Theoretical studies of the growth of GaAs on High-Index
Surface Silicon**

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The integration of III-V semiconductor devices in silicon (Si) has been of great interest for a long time due to its technological applications as in photonic integrated circuits and high electronic mobility transistors. From this perspective, the grow of high-quality III-V semiconductor films on Si is very imperative. A major challenge in growing high-quality films is the lattice constant mismatch. This lattice mismatch can lead to defects such as threading dislocations which in turn can degrade or prevent the III-V semiconductor devices from functioning [1]. One promising candidate to diminish these defects has been the growth of the III-V semiconductors on high index Si surfaces (Si-HI), for example, it has been reported experimentally the growth of inversion boundaries free GaAs in Si-HI [2]. Also, via theoretical calculations, it was shown that the crystallographic plane of growth is important to enhance the stability and fracture toughness of interfaces [3].

In this work, we present an ab initio study of the differences in stability of the interface of GaAs on Si-HI. The proposed models consist of GaAs/Si heterostructures with interfaces parallels to high-index planes. The optimal geometry, adhesion work, interfacial energy, interfacial distance and interface electronic structure were calculated by using density functional theory.

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**[TSM-170] Band structure and Strain distribution of InAs quantum dots
encapsulated in (Al)GaAs asymmetric matrixes**

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The study quantum dots (QDs) has been of great interest in the past two decades due to their exciting physical properties and interesting potential in the development of optoelectronic devices. It has been reported that self-assembled quantum dots (SAQDs) have been the main nanostructures to be considered for such applications. Also, to obtain effective experimental QDs' devices is necessary to grow a successful vertical stacked QDs in the active region of the devices [1]. Nevertheless, structural parameters get more challenging as each layer of QDs is added, since diffusion, segregation, alloy intermixing, or strain effects are wholly involved. In this work, finite element method numerical simulations of InAs QDs embedded in (Al)GaAs matrix are performed to analyze the strain distribution and the electronic bands in multi-stacked heterostructures. As input data, experimental parameters such as the QDs shapes, wetting layer (WL) and spacer layer (S) thickness were employed. The biaxial (ϵ_{xx}) and hydrostatic (ϵ_{hydro}) strain tensors were calculated for pyramidal and truncated pyramidal QDs shapes. The results revealed that the maximum local strain value for pyramidal shapes QDs were obtained at the apex, and it resulted three times larger than the truncated pyramids. For the former, the strain field was observed to be spread from the upper corners of the QDs towards the cap layers. Likewise, the relationship between strain energy and electronic structure was investigated. ϵ_{xx} resulted more affected with the variations in the InAs QDs geometry, which agrees with changes in the heavy hole (HH) and light hole (LH) between the simulated heterostructures. The strain distribution from our simulated samples can be compared with the work done by Liu for a single InAs/GaAs hetero system [2], which sustains that the main contribution of stress of the InAs QD and WL is due to elastic strain energy with their capping layers. This work shows a fairer way to picture the strain fields of InAs/(Al)GaAs multi-stacked heterojunctions.

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**[TSM-177] Strain effect on Cr₂N MXene: insight from First-Principles
Calculations**

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Structural, electronic and magnetic properties of two-dimensional Cr₂N MXene under strain were studied. Spin-polarized total energy calculations have been done using the periodic density functional theory plus Hubbard correction (GGA+U) with $1 < U < 5$ eV, as developed in the PAW (projector augmented wave method and a plane wave bases set) of the VASP code. The uniaxial and biaxial strain was considered from -5% to 5%. The phonon dispersion was calculated, where the nontrivial imaginary frequency was found for biaxial strain, but from -5% uniaxial strain, the system is unstable. Furthermore, the phonon density of states displays an interesting relation between strain and phonon gaps. Electronic properties of the dynamically stable systems were investigated by calculating the total density of states (DOS) and projected DOS. The DOS calculations showed a metallic and antiferromagnetic behavior of the Cr₂N MXene under strain. These properties widen the potential applications in the spintronics area provided that this can be grown on substrates with high lattice parameters mismatch conserving the magnetic properties. The authors thank DGAPA-UNAM projects IA100920 and IN110820 for partial financial support. Calculations were performed in the DGCTIC-UNAM Supercomputing Center, projects No. LANCAD-UNAM-DGTIC-368 and LANCAD-UNAM-DGTIC-150.



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**[TSM-178] Modeling the structural and electronic properties of the
alanine-black phosphorene interactions: Doping effects**

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Structural and electronic properties of the alanine adsorption on the black phosphorene layer are investigated using ab-initio total energy calculations. Studies have been performed within the periodic density functional theory (DFT) according to the PWscf code of the quantum espresso. The exchange-correlation potential energies are treated within the generalized gradient approximation (GGA) with the Perdew, Burke and Ernzerhof (PBE) functional. Electron-ion interactions are dealt with the pseudopotential approach. In addition van der Waals effect is included in the calculations provided that molecules are polar. To start studies the alanine is allowed interacting with the pristine phosphorene with results indicating that only weak interactions are present. To enhance the interactions between the molecule and the phosphorene metallic (aluminum, gallium and boron) atoms as impurities are incorporated in the phosphorene atomic structure to transform the layer into a more reactive material. In fact this is achieved and as a result the binding energies increase, in such a way that chemisorption is obtained. In this way the most reactive system corresponds to that doped with Al. The electronic properties are explored considering the total density of states and the projected density of states. No significant changes are obtained concerning the band gap energies as a consequence of the alanine adsorption.



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[TSM-192] Transition metal-decorated germanene for NO scavenging and sensing

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The chemical interactions between NO, O₂, and N₂ gas molecules and Cu-, Ag-, and Au-decorated germanene were investigated by using density functional theory simulations, and its potential applications as a gas sensor or scavenger were addressed. All studied molecules were physisorbed on pristine germanene where the more favorable adsorption site was the hollow one. The results show that the studied molecules have larger adsorption energy in Cu-, Ag-, and Au-decorated germanene than in the pristine monolayer. Therefore, molecule-metal-germanene complexes are more energetically favorable and are thus predicted to have an enhanced sensing capability. The larger NO adsorption energy on Cu-, Ag-, and Au-decorated germanene, in comparison with N₂ and O₂ cases, indicates its good selectivity towards NO. We investigated the work function and desorption time for the studied gases from Cu-, Ag-, and Au-decorated germanene to estimate its potential application as a NO sensor in toxic gas-insulated switch-gear. The results suggested that molecule-TM-germanene complexes are stable at ambient conditions and they are candidates for sensing and scavenging nitrogen monoxide



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**[TSM-194] Amphetamine molecule detection by doped and
functionalized silicon nanowires: a DFT study**

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Amphetamine (AA) is one of the most potent sympathomimetic amines in inducing an excited state of the central nervous system. In the past years, there were an estimated 28.9 million users of amphetamines, corresponding to 0.6 percent of the global population aged 15–64. Thus, the development of highly sensitive, fast response, hand-portability sensors for the detection of this drug agent is an essential task. Consequently, in this work, we present computational results of AA adsorption on the doped and the functionalized surface of silicon nanowires (SiNW) to theoretically explore the effect of modified surfaces on adsorption and electronic properties. The formation energy, adsorption energy, electronic structure, density of states, and atomic Voronoi charge population are calculated and analyzed systematically, and the results are further compared with that from the undoped surface of SiNW to reveal the effect of doping and functionalizing the surface. The biggest improvement in adsorption energy is given by the B-functionalized case, however, this value is too big to be considered for a reusable device, because too much energy would be necessary to remove the AA molecule from the surface. Also, the remaining five cases present a considerable improvement in the adsorption energy compared to that of the undoped case. Finally, in all cases have significant changes in the bandgap energy by the presence of the AA molecule compared to the SiNWs without the molecule adsorbed. These changes indicate that the transition from the SiNW without the AA molecule to the SiNW with the molecule could be electrically detected. SiNWs may be a potential nanomaterial for amphetamine sensing applications. We believe that this study can contribute to future experimental and theoretical studies on SiNW as a sensing material in the field of drug detection and the development of electronic devices.



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**[TSM-208] Mechanical behavior of linear atomic chains under uniaxial
stress**

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Nanostructures have driven the development of nanoscience and nanotechnology in various fields of physics, chemistry, electronics, optics, mechanics, biology and medicine, to name just a few, due to their physical and chemical properties very particular. Nanostructures such as carbon nanotubes and graphene, are just a few examples that demonstrate the structural versatility of carbon, which can form a wide variety of nanostructures based on the carbon hybridizations. The stretching bond force constants (Kr) in the chemical bonds allow us to quantify the opposition to the change of the charge distribution between the atoms, when these are subjected to a bond length changes. In other words, Kr values describe the stiffness of the chemical bond when the bonds are under stress strain. In this study, the Kr values of linear chains of carbon (LCC), boron (LBC), and boron nitride (LBNC) using density functional theory were compared and the effect of employing different exchange-correlation functionals for Kr calculation is discussed.



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**[TSM-228] Antiferromagnetic coupling in the initial stages of the MnN
epitaxial growth on the CrN (001) surface**

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The spintronics is an efficiency alternative for data storage and transfer. Spintronics systems often are based on ferromagnetic materials. However, to continuously reduce the device size it is desirable to minimize the ferromagnetic materials interference with each other. A possible solution is to replace the ferromagnetic materials with antiferromagnetic materials, provided that these latter may exhibit numerous interesting features. CrN and MnN are antiferromagnetic materials, with interesting electronic and magnetic properties. Therefore, these compounds are employed in ferromagnetic/antiferromagnetic systems, which exhibit the exchange bias effect at room temperature. However, the spin coupling and the possible exchange bias effect between CrN and MnN have not been investigated yet. Taking into account the above mentioned, we have performed spin polarized first principles calculations to study the structural and electronic properties, and spin coupling in the initial stages of the MnN epitaxial growth on CrN (001)-(1x1). Results indicate that the Mn may transform from a paramagnetic to a ferromagnetic system, when adsorbed on a surface. Also, the first CrN layer switches from antiferromagnetic to ferromagnetic alignment. Surface formation energies show that epitaxial growth of θ -MnN on CrN (001)-(1x1) surface is favorable for N-rich conditions and intermediate conditions. The MnN double layer exhibits an antiferromagnetic behavior, with the magnetic moments coupled parallel and alternating along c direction. Moreover, the exchange bias effect is manifested in the first CrN layer. The calculated project densities of states spectra show a half metallic character in first CrN layer. The Mn magnetic moments are in the range from 2.8 μ_B to 3.3 μ_B . This work provides an antiferromagnetic system for the possible applications in spintronics.



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**[TSM-2] THEORETICAL STUDY ABOUT MATERIALS FOR HYDROGEN
PRODUCTION**

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Density functional theory calculations were performed to obtain adsorption free energies for the MoS₂ monolayers based systems. Band structure calculations show that Mn and Co doped systems improve their conductivity properties. Calculations were performed to predict adsorption free energies and exchange density current for each material. We report theoretical Tafel slopes associated to their hydrogen evolution reaction (HER) performance, 76 mV, 62 mV and 63 mV for MoS₂, Co-MoS₂ and Mn-MoS₂ respectively. Quantum Theory of Atoms in Molecules (QTAIM) was used to characterize S-H bonds. We show that Mn and Co doped systems have an increment of not-covalent S-H bondings, that is to say creation of active sites on the basal plane.



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[TSM-17] STRUCTURAL AND ELECTRONIC PROPERTIES OF EUROPIUM

DOPED TIN OXIDE: FIRST PRINCIPLE INSIGHTS

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The CRYSTAL17 computer code is used to apply the density functional theory to rutile tetragonal tin oxide (SnO_2) with space group $P42/mnm$. First, the crystalline structure of SnO_2 was modeled in a unit cell, which contains 2 atoms of tin and 4 atoms of oxygen. We employed different bases using the PBE functional to have greater agreement with the lattice constant experimental. Second, in order to investigate the impacts of the Eu^{3+} impurity, the SnO_2 structure with an oxygen vacancy (Vo) and two europium (Eu) atoms were meticulously modeled in a $3 \times 3 \times 3$ supercell ($\text{Eu}_2\text{Sn}_{34}\text{O}_{71}$). The total energies of multiple $\text{Eu}_2\text{Sn}_{34}\text{O}_{71}$ supercell configurations were calculated and compared. It was discovered that when two Eu atoms are bound together and the Vo is close to an Eu atom, the total energy is at its lowest. To account for the six unpaired f electrons in the Eu^{3+} cations, all Eu doped supercell simulations were spin-polarized. The electronic properties such as the band structure, density of state (DOS), bandgap, and effective mass were predicted using HSE06 functional. The band structure and DOS predicts that SnO_2 and $\text{Eu}_2\text{Sn}_{34}\text{O}_{71}$ supercells exhibit insulator and semiconductor character, respectively. Furthermore, the $\text{Eu}_2\text{Sn}_{34}\text{O}_{71}$ supercell permits intraband f-f transitions that are otherwise prohibited in atomic Eu. This result is consistent with photoluminescence found for Eu-doped SnO_2 films and nanoparticles in the visible red range. The characteristics of the Eu-doped SnO_2 compound suggest that it could be a suitable phosphor material for reducing thermalization losses in solar cells.



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**[TSM-58] Characterization of the structural and magnetic properties of
SrRuO₃ by DFT**

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In the stoichiometry of the ABO₃ perovskite family, the roving ferromagnetic SrRuO₃ (SRO) stands out. SrRuO₃ is a widely known ferromagnetic offering a wide range of applications in spintronics. This material has now been explored due to its similar properties to AlTiO₃. SRO crystallizes in orthorhombic, tetragonal and cubic structure. In this work he focused on the orthorhombic and cubic structure, which were calculated using the VASP software package. The surfaces with the highest magnetization were calculated. DOS plot were performed for both structures and the structural and magnetic properties of the studies systems were compared.



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[TSM-59] Theoretical modelling of GeC monolayers decorated with metal atoms for hydrogen storage

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After hydrogen physisorption on graphene systems was experimentally demonstrated, exploring new kinds of bidimensional and layered materials for solid-state H₂ production and storage has considerably increased. Germanium carbide monolayers (GeC-MLs) can offer attractive opportunities for H₂ adsorption compared to graphene. However, this possibility has not been explored in detail. In this work, the adsorption of H₂ molecules on GeC-MLs decorated with alkali metal (AM) and alkaline earth metal (AEM) adatoms was investigated using the density functional theory. Results showed that the AM adatoms were chemisorbed on the GeC-ML, whereas AEM adatoms were physisorbed. The H₂ molecules presented negligible adsorption energies on the weakly adsorbed AEM adatoms. Conversely, the AM adatoms improved the H₂ adsorption, possibly due to a large charge transfer from the adatoms to the GeC-ML. The potassium-decorated GeC-ML exhibited the most optimal H₂ storage capacity, adsorbing up to six molecules and with a lower possibility of forming metal clusters than the other studied cases. These results may aid in the development of new efficient hydrogen-storage materials [1,2].

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**[TSM-73] I-V Electrical properties on MOSFET devices for resizing
purposes using LTSPICE**

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The free license LTSPICE software and Octave programming code have been used as tools on MOSFET's design. In this work, materials simulation allows to exemplify the physical phenomena at any interface or junction. Investigate their inner parameters such as geometry, voltages, parasitic capacitances, currents, factors, and constants, which are presented, it could be analyzed to propose a new assembly for MOSFET devices. Two principal models were simulated with the architectures Al/SiO₂/Si and Al/HfO₂/Si. Their geometrical parameters for the oxide film thickness were 150 nm and 50 nm, three different channel geometries: 60 μm L/40 μm W, 30 μm L/20 μm W, 20 μm L/10 μm W with a total of 12 simulations based on SPICE level 3 model were constructed and their I-V curves analyzed.

[TSM-101] Atomic vibration frequencies in CdTe and GaAs thin films

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The study of materials with applications or use in clean energies have received greater attention in recent decades. Particularly in solar energy, the materials for the manufacture of solar cells are of interest, whose greatest right is the efficiency when converting solar energy into electrical energy. In this work we carry out molecular simulations with some of these materials, first creating the bulk structures of Cd, Te, Ga and As. Once their geometry is optimized and we also obtain their densities of electronic states and vibration frequencies; These vibrational frequencies are within the frequency range of the visible light spectrum.



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[TSM-176] DOS of two coupled Fibonacci chains

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The periodic material layer stacking has been studied for graphene, silicene and germanene, just to name a few, where new phenomena arises different from that of a single layer. In this work, we studied the spectral behaviour of two stacked Fibonacci chains from a tight binding Hamiltonian approach. β is the hopping integral between the two chains; if $\beta=0$, the single chain DOS is reproduced, but for $\beta \neq 0$, the coupling effects are shown. The two chains can experiment an edge dislocation, which consists of a displacement of a lattice parameter.

[TSM-179] Ab initio elastic constants for BaTiO₃ and PbTiO₃

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The Global Industry report in 2016, reported that the market for piezoelectric devices globally was valued at 1.17 billion us dollars. It is also important to highlight from the report that 60% of the piezoelectric devices are made of ceramic materials. the electronic industry is the main employer of this type of materials. In the field of research, piezo electrics are studied for their properties of energy conversion, both on a macro and micro scale. A simple way to determine the piezoelectric quality of a material is through the coupling coefficient, which determines the fraction of mechanical energy which is transformed into electrical energy. Classic piezoelectric materials such as quartz have a low coefficient, compared with composite materials such as barium titanate, BaTiO₃. These materials have a higher coefficient and therefore are more appropriate for conversion and obtaining uses of energy.

In this work we present the elastic constants C_{11} , C_{33} , C_{44} , C_{66} , C_{12} and C_{13} for BatiO₃ and PbTiO₃ calculated with ab-initio DFT VASP code with PBESol approximation for exchange correlation approximation. Results are in good concordance with experimental values and other calculations.



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[TSM-184] H₂ Interaction with Carbon BCC-C6 in slab structure.

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BCC-C6 is a exotic phase of carbon which have been proposed from a meteorite material that fell in Popigai, Russia in 2003 [1]. From x-ray diffraction studies and Raman spectroscopy of these samples, it is concluded that there is a crystalline phase whose structure is cubic centered on the faces with a Pm3m symmetry and lattice parameters 14,697Å. Subsequent theoretical calculations showed that this carbon phase could actually have a lattice parameter of 4.34 Å [2] and 3.8 Å [3]. A phononic vibration frequency analysis was carried out, obtaining as a result that all spectrum branches are positive and the bulk phase of the BCC- C6 is meta-stable. Also, was showed that each face of the BCC-C6 phase has a relatively low surface energy, with the thin layers (111) and (100) having the lowest surface energies.

Because porosity, this structure would be suitable for hydrogen storage. The study of interaction of the H₂ molecule with the carbon phase BCC-C6 were carried out through computational calculations that involve quantum theory. In particular, the method that will be used is called Functional Density Theory (DFT). A H₂ molecule are studied in interaction with monolayers of surfaces 110 and 111 for adsorption energy calculation. Such energies are obtained as -0.39 eV and -0.42 eV for 110 and 111 surfaces.



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**[TSM-206] Electronic properties of linear carbon chains inside of carbon
nanotubes**

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The electronic and structural properties resulting from Linear Carbon Chain (LCC) insertion into a semiconducting Single-Walled Carbon Nanotubes (SWCNTs) named as Carbon Nanowires (CNWs), using density functional theory (DFT) were studied. Here all carbon nanotubes and carbon chains exhibited a semiconductor behavior in isolated state; however, the semiconductor transitions to metallic character were found when the CNWs were conformed. The effect resulting from considering the conformational stress and charge transfer on the band gap of CNWs was analyzed. The electronic character from CNW with (7,0) nanotube is affected by the structural strain and charge transfer with a slightly higher contribution. CNWs made up of (8,0) and (11,0) are primarily affected by strain, and their electronic states distribution retain the band gap associated with their isolated semiconducting nanotubes, leading than only their LCCs electronics bands to cross the Fermi level. Whereas, CNWs formed from (10,0), (13,0), and (16,0) were also mainly affected by strain, showing only a few empty states slightly above the Fermi level in their electronic states distributions, due to charge transferred from the LCC. A global metallic behavior for all CNWs with a permanent contribution from the electronic states of LCCs was found. However, an influence of nanotubes diameters with their contribution to the global metallization was determined.



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THIN FILMS

Chairmen:

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Dr. Jorge Ramón Parra Michel (Universidad de La Salle Bajío), jrparra@delasalle.edu.mx

The purpose of this symposium is to provide an international forum for discussion and exchange of ideas on the up-to-date research and developments of processing and characterization of advanced thin films. The physical properties of thin films are critically dependent on the deposition conditions and post-treatment details therefore discern the correlations between the experimental conditions and film properties are of great interest for the field. The participants from various universities, industries and research laboratories are welcome to submit contributions for both oral and posters presentations to discuss recent advances, developments, field applications, and future challenges for the thin film technologies. The topics include, but are not limited to, every kind of thin films used in:

- Energy applications
- Protective coatings
- Memory storage
- Optoelectronic devices
- Sensors and actuators
- Biomedical applications.



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**[THF-7] Electrically conductive improvement of silver nanowires thin
films through mechanical and thermal post-deposit techniques.**

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The industry looks for materials, which could be used as thin films highly electrically conductive and transparent to use in optoelectronic devices like electrodes. For that reason, we have worked with structures of silver nanowires (Ag NW) to make thin films, obtaining promising results. We fabricated the Ag NW thin films by the Spin Coating process, which is a cheap and easy method. One of the purposes is to find the best parameters of film fabrication, here each film was made with a quantity of three drops of material dissolved in ethanol, scattered over the glass by rotation with an angular frequency of 3000RPM for 3 min at room temperature. Just a solvent fraction is evaporated in the processes of rotation; therefore, the films are dried on a hotplate at 100 °C for 10 min. After fabrication, the films are characterized as follows: the electrical properties were measured by the four-point probe technique, finding sheet resistances lower than 30 Ω /sq, the optical properties by transmittance which gave an average value of 80% at 550 nm wavelength, and the morphological properties with SEM. These results allow us to augur the films as promissory candidates to replace the expensive and scarce ITO, current material used to fabricate the transparent electrodes.

Despite these results, there are some drawbacks to solve, for example, the high contact resistance between nanowires. Because of this last, we have probed two different extra processes to improve the electrical contact between nanowires. The first one is the nanowire welding by heat treatment. In this method the films are exposed to high temperatures (120-190 °C) during different time intervals, achieving a kind of junction in some of the contacts and reducing the sheet resistance in a percentage magnitude of up to 50,1%. The second applied method is the application of pressures on the films; in this method, we applied a force between 2 and 10 Ton-Force during different time intervals over the film surfaces achieving a sheet resistance decrease in a percentage magnitude of up to 75,9%. The results show an improvement in the electrical conductivity of the metallic nanowire films after the welding processes.



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**[THF-21] Low-temperature synthesis of ZnO nanostructures and their
analysis as a detector of H₂S gas**

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The detection of pollutant gases is important for the protection of the environment and people's health, so the development of low-cost and reliable portable prototypes is a current research topic. In particular H₂S gas, it is produced in many of the industrial processes and is a waste known as knock down gas. People exposed to H₂S in prolonged times and inhaling high concentrations may have immediate loss of consciousness and even cause their death. An economical and reliable way to measure exposure levels is by using sensors based on metal oxides. This work reports the characterization of ZnO nanostructures obtained through a green synthesis method: mechanical grinding (MQ). Synthesis of ZnO was produced with zinc chloride (ZnCl₂), sodium carbonate (Na₂CO₃) and sodium chloride (NaCl) at room temperature and grinding times of 20, 40 and 60 minutes. 10 layers of ZnO were placed on glass substrates in thin films by the screen printing technique and were characterized by DRX, Raman and SEM. Structural analysis revealed the presence of the wurzite hexagonal crystalline structure (ICDD 36-1451, confirmed with the three Raman vibrational modes. In morphological analysis, the growth of nanostructures from 30 to 100 nm was identified. Hydrogen sulfide gas (H₂S) detection tests were performed, detecting from 3 to 7 ppm H₂S.



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**[THF-152] Photocatalytic applications and characteristics of TiO₂ thin
films by the sol-gel method**

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TiO₂ is one of the most used materials for the realization of thin films, particularly by the sol-gel method. Extensive research has been made into the photocatalytic properties and applications of this nanomaterial. Different precursor substances can be used to generate TiO₂ thin films. The present work seeks to explain the different applications and characteristics that TiO₂ films have when created by different precursors, as well as how these change when TiO₂ is used in conjunction or doped with other materials, like SiO₂ and metal ions of Fe and Co.



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[THF-158] Morphology, texture and optical properties of ZnO

nanostructures obtained from thermal oxidation of Zn-nanodisks

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Zinc oxide (ZnO) nanostructures have attracted considerable attention due to their good oxidation resistibility, thermal stability, good biocompatibility, low toxicity, as well as their optical, chemical, and electrical properties. It is a transparent semiconductor with a direct band gap ($E_g = 3.37$ eV) and good conductivity at room temperature. Some of its technological applications span from gas sensors, varistors, and piezoelectric devices, to photodiodes. Thermal oxidation of Zn offers several advantages compared to the other approaches, such as the production of single-phase ZnO with larger amounts of the product in lesser time. Costs also are significantly lowered without losing control of the morphology. Different morphologies could be obtained by control of the oxidation time, reaction temperature, cooling rate, or the processing atmosphere, without the use of chemical precursors and catalysts, thus minimizing chemical waste and release of toxic gases to the atmosphere. In this work, thin films consisting of hexagonal-nanodisks of metallic Zn have been obtained with different thicknesses and sizes of the disks. It is shown that the thickness of metallic foils influences the global properties of the obtained nanostructured ZnO thin films. The effect of this parameter on the morphology, texture, grain size, and optical properties of the produced ZnO films is discussed. The main results are summarized as follows:

- Zinc oxide nanostructures show an on-axis preferential growth depending on the deposition conditions of metallic zinc
- Film roughness is favored in some cases by preferential growth and, in turn, the formation of ordered microcavities can be accomplished
- Microcavities support strong (optical) scattering effects which enable random lasing. Optical scattering influence both, the overall intensity and the spectral features of measured absorption (or extinction) spectra



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[THF-175] In-situ and real-time control of fabrication of one-dimensional porous silicon photonic crystals

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The possibility to modulate the refractive index of porous silicon (P-Si) makes it an attractive material for the fabrication of 1D photonic crystals (PhCs)[1], such as distributed Bragg reflectors (DBRs) and optical microcavities (MCs). However, several experimental factors that are difficult to control such as the Si wafer quality[2], the temperature of the electrolyte[2], variations in the etch rate and passive chemical etch[3] have a critical impact on the reproducibility and quality of P-Si samples. For example, a porosity gradient due to chemical etching causes the optical thickness to change with depth. Therefore, it is desirable to have an in-situ monitoring system to control in real-time that the fabrication sample has the desired optical response. In this work, we developed an in-situ monitoring and real-time control system for electrochemical etching of P-Si based on reflectivity and electrical measurements. This system allows us to observe and study the evolution of P-Si photonic crystals as they are formed during the etching process. The measured spectra of each layer of the sample are compared in-situ and in real-time to their theoretical counterpart predicted by the transfer-matrix method. Based on these comparisons, the thickness of each layer can be adjusted in real-time by modifying the etching time. This method has allowed us to diminish the negative effects of porosity gradients and proves an efficient way to tune the central wavelength of P-Si photonic crystals without the need of painstaking and time-consuming calibration processes.

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**[THF-188] Study of Ti_{1-x}Hf_xO₂ films for high-k gate insulators
applications**

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High-k gate insulators, dielectric constant (k), are increasingly being adopted for transistor designs as they offer superior control over leakage current and channel electrostatics, such as Al₂O₃. One promising material for high-k gate insulators is titanium oxide (TiO₂) due to its high permittivity (k = 50-60). The addition of Hf into TiO₂ form a complete solid solution, Ti_{1-x}Hf_xO₂, that could have intermediate properties between the TiO₂ and HfO₂ because of the low k (k = 15-27) and wide band gap (5.3-5.9eV) of HfO₂ [1]. Films of these compounds have been prepared on substrates using various growth methods, such as atomic layer deposition (ALD) [2] and spin coating [3-4]. The spin coating technic presents advantages such as large coating area, low-temperature processing, and low cost.

In this work, Ti_{1-x}Hf_xO₂ solid solution films were prepared by spin coating using silicon wafers as substrate with x = 0, 0.25, 0.50, 0.58, 0.66, 0.75, 0.85, 1 of Hf, later films were annealing to obtain crystalline films. Structural characterization of the films was done with grazing incidence x-ray diffraction (GIXRD) and Raman spectroscopy. At x = 0 and 1, pure phases of anatase TiO₂ and monoclinic HfO₂ were obtained. At a concentration greater than 0.58 Hf we observe a change in crystalline phase. A phase between TiO₂ to HfTiO₄, a compound that is expected to have the intermediate properties between the TiO₂ and HfO₂.

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**[THF-15] Effect of nitrogen doping on physicochemical properties of ZnO
thin films**

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ZnO is a semiconductor material with high chemical and thermal stability, it is also a low cost and low toxicity compound, which makes it an attractive material for various applications such as gas sensors, solar cells, photocatalyst, light-emitting diodes (LED's), etc[1,2]. ZnO can be produced in different ways. Currently, thin films have aroused great interest in the scientific community, since depending on the synthesis method their properties can be modified and/or controlled allowing their use in different technological fields. Among the different techniques, atomic layer deposition (ALD) occurs in the gas phase. It is characterized by a time-sequenced introduction of precursors onto the deposition zone where self-limited reactions occur[3]. The self-limited growth mechanism of this technique results in excellent accommodation, high crystallinity, uniformity, and specific film thickness control. In addition, the properties of a material can be improved by incorporating doping elements, providing to the material new characteristics, generating multifunctional materials. Recently, nitrogen is emerging as a key element in the doping of materials due to its low cost and high chemical stability[4]. The present work focuses on the characterization of the physicochemical properties of nitrogen-doped ZnO thin films, synthesized through the combined use of the ALD technique and hydrothermal methods, followed by doping through a discharge of nitrogen plasma. The N-ZnO thin films shown interesting features for possible application in various technological fields.

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[THF-34] Performance evaluation of $Zn_xCd_{1-x}S$ as window layer and $Cu_{2-x}Te$ as p + layer in CdTe-based photovoltaic devices

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The thin film solar cells based on CdTe show a great alternative to the more common commercial cells based on silicon, as it is the second technology with an impact on the market, and it still has a possible development to reach its theoretical limits. In laboratory work, the best efficiencies for this technology have been achieved using techniques such as CdTe deposition through closed space sublimation (CSS). This thesis project includes the development of a solar cell based on the CdS/CdTe heterostructure, modifying the window layer by a $Zn_xCd_{1-x}S$ film, improving the optical and electrical properties of the device. This solar cell will be executed on a 3mm commercial glass substrate with FTO conductive film, the deposit of the CdS and $Zn_xCd_{1-x}S$ films will be used by the chemical bath deposit technique (CBD). Subsequently, using the closed space sublimation technique (CSS), the CdTe film will be deposited; and, once this heterostructure is obtained, a p+ type layer will be deposited by cathodic erosion on the CdTe layer obtained, this in order to improve the conversion efficiency of the device. The material to be tested as a p+ layer will be $Cu_{2-x}Te$. Once the different devices have been manufactured, the efficiency of each one with the different additional layers will be evaluated and they will be compared against the solar cell without the addition of any p+ layer, this in order to evaluate if the improvement is significant.



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[THF-41] Optical, structural, and morphological properties of CdSe thin films grown by thermal evaporation.

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The present work is about the structural, optical, chemical, and morphological properties of CdSe thin films obtained by the CdCO₃ precursor thin films transformations in cadmium selenide (CdSe) thin films by thermal evaporation for possible application in solar cells, TFTs, LEDs, and others. The direct bandgap of CdSe thin films are 1.82 and 1.86 eV, respectively, and are related to direct transitions of electrons between valence and conduction bands in concordance with the value reported in the literature. SEM studies show the morphology of CdSe thin films, and the expected chemical composition for CdSe thin films is proving by the low- and high-resolution XPS spectra and EDS.

[THF-65] Aluminium Doped ZnO thin films ultrahighly oriented in c-axis (002) with high transparency and low electrical resistivity

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Aluminium doped ZnO (AZO) thin films deposited on glass substrates are synthesized by means of the Spray Pyrolysis technique. The incorporation of aluminium at the average of 3.6 % of atomic concentration is well determined by EDS measurements. The films are highly oriented along the (002) direction, which resembles an epitaxial growth as corroborated by X-ray diffraction spectra and Atomic Force Microscopy images. The optical transmittance was of the order of 85 %. The lower electrical resistivity value of $1.016 \times 10^{-2} \Omega\text{-cm}$ was measured.



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[THF-75] Study of CdS thin films doped with metals using CBD and a coupled system of SILAR-CBD by optical, morphological, and structural characterization.

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The current situation demands the study of new materials that can be used in modern devices and represent an improvement for these, but not only the synthesis of materials is pursued with the purpose of innovating in various fields, but the need for the development of clean and environmentally friendly technologies has taken a role of great importance. CdS films are leading semiconductors in optoelectronic and photovoltaic applications, being used in solar panels, photodetectors and transistors, to name a few examples. The optical properties of these films are remarkable, presenting band gap energies considered to be in the average. An interesting way to promote their electrical and optical properties is by doping the films with certain elements such as metals, including copper, indium, gallium, tin, among others. There are several methods to carry out this process, in this work we analyze in detail between two methods, in one of them the films are synthesized by chemical bath deposition to subsequently doping the films by SILAR technique, on the other hand, the second way incorporates the doping of the film directly in the chemical bath deposition by altering the base formulation of CdS. It should be noted that the CBD technique represents an inexpensive but effective way to synthesize the films, requiring temperatures ranging from room temperature to 90 degrees Celsius. The comparison of both processes will be discussed by analyzing the optical, morphological, structural and electrical properties of the films obtained by characterization techniques such as UV-Vis spectroscopy, reflection and transmission spectroscopy, Energy Dispersive X-ray Spectroscopy (EDXS).

Keywords: Chemical bath deposition, SILAR, doping, solar cells, photodetectors.



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[THF-85] A study of the Si Sputtering Yield Amplification

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The *Sputtering Yield Amplification, SYA*, is a phenomenon based on doping a sputtering target with atoms of higher atomic mass with the aim to increase the ejection of target atoms. As a result of this doping, the depth and the direction of the collision cascade to the surface's target are changed. In this work, we present a new way of generating the SYA, only by increasing the working pressure and adding small pieces of W, as dopant element, on the Si target's racetrack we studied the physical phenomena necessary to promote the phenomenon in two different deposition chambers and two sizes of sputtering targets. Based on the collisions the target atoms have with the working gas atoms in the gas phase, we made a calculation on the number of W atoms returning to the racetrack from the number of deposited atoms on the substrate in order to determine their effect on the cascade of collisions. In addition, calculations with the Simulation of Metal Transport code were developed to determine the location over the Si target the returning atoms were deposited. By analyzing reference samples placed on the racetrack, via XPS and RBS, we found that the percentage of SYA, measured with the Co-Sputtering Simulation software, depends on the number of dopant atoms deposited as well as the depth distribution these atoms had in the racetrack surface. The system pressure threshold to observe SYA was estimated via plasma-emission spectroscopy



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[THF-109] Intrinsic Photovoltaic effect of SiOx films deposited by HFCVD

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In this work, the presence of photovoltaic effects in MOS-type structures manufactured using off-stoichiometric silicon oxide (SiO_x) deposited by HFCVD technique is reported. Current-voltage measurements under dark and illumination conditions were carried out. The reported MOS-type structures with SiO_x as dielectric layer undergo a change in the charge conduction mechanisms of the injection current, exhibiting a transition from the Hopping to Schottky mechanism, which is dependent on the hydrogen amount and the deposition parameters of SiO_x films. It was found that in the range of low applied voltages the Space Charge Limited Conduction mechanism (SCLC) is present. Additionally, the photovoltaic effect was also obtained and studied from these types of structures, being corroborated by making current-time and voltage-time measurements without applied bias, where the current and voltage values correspond to those obtained from the IV curves. The structures with SiO_x films having thermal annealing exhibit the photovoltaic effect. The obtained results are suitable for photovoltaics applications with additional advantages of short time of deposit (3 minutes) by HFCVD, and a single MOS-type structure.



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[THF-118] Effect of the temperature deposition on the physicochemical properties of ZnSe films

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Chalcogenide materials belongs to II-VI groups of the periodic table are promising semiconductors for electronic and optoelectronic devices due to their optical properties. Zinc Selenide (ZnSe) is a n-type semiconductor with a visible band gap (2.7 eV) which is composed with naturally abundant elements. ZnSe films has been made by different techniques such pulse layer deposition (PLD), thermal evaporation, and chemical bath deposition (CBD). CBD is a low-cost technique where the processing parameters (temperature, deposition time, and ions precursors) can be controlled to obtain high quality chalcogenide films. In this work, ZnSe thin films were deposited on glass substrates by a CBD method varying the deposit temperature at 60 °C and 70 °C. The chemical reagents employed were zinc sulphate and sodium selenosulfate as a Zn²⁺ and Se²⁻ ions, respectively. KOH as reducing agent and hydrazine as complex agent. The deposition time was modified at 2 h, 3h and 4 h to assess the thickness, morphology and optical properties of ZnSe films. At the end, the films were washed with deionized water and dried in air atmosphere. The influence of the temperature deposition on the physicochemical properties was evaluated by structural (XRD), optical (UV-Vis), morphological (FESEM) and superficial (XPS) analysis.

Keywords: ZnSe films, XPS analysis, Chemical bath deposition



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**[THF-139] Synthesis and study of the ferroic properties in thin films of
BiFeO₃**

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The study of mixed oxides with perovskite structure is significantly interesting due to the various possibilities of modeling their properties through ion exchange in their structure. Different methodologies are being sought to obtain these mixed oxides either in the form of single crystals, powders or thin films. BiFeO₃ is the first ABO₃ ferroelectric perovskite discovered with trivalent A and B ions, where the polarizability of Bi³⁺ and the presence of Fe³⁺ with its uncompensated spin give rise to ferroelectric and ferromagnetic properties simultaneously. It has the advantage of having a high melting point and a high Curie temperature (T_C), additionally it is a ferroelectric/ferroelastic compound with a rhombohedral distortion described by the space group R3c from the temperature of liquid helium up to 823°C, it has a helical magnetic structure and a 3m Shubnikov group. In this work, the preparation of thin films of BiFeO₃ was carried out by the spray pyrolysis technique, and their ferroelectric properties were analyzed.

The thin films of BiFeO₃ were prepared by means of the spray pyrolysis technique, on glass substrates. The precursor reagents were bismuth and iron nitrates, dissolved in dimethylformamide. Deposits were made in the range of 300°C to 500°C with a subsequent annealed treatment at 550°C. Homogeneous films with good adhesion to the substrate were obtained. The elemental composition, surface morphology, and crystalline structure of the films were analyzed as a function of concentration and deposition temperature. The samples were characterized by the X-ray diffraction technique (XRD) showing the rhombohedral structure. The measurements of the ferroelectric properties of the prepared films were carried out by determining the remanent polarization values and the coercive field (P vs E).



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**[THF-141] Growth parameters to obtain crystalline ZnO films synthesized
by hydrothermal method**

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With the development of the industry, environmental problems have become more complicated, the removal of toxic compounds from water is a currently a research topic. An alternative to reduce water pollution is photocatalytic treatment using zinc oxide (ZnO) as a photocatalyst material in film form. The advantage of using layers of photocatalyst is that it avoids final separation operations, it is recovered and reused. In this work the characterization of the ZnO films (seed layers-CS) by sol-gel, deposited on glass substrates by spin coating in 3, 5 and 7 layers is reported, these CS were used as a base to grow ZnO nanorods by hydrothermal method. The adhesion test of the CS films and with hydrothermal growth was carried out under the ASTM D3359-09 standard, and the quality of the films corresponds to level 5 for both cases. The films obtained have a ZnO hexagonal wurtzite structure, confirmed by Raman vibrational modes; the strongest planes are shown along orientations (100), (101), and (002). For both CS and hydrothermal growth, a plane orientation change occurs as the number of layer increases. Respecting the surface morphology, the grain size of the CS varied from 97-120 nm and the average dimensions of the nanorods took values of 90-120 nm in diameter and 420-543 nm long, and the thickness of the films is up to 200 nm. This material thus obtained will be evaluated in its photocatalytic properties of the degradation of methylene blue with UV light as a source of activation.



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**[THF-160] Electrical properties of ITO thin films deposited by DC
magnetron sputtering and their photoelectrochemical behavior.**

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ITO thin films were deposited on a glass substrate by DC Magnetron Sputtering to be used as photoelectrochemical electrodes. The deposits were made, varying the power deposition from 5w to 40w for 30 minutes to study their electrical properties. After deposition, ITO thin films were heat treatment at 400°C to improve the structural and electrical properties. The resistivity of the films was improving its resistivity from 2MΩ to 20kΩ after the heat treatment. The transmittance percentage was higher than 80% for all films, which complies with this transparent semiconductor oxide (TCO). The thickness of the ITO films was measured on a profilometer obtaining thickness until 69.2 nm. ITO thin films were probe in electrochemical tests to determine the electrical properties and considering using these films as electrodes in the photoelectrochemical tests.



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[THF-202] Structural and optoelectronic properties of Al-doped In₂S₃ thin films prepared by chemical bath deposition for photovoltaic applications.

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Nowadays, research in environmentally friendly materials for photovoltaic device applications, is an important issue which have received a special interest in order to process toxic-free solar cells at lower cost. Due to its thermal stability, optical transparency and wide band gap in the range 2.0-2.9 eV, n-type In₂S₃ semiconductor compound, could be considered an admissible option to be used as buffer layer.

In₂S₃ films have been prepared by different methods, such as sputtering, physical vapor deposition, electrodeposition, spray pyrolysis and chemical bath deposition (CBD). The CBD method is an attractive technique in the manufacture of films due to its feasibility to produce a low cost large-area thin films. The properties of In₂S₃ can be improved by the addition of several materials

The present work focuses on the elaboration of films of the semiconductor compound In₂S₃, using chemical bath deposition technique. The main objective of this research is to obtain a semiconductor heterostructure on flexible substrates that can be applied as a photovoltaic device.

[THF-214] Physical properties of Ti-Al-Cr-N thin films prepared by reactive co-sputtering

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Thin films of Ti-Al-Cr-N have been synthesized onto glass substrates by reactive magnetron sputtering of pure Cr and TiAl alloy targets. The experimental process included the Cr-target power control to modify the coating composition. The composition and microstructure of coatings were analyzed by Auger Electron Spectroscopy (AES) and X-ray diffraction (XRD), respectively. The electrical resistivity was measured by the four-point probe method and their optical properties were characterized by ultraviolet/visible (UV/Vis) spectroscopy. The results have shown the influence of Chrome concentration on microstructure and its consequences on the electrical and optical properties.



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**[THF-215] Mechanical and tribological properties of Ti-Al-Cr-N thin films
deposited by co-sputtering**

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Thin films of Ti-Al-Cr-N were deposited onto glass and silicon substrates by means of reactive magnetron sputtering. This investigation was carried out by adjusting the Cr-target power in order to increase the Cr amount in the films. The microstructure of the films was investigated via X-ray diffraction (XRD). The elemental composition of the coatings was determined using auger electron spectroscopy (AES). The surface morphology and the roughness were studied using scanning electron microscopy (SEM) and optical profilometry respectively. The mechanical properties were evaluated by means of nanoindentation, and the wear resistance was studied with pin-on-disk technique. The film morphology changed to fine columnar as chromium increased. As a general observation, the hardness, resistance to plastic deformation (H3/E2) and wear resistance of the samples increased as the chromium increased

**[THF-216] Mechanical behavior of TiAlCrN thin films co-deposited with
Cu on hardmetal via co-sputtering**

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In this investigation, TiAlCrN coatings with different copper (Cu) contents were deposited by means of reactive magnetron sputtering. The microstructure of the films was investigated via X-ray diffraction (XRD). The elemental composition of the coatings was determined using X-ray fluorescence (XRF). The surface morphology and the roughness were studied using scanning electron microscopy (SEM) and optical profilometry respectively. The mechanical properties were evaluated by means of nanoindentation and the wear resistance was studied with pin-on-disk technique. The film morphology changed to fine columnar as copper increased. The addition of Cu to the TiAlCrN coatings led to increasing the hardness, resistance to plastic deformation (H3/E2), and wear resistance.



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**[THF-240] CBD-CdS/ZnS and SILAR-CdS/ZnS thin films and their
application in solar cells devices: a comparative study**

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The use of buffer layers that totally or partially replace the traditional CdS thin films in the thin-film solar cells, has attracted the attention of the photovoltaic community due to the combination of desirable physical properties and to reduce the problems related with the toxicity of Cd. However, currently the best efficiencies obtained in the second generation of photovoltaic devices remains with the use of CdS as buffer layer. Therefore, a compromise between these two great issues must be reached. In this context the propose of the use of bilayers CdS/ZnS has been considered as an alternative to the traditional CdS one. In this work we present a comparative study of the properties of CdS/ZnS thin films, deposited by CBD, and the combination of CBD with SILAR method, with the aim of establishing the growth processes that guarantee the obtention of Cd_{1-x}Zn_xS ternary compound as alternative buffer layers to CdS in high efficiency in Sb₂Se₃ solar cells.



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Camarillo Salazar Erika *TSM-61*
Campos Enrique *NSN-112*
Campos Enrique *PLV-138*
Campos-González E. *NSN-199, PLV-193, SIT-195, SIT-197*
Campos-Gonzalez Enrique *PLV-104*
Camps E. *NSN-199, PLV-193, SIT-195, SIT-197*
Camps Enrique *PLV-138*



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Camps Enrique *PLV-104*
Camps Carvajal Edgar Enrique *MUL-70*
Cano Salazar Jesus Adrian *SEM-124*
Cano Salazar Jesus Adrian *SEM-122*
Cano-Rico Alan *NSN-174*
Cano-Rico Alan *SEM-173*
Canto G.I. *TSM-206*
Capote Rodriguez Gil *THF-216*
Carbajal Arizaga Gregorio Guadalupe *CHM-74*
Carbajal-Valdez Rigoberto *NSN-150*
Cardenas Flechas Leydi Julieta *NSN-27*
Cardenas Flechas Leydi Julieta *NSN-29*
Cárdenas-Martínez Jessica *RWE-274*
Carmona Carmona Abraham *SIT-129*
Carmona Carmona Abraham Jorge *CHM-142*
Carmona Tellez S. *SEM-119*
Carmona Téllez Salvador *LPM-156, LPM-157*
Carmona Téllez Salvador *LPM-123, LPM-166*
Carmona-Carmona Jorge A *SIT-204*
Carmona-Carmona Jorge-Abraham *SIT-116*
Carodona Peña Lizbeth Berenice *SEM-258*
Carrasco Jaim Omar Ali *RWE-56*
Carrasco Rodríguez Raymundo *LPM-218*
Carreño Carmona Irlanda *RWE-234*
Carreño Carmona Irlanda *RWE-235*
Carreón Álvarez María Alejandra *NSN-37, RWE-45*
Carrillo Flores Diana María *MUL-213*
Carrillo López Jesús *RWE-32*
Casais-Molina M.L. *NSN-203*
Casallas Moreno Yenny Lucero *NSN-220, NSN-253, SEM-89, SEM-122, SEM-124, SEM-219*
Casallas-Moreno Y.L. *SEM-57*
Castañeda Guzman Rosalba *MUL-280*
Castañeda Valderrama Rocío *NSN-37, RWE-45*
Castañeda-Priego Ramón *NSN-12*
Castillo Jhonathan *MEM-263*
Castillo Santo Jesús *SEM-25*
Castillo Alvarado Fray de Landa *TSM-2*
CASTILLO SÁNCHEZ MARTÍN DARIO *SIT-8*
Castro Guerrero Carlos Fernando *SIT-30*
Castro-Camus Enrique *SEM-164*



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Ceballos Sanchez Oscar *NSN-120*
Ceballos-Sanchez Oscar *THF-118*
Cerde Mendéz Edgar Armando *SEM-187*
Cerde-Méndez Edgar Armando *THF-175*
Cervantes Álvarez Fernando *NSN-279*
CERVANTES LÓPEZ JOSÉLUIS *THF-21*
Cervantes-López José Luis *THF-15*
Céspedes-Pérez Pablo César *NSN-227*
Chavelas-Gonzalez Pamela *SEM-239*
Chávez Chávez Arturo *SEM-207*
Chávez Urbiola Iker *MEM-84, THF-75*
Chavez Urbiola Iker Rodrigo *SEM-31*
Chávez -Chávez A. *NSN-199, SIT-146, SIT-195, SIT-197*
Chávez -Cruz M. del C. *TSM-101*
Chávez -Urbiola Iker Rodrigo *RWE-36*
Cigarroa Mayorga Oscar Eduardo *NSN-106*
Cigarroa Mayorga Oscar Eduardo *RWE-113*
Cigarroa-Mayorga Oscar Eduardo *SIT-11*
Comas-Garcia Mauricio *BIO-18*
Compeán García Vicente Damián *SIT-256*
Conejeros Sergio *TSM-17*
Contreras Gerardo *PLV-81, PLV-82, PLV-83*
Contreras Chávez Rafael *BIO-278*
Contreras Puente Gerardo *RWE-19*
Contreras-Navarrete José de Jesús *NSN-143*
Contreras-Navarrete José de Jesús *NSN-149, NSN-154*
Contreras-Rascón Jorge Indalecio *NSN-250*
Cordero García Adrián *THF-141*
Correa Pacheco Zormy Nacary *CHM-225*
Correa-Pacheco Zormy Nacary *NSN-148*
Cortazar Martínez Orlando *CHM-142*
Cortazar Martínez Orlando *SIT-129*
Cortazar-Martinez Orlando *SIT-116, SIT-204*
Cortes Mestizo I.E. *NSN-163, RWE-165, SEM-168*
Cortes Suarez Jorge Victor *SIT-96, SIT-97*
Cortes-Mestizo Irving E *NSN-174*
Cortes-Mestizo Irving E. *NSN-167, NSN-172, SEM-164, SEM-173, TSM-170*
Courel Piedrahita Maykel *RWE-249*
Coyopol Solis Antonio *SEM-114*
Crisóstomo Margarita C. *TSM-194*



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Cruz Julio *PLV-86*
Cruz Julio *THF-85*
Cruz -Irisson Miguel *NSN-132, NSN-190*
Cruz Gabarain Lorena Conchita *CHM-272*
Cruz García Cristian Felipe *SIT-40*
Cruz Irisson Miguel *NSN-131, RWE-92*
Cruz Irisson Miguel *TSM-59*
Cruz Orea Alfredo *CHM-225*
Cruz Ortiz Giovanni Alejandro *RWE-47*
Cruz-Cárdenas Julio *CHM-88*
Cruz-Hernández Esteban *TSM-169*
Cruz-Hernández Esteban *NSN-211, NSN-212*
Cruz-Irisson Miguel *TSM-194*
De Anda Gil Jessica *LPM-80*
De la Mora Ramírez Tomas *SIT-99*
De la Mora Ramírez Tomas *SIT-99*
De La Vega Luis Ricardo *SIT-40*
de Melo Osvaldo *NSN-220*
de Moure Francisco *PLV-81, PLV-82*
de Moure Flores Francisco Javier *BIO-136, PLV-83, RWE-19*
de Moure-Flores Francisco *THF-202*
De Santiago Varela Francisco *TSM-59*
de Urquijo Ventura Maria da la Soledad *MEM-111*
Dehonor Márquez Ethnice *BIO-262*
DEL ÁNGEL MERAZ EBELIA *THF-21*
Del Pozo Zamudio Osvaldo *SEM-187*
Del Río De Santiago Antonio *THF-139*
Del Rio-De Santiago A. *RWE-69*
Delgado Arroyo Filemón *SIT-30*
Delgado-Ramos B. B. *NSN-137*
Díaz Gabriel *NSN-115*
Diaz Alonso Daniela *MEM-128, SCD-276*
Diaz de León Jorge Noe *MUL-3*
Díaz Flores Laura Lorena *THF-141*
DIAZ FLORES LAURA LORENA *THF-21*
Díaz Gongora José Antonio Irán *LPM-185*
Diaz-Reyes Joel *BIO-135, NSN-137, NSN-150*
Díaz-Reyes Joel *LPM-251, NSN-250, NSN-252*
Dominguez David *MUL-3*
Dominguez Jimenez Miguel Angel *SCD-108*



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Domínguez Robledo Oscar Iván *THF-34*
Domratcheva-Lvova Lada *NSN-143, NSN-145, NSN-149, NSN-154*
DOÑU MARCO ANTONIO *SIT-127*
Doñu Ruiz Marco Antonio *SIT-97, SIT-98, SIT-99, SIT-140*
Doñu Ruiz Marco Antonio *SIT-96*
Dueñas Bueno Rodrigo *SIT-254*
Duran Ledezma Angel Adalberto *LPM-264*
Duran Ledezma Angel Adalberto *LPM-44*
Dutt Ateet *RWE-241*
E. Solis Omar *LPM-44*
Echartea Reyes Olga Alondra *LPM-248*
Edgar Briones *NSN-196*
Elías Espinosa Milton Carlos *SIT-140*
Elizalde Galindo José Trinidad *MUL-186, MUL-213*
Elsie Araujo *NSN-196*
Enrichi Francesco *LPM-80*
Escalante Garcia Ismailia L. *RWE-69*
Escalante García Ismailia Leilani *NSN-260*
Escamilla-Alvarado E. *TSM-101*
Escobar Aguilar Manuel *MEM-128*
Escobar Alarcón Luis *PLV-284*
España-Sánchez Beatriz Liliana *RWE-274*
Esparza Diego *LPM-44, LPM-264*
Esparza Rodrigo *RWE-274*
Esparza Alegría Enrique *PLV-284*
Espinosa Ceron Y. *SEM-119*
Espinosa Roa Arián *SEM-33*
Espinosa Vega L.I. *NSN-163, RWE-165, SEM-168*
Espinosa-Almeyda Y. *MUL-63*
Espinosa-Vega Leticia I. *NSN-172, NSN-174, SEM-164, SEM-173, TSM-170*
Espinosa-Vega Leticia I. *NSN-167*
Esquivel Escalante Karen *BIO-136*
Estrada-Ayala Fernando Esteban *RWE-209*
FABIÁNANGUIANO JOSÉARTEMIO *RWE-283*
Falcón Franco Lázaro Abdiel *MEM-54*
Falcony Ciro *LPM-80*
Falcony Guajardo Ciro *LPM-117*
Falcony Guajardo Ciro *LPM-287*
Farías Mario *ALD-4*
Farias Mancilla Jose Rurik *MUL-213, RWE-245*



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Favela Lopez Juan Jazziel *SEM-122*
Favela López Juan Jazziel *SEM-124*
Félix Quintero Héctor Aníbal *MUL-180*
Feregrino Pérez Ana Angélica *BIO-136*
Fernández Benavides David Andres *MEM-128*
Fernando González *NSN-196*
Ferrerira García Maria Guadalupe *MEM-128*
Flores Acosta Mario *NSN-53, THF-41*
Flores Arciniega José Luis *NSN-62*
Flores Arcos Daniel Misael *SIT-98*
Flores Arcos Daniel Misael *SIT-98*
Flores Contreras Ian Carlos *RWE-273*
Flores Hernández Cynthia Graciela *SCD-182, THF-75*
Flores Hernandez Cynthia Graciela *SCD-183*
Flores Hernández Cynthia Graciela *BIO-77*
Flores Martínez Martín *SIT-99*
Flores Medina Dulce Alejandra *MEM-54*
Flores Ramírez Daniel *SEM-89*
Flores Ruiz Francisco Javier *MUL-70*
Flores Ruvalcaba Abbi Azalia *TSM-73*
Flores Urquizo Israel Alejandro *MUL-186*
Flores-González Maribel *BIO-135*
Flores-Ruiz Francisco Javier *NSN-48*
Florez Rios John Fredy *SEM-207*
Fonseca Hernández Gerardo Antonio *BIO-77*
Francisco Javier De Moure Flores *THF-34*
Fu Zhiwei *RWE-286*
Fuentes Moyado Sergio *NSN-28*
Gabriela Pineda Chacon Gabriela *SCD-182*
Galaz Bórquez Francisco Ernesto *SEM-25, SIT-24*
Gallardo-Hernández Salvador *SIT-11*
Gallardo-Hernández Salvador *BIO-257*
Gallegos Espinoza Damián Lorenzo *TSM-73*
Galvan Thaire Valeria *NSN-189*
Gamboa Fidel *TSM-22*
Garate-Velez Lorena *BIO-18*
Garay Tapia Andrés Manuel *SEM-33*
Garay-Cervantes Lilián Andrea *ALD-205*
Garay-Cervantes Lilián Andrea *CHM-68*
Garay-Tapia Andrés M. *SCD-244*



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García Rafael *PLV-13*
GARCIA BORQUEZ ARTURO *NSN-181*
García Bustos Ernesto *SIT-99*
García Bustos Ernesto David *SIT-96, SIT-98*
García Caballero Ariadna Daniela *PLV-83*
García Cerda Luis Alfonso *MEM-54*
García Cruz Miguel Angel *SIT-40*
García Díaz Reyes *TSM-61*
García Díaz Reyes *TSM-46*
García Hernández Sergio Agustín *SIT-256*
García López Karla Berenice *LPM-166*
García Orozco Iván *NSN-261*
García Paredes Felipe de Jesus *MEM-128*
García Ramírez Mario Alberto *BIO-67*
García Ramírez Mario Alberto *CHM-74*
García Rentería Marco Arturo *MEM-54*
GARCIA ROCHA MIGUEL *BIO-121, NSN-181*
García Salgado Godofredo *SEM-114, SIT-110, THF-109*
García Sánchez Mario Fidel *RWE-234, RWE-235*
García Sánchez Mario Fidel *SCD-230*
García Valdivieso Ma. Guadalupe *BIO-133*
García Valdivieso Ma. Guadalupe *BIO-134*
García Vanegas Leopoldo *SIT-140*
García Vázquez Valentín *MUL-70, NSN-78*
García Villarreal Sergio *MEM-54*
García Zaldívar Osmany *MUL-70*
GARCÍA ZALETA DAVID SALVADOR *THF-21*
García-García Alejandra *SCD-244*
García-Gonzalez Leandro *MEM-200, NSN-145*
García-Mejía María Fernanda *SEM-6*
García-Rocha Miguel *LPM-44, LPM-264*
García-Ruiz Diana Litzajaya *NSN-143*
García-Ruiz Diana Litzajaya *NSN-145, NSN-149, NSN-154*
García-Sotelo Alejandra *SEM-239*
García-Vazquez Valentín *NSN-48*
García-Vidal Usiel Omar *NSN-151, NSN-227*
Garduño Medina Adriana *MUL-70*
Garduño Terán Ulises *RWE-235*
Garduño- Wilches Ismael *LPM-162*
Garibay Alvarado Jesus Alberto *BIO-236*



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Garnica Palafox Itzel Marisol *MEM-128*
GARNICA ROMO MA. GUADALUPE *THF-21*
Garnica Romo Ma. Guadalupe *BIO-278, NSN-277, NSN-279*
Godínez García Andres *RWE-171*
Gómez Aguilar Ramón *NSN-93*
Gómez Barojas Estela *NSN-64*
Gómez Barrales Paola Dhamar *MEM-84*
Gomez Barrales Paola Dhamar *THF-75*
Gómez-Rosas G. *SIT-195, SIT-197*
Gomez-Sosa Gustavo *SIT-116, SIT-204*
González Ronquillo Ana Lilia *NSN-78*
Gonzales-Cisneros Alejandro *LPM-264*
Gonzalez Lucy T. *NSN-9*
González Castillo Jesus Roberto *RWE-238*
González Cortés Israel *RWE-92*
González Hernández Jesús *NSN-35*
González Medrano Javier *NSN-48*
Gonzalez Méndez Santiago *MEM-10*
GONZÁLEZ MORALES MIGUEL ÁNGEL *SEM-219*
González Pérez Mario *NSN-190*
González Reynoso Orfil *CHM-74*
González Reynoso Orfil *BIO-67*
Gonzalez Solano Manuel *SEM-60*
González Zavala Fernando *PLV-284*
Gonzalez-A. Edson *NSN-14*
Gonzalez-Cisneros Alejandro *LPM-44*
Granados-Martínez Francisco Gabriel *NSN-143, NSN-145, NSN-149, NSN-154*
Guarneros-Aguilar Cesia *MEM-200*
Guerrero de León Alonso *PLV-198*
Guerrero Lara Graciela *BIO-77*
Guerrero Martínez Grecia Aranzazú *BIO-133*
Guerrero Sanchez Jonathan *TSM-58*
Guerrero-Sánchez Jonathan *TSM-177*
Guillén Cervantes Angel *RWE-19*
Gutiérrez Franco Angélica *LPM-123*
Gutiérrez Franco Angélica *LPM-156*
Gutiérrez Gil Ari Axel *MEM-84*
Gutiérrez Heredia Gerardo *MEM-10*
Gutiérrez-Fuentes Rubén *NSN-148, NSN-150*
Gutiérrez-García Carmen Judith *NSN-145, NSN-149, NSN-154*



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Gutiérrez-García Carmen Judith *NSN-143*
Gutiérrez-Ojeda Sandra Julieta *TSM-178*
Gutiérrez-Ojeda Sandra Julieta *TSM-177*
Guzmán Castañeda Jesús Israel *LPM-185*
Guzmán Cruz Andrés *NSN-270*
Guzmán Silva Tania Maria *THF-152*
Guzman-Bucio Dulce-Maria *SIT-116*
Guzmán-Fuentes Jaime Abraham *NSN-143*
Guzmán-Fuentes Jaime Abraham *NSN-149*
Hamui Leon *RWE-79*
Haro Poniatowski Emmanuel *PLV-284*
Heredia Cancino Jose Antonio *NSN-53*
Heredia Cancino José Antonio *SEM-25, SIT-24*
Hernández Eric-Noe *BIO-94*
Hernandez Acosta Humiko Yahaira *SIT-97*
Hernández Calderón Guadalupe Viviana *RWE-238*
Hernández Calderón Viviana *THF-240*
Hernandez Cocoltzi Gregorio *TSM-46, TSM-159, TSM-228*
Hernández Cocoltzi Gregorio *TSM-178*
Hernández Como Norberto *MEM-54, TSM-73*
Hernández Cruz María Guadalupe *SEM-60*
Hernández De La Cruz Jose Alonso *RWE-245*
Hernández de la Luz Alvaro David *NSN-201*
Hernandez de la Luz J. Alvaro David *SIT-110, THF-109*
Hernández Gaytán L.M. *NSN-163, SEM-168*
Hernández Gaytán L.M. *RWE-165*
Hernández Hernández Jorge *LPM-117*
Hernández López Susana *BIO-262*
Hernandez Marquez Jesus Alfredo *ALD-205*
Hernández Martínez Luis *SCD-242*
Hernández Rodríguez M.F. *SEM-119*
Hernández Rodríguez Yazmin Mariela *NSN-106*
Hernandez Simon Zaira Jocelyn *SIT-110*
Hernandez Simon Zaira Jocelyn *THF-109*
Hernandez-Arcique Aaron *RWE-209*
Hernandez-Como Norberto *MEM-263*
Hernández-Cristóbal Orlando *NSN-145, NSN-149*
Hernandez-de la Cruz Jose Alonso *RWE-66*
Hernández-Elizarrarás Erika *NSN-199*
Hernández-Gallegos Dalia Jazmin *SIT-195*



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Hernández-Hernández Arturo *SEM-239*
Hernández-López Susana *THF-158*
Hernandez-Marquez Jesus Alfredo *RWE-66*
Hernández-Rodríguez E. *SIT-155*
Hernández-Rodríguez Eric Noé *RWE-87*
Herrera Gomez Alberto *CHM-142, SIT-129*
Herrera Pérez Jose Luis *SEM-89, SEM-219*
Herrera-Gomez Alberto *SIT-116, SIT-204*
Herrera-Gomez Alberto *CHM-125*
Herrera-Perez J.L *SEM-57*
Herrera-Pérez José Luis *NSN-137*
Hidrogo Rico Mario Alberto *ALD-268*
Hidrogo-Rico Mario Alberto *RWE-66*
Higuera Mendoza Edgar Alfonso *RWE-47*
Huerta Ávila Héctor *NSN-37*
Huerta Flores Ali Margot *NSN-120*
Hughes Gregory *ALD-205*
Huguenin López E. *RWE-165, SEM-168*
Huguenin López E. *NSN-163*
Huipe Domratcheva Ernesto *TSM-176*
Ignacio-De la Cruz Juan Luis *NSN-154*
Ignacio-De la Cruz Juan Luis *NSN-145*
Iturrios Maria Isabel *TSM-194*
Iturrios Santos M. Isabel *TSM-59*
Jaime-Fonseca Mónica Rosalía *BIO-20*
Jáuregui Rosas Segundo Rosalí *MUL-180*
Jiménez Elías Oscar Daniel *NSN-260*
Jimenez Flores Yolanda *BIO-77, MEM-84, SCD-183, THF-75*
Jimenez Flores Yolanda *SCD-182*
Jiménez Olarte Daniel *RWE-238*
Jiménez Pérez Joel *CHM-225*
Jiménez Pérez José Luis *NSN-150*
Jiménez Pérez José Luis *CHM-225*
Jiménez-Pérez José Luis *NSN-148, NSN-151*
Jiménez-Pérez José Luis *NSN-227*
Juárez Pinedo Lucero *THF-139*
Juárez-Torres José Ángel *BIO-135*
Juárez-Torres José Ángel *NSN-137*
Kharisov Boris I. *NSN-9*
Kharissova Oxana V. *NSN-9*



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Kharissova Oxana Vasilievna *SIT-90*
Koffroth Cárdenas Clark *PLV-193*
Koffroth Cardenas Clark *SIT-126*
Kolli Chandra Sekhar Reddy *SEM-105*
Kolosovas-Machuca Samuel E. *NSN-167*
Kudriavtsev Yuriy *NSN-253*
Kumar Krishnan Siva *NSN-270*
Landín Ramón Ochoa *SEM-25*
Lara Javier *PLV-13*
Lara Alfaro Héctor Francisco *THF-175*
Leal Tania *NSN-132*
Leal Zayas Julio Cesar *MUL-72*
Lefranc Cabrera Joaquin *THF-75*
León Cruz Carlos *SIT-99*
León Silva Ulises *SIT-30*
Leovigildo Lozada Rosendo *LPM-166*
Leyva Elisa *NSN-76*
Licea Jimenez Liliana *CHM-49, CHM-50, RWE-43, RWE-47*
Licea Jiménez Liliana *NSN-285*
Licona Ibarra R. *SEM-119*
Loeza-Poot Mariely Isabel *RWE-87*
Longoria Rodríguez Francisco E. *NSN-9*
Lopez Javier *ALD-4, MUL-3*
López Alejandro Edicson Macedonio *SEM-60*
López Álvarez Miguel Angel *CHM-74*
López Guemez Antonia del Rocío *THF-141*
López Hernández Juan *SEM-258*
López López Máximo *NSN-220, NSN-253, SEM-122, SEM-124*
López Luna Edgar *NSN-189, SIT-256, THF-139*
Lopez Mena Edgar Rene *NSN-120*
López Perrusquia Noé *SIT-96, SIT-97, SIT-98, SIT-99*
López Perrusquia Noé *SIT-140*
LOPEZ PERRUSQUIA NOE *SIT-127*
López Picazo Pedro Iván *NSN-37*
Lopez Picazo Pedro Ivan *RWE-45*
LÓPEZ RODRÍGUEZ ANGÉLICA SILVESTRE *THF-21*
López-Bueno G. *TSM-101*
López-Cárdenas Patricia Guadalupe *NSN-191*
López-Cárdenas Patricia Guadalupe *NSN-130*
Lopez-Castillo Miguel *MEM-263*



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López-Castro Carlos Gerardo *NSN-227*
López-Gamboa Genaro *NSN-148*
López-Huerta Francisco *MEM-200*
López-López Máximo *NSN-211*
López-Lopez Máximo *NSN-102*
Lozada Morales R. *SEM-119*
Lozada Morales Rosendo *LPM-123*
Lozada Morales Rosendo L. *LPM-157*
Lozada Morales Rosendo Leovigildo *LPM-156*
Lozano Rojas Ivonne Berenice *LPM-185*
Lucio Hernández Daniel Alejandro *THF-160*
Luna López José Alberto *NSN-64*
Luna López José Alberto *SIT-110, THF-109*
Luna-García A. *TSM-101*
Luna-Sánchez José Luis *NSN-150*
Lunagómez Rocha María Antonia *THF-141*
Machorro Roberto *THF-85*
Machorro Roberto *CHM-88*
Machorro Mejía Roberto *CHM-91*
Machorro Mejía Roberto *CHM-272*
Machorro-Mejía Roberto *PLV-86*
Maldonado Cortez Demofilo *SIT-90*
Maldonado Onofre Daniel *SIT-99*
Mani González Pierre Giovanni *MUL-213, RWE-245*
Mani Gonzalez Pierre Giovanni *ALD-205, TSM-73*
Mani-Gonzalez Pierre Giovanni *CHM-68, RWE-66*
Manuel Rivas Jesus *LPM-44*
Marcelino-Pérez Gabriel *BIO-257*
Marin-Perez Jhonatan *THF-118*
Marquez Heriberto *ALD-4*
Márquez-Herrera A. *SIT-155*
Martin Andrea *LPM-162*
Martín Medina Irma *TSM-179*
Martines Cervantes Rubí *SIT-40*
Martínez Arturo *TSM-17*
Martínez Angeles Wendy Liliana *CHM-74*
Martínez Barra Alexis *BIO-136*
Martínez Flores Héctor Eduardo *BIO-278*
Martínez Gómez Álvaro de Jesús *BIO-67*
Martínez González Joel *NSN-261*



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Martínez Guerra Eduardo *THF-160*
Martínez Guerra Eduardo *ALD-268*
Martínez Juárez Javier *NSN-201*
Martínez Landeros Víctor Hugo *MEM-54*
MARTÍNEZ PACHECO CLAUDIO *THF-21*
Martínez Pérez Lilia *THF-65*
Martínez Puente Marcelo *ALD-268*
Martínez-Escobedo Verónica Nayelli *SEM-275*
Martinez-Guerra Eduardo *MEM-263*
Martinez-Landeros Victor Hugo *RWE-66*
Martinez-Lopez Angel Leonardo *SEM-57*
Martínez-Olguín Aracely Del Carmen *TSM-159*
Martínez-Orozco J. C. *RWE-69*
Martinez-Torres Pablo *CHM-210*
Matamoros Ambrocio Mayra *NSN-64*
Matías-Reyes A.E. *NSN-259*
Mayén Sandra *PLV-81, PLV-82*
Mayén Hernández Sandra Andrea *PLV-83*
Mayén-Hernández Sandra *THF-202*
Mayorga-Garay Marisol *SIT-204*
Medina Esquivel Ruben Arturo *CHM-210*
Medina Muñoz Wendy Eridani *RWE-282*
Medina-Esquivel R.A. *TSM-208*
Medina-Esquivel Ruben Arturo *RWE-209*
Mejía Silva Israel *MEM-128*
Mejía Uriarte Elsi Violeta *MUL-180*
Melendez-Lira Miguel *SEM-239*
Melendez-Lira* Miguel *SCD-237*
Melo Máximo Dulce *SIT-98*
Melo Máximo Lizbeth *SIT-98*
Méndez Francisco *NSN-143*
Méndez García V.H. *NSN-163, RWE-165, SEM-168*
Méndez López Arturo *THF-152*
Méndez Resendiz Abraham *CHM-49, CHM-50, RWE-43*
Méndez Rojas Miguel Ángel *RWE-32*
Méndez-Camacho Reyna *TSM-169*
Méndez-Camacho Reyna *NSN-212*
Méndez-Garcia Victor H. *NSN-167*
Méndez-Garcia Victor H. *NSN-172, NSN-174, SEM-164, SEM-173, TSM-170*
Méndez-García Víctor Hugo *RWE-69*



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MENDEZ-GONZALEZ M. M. *BIO-121, NSN-181*
Méndez-Hernández Julet Marcela *RWE-87*
Méndez-Rojas Miguel Ángel *NSN-103*
Mendivil Palma Maria Isabel *ALD-268*
Mendivil-Palma María *MEM-263*
Mendoza David *NSN-115*
MENDOZA ÁLVAREZ JULIO GREGORIO *SEM-89, SEM-219*
Mendoza Conde Gabriel Omar *SIT-110*
Mendoza-Alvarez J.G. *SEM-57*
Meraz Dávila Susana *BIO-136*
Meraz Dávila Susana *BIO-136*
Mercado Ornelas C.A. *NSN-163, RWE-165, SEM-168*
Mercado-Ornelas Christian A. *NSN-167, NSN-174, SEM-164, SEM-173, TSM-170*
Mercado-Ornelas Christian A. *NSN-172*
Mesa Rocha A. N. *SEM-119*
Meza Arroyo Javier *MEM-26*
Meza Ramírez Elder A. *SIT-146*
Meza Rocha Abraham N. *LPM-157*
Meza Rocha Abraham Nehemías *LPM-123*
Mijangos Zúñiga Gabriela E. *RWE-282*
Mijangos Zúñiga Gabriela Elizabeth *RWE-229*
MIMILA ARROYO JAIME *LPM-16, RWE-95*
Miranda Álvaro *NSN-132, NSN-190*
Miranda Álvaro *TSM-192, TSM-194*
Miranda Cid Alejandro *SIT-97*
Miranda Duran Álvaro *TSM-59*
Molina-Mil Trinidad *SEM-6*
Mondaca Felipe *TSM-17*
Monfil Leyva Karim *SIT-110, THF-109*
Montalvo-Urquizo Jonathan *SCD-222*
Montero del Aguila Victor *MUL-180*
Montes Regina *BIO-94*
MONTIEL GONZÁLEZ ZEUZ *SCD-221*
Montiel-González Zeuz *SCD-244*
Monzón Hernández David *MEM-128*
Mora Mora Zaira *NSN-279*
Mora-Herrera David *RWE-269*
Morales Pedro *NSN-132*
Morales de la Garza Leonardo *TSM-178*
Morales Jáquez Sonia Arlyn *MUL-213*



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Morales Méndez José Guadalupe *PLV-284*
Morales Rodriguez Hector Daniel *TSM-2*
Morales Sánchez Alfredo *RWE-32*
Morán Lázaro Juan Pablo *SEM-207*
Moran Tellez Alfonso Angel *RWE-47*
Moreno Salomón *PLV-82*
Moreno Armenta María Guadalupe *TSM-177*
Moreno Banda José Antonio *NSN-190*
Moreno Hernandez Juan Carlos *TSM-228*
Moreno Saavedra Victoria *NSN-55*
Moreno Téllez Carlos Mauricio *SIT-254*
Moreno- Rocha José Manuel *NSN-227*
Moreno-Cabrera N. E. *NSN-259*
Mota González María de la Luz *LPM-288*
Muhl Stephen *PLV-86, THF-85*
Mullins Charles Buddie *RWE-56*
Muñoz Franklin *MUL-3*
Muñoz Aguirre Narcizo *NSN-5*
Muñoz Aguirre Narcizo *THF-65*
Muñoz Hernández Germán Ardul *NSN-201*
Nakamura Jun *TSM-59*
Nava Lara Maria del Rocio *NSN-131*
Navarrete-Meza Zulema *NSN-227*
Navarro Chávez Oracio *TSM-176*
Navarro Contreras Hugo R. *NSN-144, NSN-153*
Navarro Contreras Hugo Ricardo *BIO-133, BIO-134, NSN-147*
Nedev Nicola *MEM-263*
Negrete-Martínez Cynthia I *SIT-204*
Nicho Díaz María Elena *SIT-30*
Nicolás Marín Miriam Marmara *RWE-249*
Niño González Carlos E. *NSN-144*
Noheda Beatriz *MEM-42*
Nuñez Murguía Yhoset Ricardo *SIT-96*
O'Connor Robert *CHM-68*
Ochoa Valiente Raúl *TSM-46*
Ojeda Galván Hiram Joazet *SEM-187*
Ojeda Galván Joazet Hiram *NSN-62*
Olaya Jhon *CHM-217, THF-214*
Olaya Florez Jhon Jairo *SIT-254*
Olaya Florez Jhon Jairo *THF-215, THF-216*



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Oliva González Cesar M. *NSN-9*
Oliver Alicia *SCD-244*
Olmos Domínguez Victor Hugo *SIT-140*
Olvera Rafael *RWE-19*
Olvera-Amador Ma. de la Luz *THF-202*
Olvera-Enriquez José P. *NSN-172, SEM-173*
Olvera-Enriquez José P. *TSM-170*
Ornelas Cruz Iván de Jesús *RWE-92*
Orozco Durán Gabriela Esmeralda *NSN-5*
Orozco Hernández Giovany *SIT-254*
Ortega Cervantez Gerardo *NSN-93*
Ortega-Varela Luis Fernando *NSN-143*
Ortiz Beas Juan Pedro *NSN-120*
ORTIZ LANDEROS JOSÉ *RWE-283*
Ortiz Landeros José *RWE-267*
Ortiz López Jaime *NSN-93*
Ortuño Lopez Monica Balvanera *BIO-77, SCD-183*
Ortuño López Mónica Balvanera *MEM-84, SCD-182, THF-75*
Osorio-de la Rosa Edith *MEM-200*
Otero J. A. *MUL-63*
Oviedo Roa Raúl *RWE-92*
O' Connor Robert *ALD-205*
Pacio Castillo Mauricio *RWE-32*
Pal Mou *RWE-269*
Pal Mou *NSN-270, RWE-271*
Pal Umapada *NSN-270*
Palacios-Hernández Daniel *SEM-6*
Panecatí Bernal Yesmin *RWE-32*
Paraguay-Delgado Francisco *NSN-270*
Paredes Rubio Gabriel Romero *NSN-106*
PatiñoCarachure Cristobal *NSN-261*
Pedro Huaman Juan Javier *MUL-180*
Peña Paras Laura *SIT-90*
Peña Sierra Ramón *NSN-106*
Peñuela Cristian-Esneider *BIO-94*
Peñuela-Cruz C.E. *SIT-155*
Perea Parales F.E. *RWE-165*
Perea Parrales F.E. *NSN-163*
Perea-Parrales Felipe E. *NSN-167, NSN-172, SEM-164, SEM-173, TSM-170*
Perea-Parrales Felipe E. *NSN-174*



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Pérez Claudia *PLV-81, PLV-82*
Perez Israel *TSM-22*
Perez Jaime *CHM-217*
Pérez Luis Antonio *TSM-192*
Perez Arrieta Leticia *NSN-189*
Perez Arrieta María Leticia *LPM-161*
Pérez Centeno Armando *SEM-207, SIT-126*
Pérez Garcia Alfonso *CHM-50*
Pérez García Claudia Elena *BIO-136, PLV-83*
Perez Garcia Sergio Alfonso *CHM-49, NSN-285, RWE-43, RWE-47*
Pérez Hernandez German *SEM-52, SEM-60*
Pérez López Luis Antonio *NSN-131*
Pérez Luna Victor Hugo *BIO-67*
Pérez Mendoza Gerardo Julián *SIT-97*
Pérez Orozco Juan Adrián *MEM-84*
Pérez Rodríguez Felipe *MUL-70*
Pérez Valverde Maritza Iveth *THF-188*
Pérez Vidal Hermicenda *THF-141*
Pérez-Centeno A. *PLV-193*
Pérez-Rodríguez Felipe *NSN-48*
Pérez Arrieta María Leticia *THF-139*
Piamba Oscar *CHM-217, THF-214*
Piamba Tulcan Oscar Edwin *THF-215*
Pilo González Jorge *RWE-92*
Pineda Chacon Gabriela *BIO-77, THF-75*
Pineda Chacon Gabriela *SCD-183*
Pineda Sapuyes Jose Miguel *THF-215*
Pinna Nicola *LPM-162*
Poiré-De la Cruz David Ricardo *NSN-145*
Poiré-De la Cruz David Ricardo *NSN-154*
Polito Lucas Jorge Alberto *NSN-78*
Ponce Pérez Rodrigo *TSM-159, TSM-228*
Ponce-Pérez Rodrigo *TSM-177*
Prieto Novoa Gina *THF-214*
Prieto Novoa Gina Milena *THF-215*
Puch Ceballos Felipe Román *THF-139*
Puente-López Edgar *RWE-271*
Quiñones José *PLV-81, PLV-82*
Quiñones Galván J.G. *SIT-146*
Quiñones Galván José *PLV-198*



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Quiñones Galván José Guadalupe *RWE-19, SEM-207*
Quiñones Galván José Guadalupe *SIT-126*
Quiñones-Galván J.G. *NSN-199, PLV-193, SIT-195, SIT-197*
Quiñones-Galván José *THF-202*
Quiñones-Galván José G. *PLV-138*
Quintana Mildred *NSN-76*
Quintana Mildred *NSN-76*
Quintana Ruíz Mildred *NSN-55, NSN-62, SEM-187*
Quintana-Ruiz Mildred *BIO-18*
Raboño Borbolla Joaquin *SIT-129*
Raboño-Borbolla Joaquín G *SIT-204*
Rafael Ramirez Bon *SEM-105*
Ramírez Bon Rafael *SEM-31, THF-41*
Ramirez Bon Rafael *MEM-111*
Ramirez lopez M. *SEM-57*
RAMÍREZ LÓPEZ MANOLO *SEM-89, SEM-219*
Ramírez López Manolo *LPM-218, NSN-220*
Ramirez Meda Walter *NSN-120*
RAMIREZ MORALES ERIK *SEM-52, SEM-60*
Ramírez Velasco Sergio *THF-240*
Ramírez Velasco Sergio *RWE-238*
Ramírez-Bon Rafael *RWE-36*
Ramírez-Dámaso G. *TSM-101*
Ramirez-Leda Walter *THF-118*
Ramírez-Núñez A. L. *NSN-259*
Ramos Antonio *PLV-13*
Ramos Armando *PLV-13*
Ramos Carlos *RWE-241*
Ramos Carrazco Antonio *MEM-10*
Ramos Vilchis Carlos David *RWE-246*
Rangel Ricardo *NSN-14, PLV-13, THF-15*
Rangel Cobian Victor *NSN-120*
Raya Colín José Antonio *RWE-267*
Rebollo Jacqueline *NSN-132, TSM-192*
Regalado-de la Rosa Jorge L. *SEM-164*
Reséndiz Mendoza Luis Martín *RWE-273*
Reyes Chaparro Gabriela Mariela *RWE-234*
Reyes Contreras Delfino *NSN-261*
Reyes López Simón Yobanny *MUL-213*
Reyes López Simón Yobanny *BIO-233, BIO-236*



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Reyes Montero Armando *MUL-280*
Reyes-Esqueda Jorge Alejandro *THF-158*
Reyes-López Simón Yobanny *BIO-231, NSN-232*
Rickards Jorge *SIT-40*
Righini Giancarlo *LPM-80*
Rincón Joya Miryam *NSN-29*
Rincón Joya Miryam *NSN-27*
RIOS PIMENTEL FERNANDO FRANCISCO *BIO-121*
Rivadeneira Gutiérrez Gabriela *TSM-184*
Rivas Jesús Manuel *LPM-264*
Rivera Carlos *PLV-138*
Rivera L. P. *PLV-198*
Rivera L.P. *PLV-193*
Rivera Armenta Jose Luis *BIO-77*
Rivera López Jesús Eduardo *NSN-5*
Rivera Rios Lorena *ALD-205, RWE-245*
Rivera Tello César Daniel *PLV-198*
Rivera-Rios Lorena *RWE-66*
Rivera-Rodríguez Carlos *PLV-104*
Rivero Cruz Omar Ignacio *BIO-136*
Roa-Velazquez Daniela *BIO-257*
Robles Águila Maria Josefina *NSN-201*
Rocha Rangel Enrique *SEM-258*
Rodríguez Bibiana *LPM-288*
Rodríguez Karen *PLV-82*
Rodríguez Karen *PLV-81*
Rodríguez Barraza Laura Elena *NSN-53, SIT-24*
Rodríguez del Ángel Jimena *MEM-42*
Rodríguez Fernández Luis *SIT-40*
RODRÍGUEZ FRAGOSO PATRICIA *SEM-89, SEM-219*
Rodríguez García Bibiana *LPM-287*
Rodríguez Hernandez Juan Ignacio *TSM-2*
Rodríguez Jiménez Rafael Aurelio *RWE-32*
Rodríguez Lehovec Alejandro *THF-141*
Rodríguez López Ramón *CHM-91*
Rodríguez Reyes Daniel Alberto *LPM-161*
Rodríguez Rosales Karen *PLV-83, RWE-19*
Rodríguez Victoria Angel Pedro *NSN-201*
Rodríguez-Fragoso P *SEM-57*
Rodríguez-Hernandez Paola *THF-202*



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Rodríguez-López Jorge *THF-15*
Rodríguez-López Ramon *CHM-88*
Rodríguez-Ramos R. *MUL-63*
Rodriguez-Santos Karla Y. *SEM-164*
Rodriguez-Santos Karla Y. *NSN-167*
Rojas Blanco Lizeth *SEM-52, SEM-60*
Rójas-Hernández E. *TSM-101*
Román López Jesús *LPM-185*
Romano Trujillo Roman *SEM-114*
Romero de la Cruz María Teresa *TSM-46, TSM-61*
Romero de la Cruz Maria Teresa *TSM-58*
Romero Ibarra Issis Claudette *RWE-113, RWE-229*
Romero Lopez Anabel *RWE-32*
Romero Romo William *LPM-157*
Romero-Ibarra Issis C, *RWE-282*
Romero-Ibarra Issis Claudette Romero *SCD-226*
Rosas Reyna César Artemio *THF-65*
Rosendo Andrés Enrique *SEM-114*
Rubio Padrón Miguel Angel *NSN-247*
Rubio Rosas E. *SEM-119*
Rubio-Pereda Pamela *TSM-178*
Rubio-Ponce* Alberto *SEM-239*
Ruelas-Lepe Ruben *THF-118*
Ruiz Luna Haidee *NSN-260, RWE-171*
Ruiz Ramirez Luis Roberto *BIO-233*
Ruiz-Medrano Roberto *BIO-257*
Ruvalcaba Manzo Sayra Guadalupe *THF-41*
Sabina F. J. *MUL-63*
Salazar Fernando *TSM-192, TSM-194*
Salazar Posadas Fernando *NSN-132, NSN-190, TSM-59*
Salazar Posadas Fernando *NSN-131*
Salcido Vall Oscar Rene *NSN-53*
Salcido Valle Oscar René *SEM-25, SIT-24*
Saldaña Jiménez José Antonio *MUL-180*
Saldaña-Robles A. *SIT-155*
Samanamud Moreno Fanny Valentina *MUL-180*
Sánchez Fraga Rodolfo *TSM-73*
Sánchez González Yudania *THF-240*
Sánchez Huitron David *SIT-96*
SANCHEZ HUITRON DAVID *SIT-127*



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Sanchez Martinez Araceli *NSN-120*
Sánchez Mora Enrique *NSN-64*
Sánchez Tizapa Marciano *RWE-45*
Sanchez Tizapa Marciano *NSN-37*
Sánchez- Alarcón Raúl Ivan *LPM-162*
Sánchez-Dena Oswaldo *THF-158*
Sanchez-Martinez Araceli *THF-118*
Sánchez-Martinez Elihu Hazel *NSN-211*
Sánchez-Ramírez José Francisco *BIO-135, LPM-251, NSN-137, NSN-150, NSN-151, NSN-252*
Sánchez-Torres Juan Diego *NSN-130*
Sánchez-Valdés C. F. *MUL-63*
Sánchez-Yáñez Juan Manuel *NSN-145*
Sang Inés Roberto *CHM-88, THF-85*
Sang Inés Roberto *PLV-86*
Sang Inés de Castro Roberto *CHM-91, CHM-272*
Santana Guillermo *RWE-235*
Santana Guillermo *RWE-241*
Santana José Eduardo *TSM-192, TSM-194*
Santana Aranda Miguel Ángel *SEM-207*
Santana Rodríguez Guillermo *RWE-246*
Santana-Aranda M.A. *PLV-193*
Santillán Pacheco Mauricio Gabriel *MEM-84*
Santos José *PLV-81, PLV-82*
Santos Cruz José *PLV-83, RWE-19*
Santos-Curz José *THF-202*
Santoyo Jaime *NSN-112*
Santoyo-Salazar J. *NSN-259*
Sastré-Hernández Jorge *SEM-6*
Secundino-Sánchez Orlando *NSN-150*
Secundino-Sánchez Oscar *LPM-251, NSN-252*
Segura Sosa Juan *TSM-61*
Serrano Fernando Adán *TSM-192*
Serrano Quezada Thelma E. *NSN-9*
SERVIN DE DIOS FANNY *SEM-52*
Sigala Valdez Jesus O. *RWE-69*
Silva Vidaurri Luis Gerardo *NSN-285*
Silva-Holguin Pamela Nair *BIO-231*
Simakov Andrey *NSN-144, NSN-153*
Smolentseva Elena *NSN-147, NSN-153*
Snelgrove Matthew *ALD-205, CHM-68*



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Solís Alfredo *NSN-14*
Solis Omar E. *LPM-264*
Solis-Sanchez Luis Octavio *RWE-69*
Solorio-Grajeda Daniela *NSN-232*
Soriano Romero Omar *LPM-123, LPM-157*
Sosa Akari Narayama *TSM-192, TSM-194*
Sosa Victor *TSM-22*
Sosa Sanchez Jose Luis *SCD-108*
Soto Gerardo *MUL-3*
Soto Cruz Blanca Susana *SCD-108*
SOTO-PUEBLA DIEGO *CHM-265*
Soto-Valle Genaro *THF-85*
Sprick Sebastian *RWE-286*
Takeuchi Noboru *TSM-228*
Talamás-Rohana Patricia *SIT-11*
Tamayo Meza Pedro A. *NSN-5*
Tapia J. A. *NSN-203*
Tapia J.A. *TSM-206, TSM-208*
Tapia González Jorge *TSM-179, TSM-184*
Tapia Gonzalez Jorge Alejandro *CHM-210, RWE-209*
Tenopala Perlata Jorge Eduardo *LPM-185*
Tiznado Hugo *ALD-4, MUL-3*
Toledo-Guizar Pablo *MEM-263*
Torres Guerra Leticia Myriam *THF-160*
Torres Ochoa Jorge Alejandro *CHM-142*
Torres Ochoa Jorge-Alejandro *SIT-129*
Torres Rosales Ángel Andrés *THF-175*
Torres Rosales Ángel Andres *SEM-187*
Torres-Ochoa Alejandro *SIT-204*
Torres-Ochoa Jorge-Alejandro *SIT-116*
Torres-Sánchez Juan Diego *NSN-191*
Torres-Torres Carlos *SCD-244*
Torres-Torres David *SCD-244*
Torres-Torres Jesús-Alejandro *SCD-244*
Tostado Plascencia Miriam Marcela *NSN-37, RWE-45*
Tovar Sifuentes Estefany *SIT-90*
Trejo Baños Alejandro *NSN-131, NSN-190, RWE-92*
Trejo Luna Rebeca *SIT-40*
Urbina Vázquez Veronica Jazmin *BIO-134*
Valdez Benjamin *MEM-263*



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Valdez Torija Eduardo Alejandro *SEM-114*
Valdez-Perez Donato *NSN-174*
Vales-Pinzon Caridad *RWE-209*
Vales-Pinzon Caridad *CHM-210*
Vallejo Bastidas Fabio Fernando *THF-216*
Valverde Alva Miguel Ángel *MUL-180*
VARGAS ARANA CONAN *MUL-71*
Vargas Ortiz Ramón Álvaro *MUL-72*
VARGAS ORTIZ RAMON ALVARO *MUL-71*
Vazquez Jorge *ALD-4*
Vázquez Barragán Nicolás Enrique *RWE-19*
Vázquez Delgado Marco Antonio *MUL-70*
Vázquez Escudero Agustín *NSN-261*
Vazquez Vazquez Eric Fernando *RWE-113*
Vázquez-Cuchillo Odilón *NSN-252*
Vega Becerra Oscar Edgardo *CHM-50*
Vega Becerra Oscar Eduardo *RWE-43*
Vega-Jiménez K. A. *TSM-101*
Vega-Loyo L. *NSN-259*
VELÁZQUEZ VÁZQUEZ MARÍA DE JESÚS *SIT-8*
Verduzco-López Yadira *RWE-241*
Vidal Borbolla Miguel Ángel *SIT-256, THF-188*
Vigil Galán Osvaldo *RWE-238, RWE-249, THF-240*
Vigueras Santiago Enrique *BIO-262, NSN-261*
Vigueras-Santiago Enrique *THF-158*
VILLA MARTÍNEZ GERARDO *LPM-218, NSN-220, SEM-89, SEM-219*
Villa-Martinez G *SEM-57*
Villanueva Cab Julio *RWE-32*
Villarreal Faz M. *NSN-163, RWE-165*
Villarreal Faz M. *SEM-168*
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VillicañaMéndez Maricela *NSN-277*
Vorobiev Pavel *RWE-36, SEM-31*
Vorobiev Pavel *RWE-47*
Vorobiev Yuri *RWE-36, SEM-31*
Vorobiov Yurii *RWE-47*
Wang Xiaoyan *RWE-286*
Willars Rodriguez Francisco Javier *SEM-31*
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Woicik Joseph *ALD-205*
Woo-Garcia Rosa *MEM-200*
Xoconostle-Cázares Beatriz *BIO-257*
Yadav Pravind *ALD-205*
Yáñez Soto Bernardo *NSN-62*
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Yee Rendon Cristo M. *NSN-189*
Yee Rendón Cristo Manuel *NSN-253, SEM-122, SEM-124*
Yee-Rendon Cristo M. *NSN-172, NSN-174*
Yee-Rendón Cristo Manuel *NSN-211*
Zambrano-Arjona M.A. *TSM-206*
Zambrano-Arjona Miguel Angel *CHM-210, RWE-209*
Zamora Barrera Karen *LPM-218, NSN-220*
Zamora-Peredo Luis *NSN-154*
ZAMUDIO TORRES ILDEFONSO *SEM-52*
Zapata Diego *NSN-76*
Zavaleta Espejo Gina Genara *MUL-180*
Zayas Ma. E. *SEM-119*
ZEIFERT BEATRIZ *RWE-283*
Zelaya Orlando *NSN-112*
Zepeda Trino *NSN-14*
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