BOOK OF ABSTRACTS

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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 an enormous support from all the members of the SMCTSM which made the XV-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 XV ICSMV

Organizing Committee SMCTSM

September 2022

PLENARY TALKS

Matteo Cargnello, PhD

Stanford University, Stanford, CA

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Eduard Llobet, PhD

Universitat Rovira i Virgili, (URV) Spain

Gas sensing properties of CVD grown tungsten oxide nanowire films

Eden Morales-Narváez, PhD

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Nanophotonic materials for (bio)sensing

Elías Pérez, PhD

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Karim Sapag, PhD

Universidad Nacional de San Luis, San Luis, Argentina

Adsorption and Nanoporous Materials for Energy, Environment and Health Applications

M. Laura Soriano, PhD

Universidad de Córdoba, Spain

Format of carbon based nanodots in sensing matters

Thomas J. Webster, PhD

Hebei University of Technology, China, Vellore Institute of Technology, India

25 Years of Commercializing Nanomedicine: From Tissue Engineering to Fighting COVID-19

MATTEO CARGNELLO, PhD

BIO

Matteo Cargnello received his Ph.D. in Nanotechnology in 2012 at the University of Trieste, Italy, under the supervision of Prof. Paolo Fornasiero, and he was then a post-doctoral scholar in the Chemistry Department at the University of Pennsylvania with Prof. Christopher B. Murray before joining the Faculty at Stanford University in January 2015. He is currently Assistant Professor of Chemical Engineering and, by courtesy, of Materials Science and Engineering and Terman Faculty Fellow. Dr. Cargnello is the recipient of several awards including the Sloan Fellowship in 2018, the Mitsui Chemicals Catalysis Science Award for Creative Work in 2020, and the Early Career Award in Catalysis from the ACS Catalysis Division in 2022. General goals of the research in the Cargnello group pertain to solving energy and environmental challenges. Uniform and tailored nanocrystals and nanostructures are synthesized, studied and used for energy and environmental applications through catalytic processes, with emphasis on how to precisely control their structure to understand and exploit interactions between well-defined building blocks.

Understanding and Engineering Catalytic Materials Using Nanocrystal Precursors

Catalytic processes are central to the goal of a sustainable future. A promising approach in developing catalytic materials is represented by the design of catalytic sites based on the knowledge of structure-property relationships, and in the precise synthesis of thes sites at the atomic level. Colloidal nanocrystals, with tunable active sites and compositions, can help in this mission. The goal of this talk is to show how this approach can provide not only fundamental understanding of catalytic reactions, but also a way to precisely engineer reaction sites to produce efficient catalysts that are active, stable and selective for several important transformations. Advances in the synthesis of these materials will be presented. Examples of the use of these building blocks as supported systems or in combination with hybrid organic materials will be shown, both to understand trends in methane and CO 2 activation, and in the preparation of optimized catalytic systems combining multiple active phases. In all these examples, important efforts to obtain precious structure-property relationships will be highlighted, with this knowledge used to prepare more efficient and stable catalysts for reducing the emission of greenhouse gases and for the sustainable production of fuels and chemicals.

EDUARD LLOBET, PhD

BIO

IEEE Senior Member, PhD from the UPC-Barcelona Tech (1997). Full Professor of Electronics (2009) at the Universitat Rovira i Virgili in Tarragona (Catalonia, Spain). Distinguished Professor (2019). Group Leader with research interests in nanomaterials (metal oxide nanowires, 2D and 3D transition metal di-chalcogenides, functionalized graphene) and their integration in microsystems for detecting pollutant/hazardous gases at trace levels. From 2010 to 2014 he was the Director of the Centre for Research in Materials Engineering and Micro / Nano Systems (URV) and vice-president of the Spanish IEEE Sensor Chapter. President of the Spanish Network of Microsystems and Nanotechnology (IBERNAM). Co-author of over 250 peer-reviewed journal papers (h = 56), editor of 3 books, has given some 35 invited lectures at international conferences and led over 35 regional, national and international projects. Founder of the spinoff Green Smart Data. In 2012 he received the URV's RQR award and the ICREA Academia award (in 2012 and 2018).

Gas sensing properties of CVD grown tungsten oxide nanowire films

Single crystalline, tungsten oxide nanowires (NWs) loaded with metal oxide nanoparticles (NPs) are very promising for developing a new generation of inexpensive, yet highly sensitive and more stable gas sensors. By supporting p-type metal oxide NPs (e.g. Pd, Cu, Ni, Co or Ir oxides) on n-type metal oxide NWs, both chemical and electronic sensitization effects can be obtained, which can dramatically tune the response to target gases of the resulting hybrid nanomaterials, thus enabling the engineering of selectivity. I will discuss the aerosol-assisted chemical vapour deposition (AACVD) technique, which enables growing single crystalline, n- type metal oxide NWs supporting homogeneously distributed, mono-modal, p-type metal

oxide NPs in a wide range of loading levels. SEM, TEM, XRD, XPS, Raman, ToF-SIMS and PL are used to analyse the morphology, crystalline phase, chemical composition and defects. Their gas sensing properties (response, selectivity and stability) towards different species (e.g., ethanol, ammonia, nitrogen dioxide, hydrogen sulphide will be discussed in detail. In addition, some recent, in-operando, NAPS-XPS results will be shown and the derived gas-sensing mechanisms will be presented.

EDEN MORALES NÁRVAEZ, PhD

BIO

Eden Morales Narváez received a degree in Bionics Engineering from the National Polytechnic Institute (IPN) of Mexico in 2006 and the PhD in Biomedical Engineering from the Polytechnic University of Catalonia (UPC), Spain in 2013. He was a Postdoctoral Researcher at Nanobioelectronics and Biosensors Group (led by Prof. Arben Merkoçi), Catalan, Institute of Nanoscience and Nanotechnology (ICN2), Barcelona Spain. He started his independent career in late 2016 as a Full Research Scientist at Center for Research in Optics (CIO) and head of the Biophotonic Nanosensors Laboratory, León Mexico. His research is focused on the development and application of advanced materials for (bio)sensing, particularly using nano(bio)photonics at the cutting-edge. He is particularly interested in healthcare 4.0, nanotechnology, food analysis, environmental monitoring and green technologies, among other fields. He is a lecturer in Biophotonics and Photonic Materials at CIO. He has edited a book on Wearable Sensors and he is also part of the Editorial Board of several journals, including Biosensors and Bioelectronics X, JPhys Photonics, Green Analytical Chemistry, Biosensors and Frontiers (Nanobiotechnology Section). He has also been awarded as an Emerging Leader 2020 by IOP Publishing.

Nanophotonic materials for (bio)sensing.

Nanophotonic materials and their properties endow researchers and technologists with outstanding tools to develop advantageous (bio)sensing systems and detect a myriad of analytes related to health care, environmental monitoring and safety and security. We will discuss the rationale behind nanophotonic materials in biosensing and I will share with all of you my perspectives on this exciting topic.

ELÍAZ PÉREZ, PhD

BIO

E. Perez is a Physicist by the UAM-I. His PhD studies were on Physico-Chemistry of Macromolecules in the Institute Charles Sadron, France. Two postdoctoral positions followed his formation: in the University of Konstanz, Germany, and INSERM 424 in Strasbourg France. He spent a sabbatical year at the Institute Curie, Paris, France. His current position started in April 2000 attending graduate and undergraduate students in his laboratory. He teaches with the Faculty of Sciences and Chemistry in the UASLP, but also participates in the Material Science Postgraduate Program in the same University.

Dependence of the liquid polarity in the wetting on a rough surface: a effective surface tension approach

Surface wetting is characterized by the liquid (usually water) contact angle on the surface, and it has been the subject of numerous studies for many years, Young's equation (1805) describes many of that phenomenon. However, this equation is no longer valid for rough and inhomogeneous surfaces. Instead, Wenzel (1936) and Cassie–Baxter (1944) have proposed alternative equations that take into account the roughness and inhomogeneity, respectively. In this talk we present an approach based on the equation of state (EQS) that describes very well the wetting of liquids on a rough surface using an effective surface tension, this implicitly contains information about roughness, liquid-surface interaction and inhomogeneities. Indeed, experimental results show that the liquid and surface polarity is an important issue in wetting on rough surfaces. These results shown that low polar liquids show little dependence on roughness of a low polar surface, while the high polar liquids are very sensitive to it. As consequence, the calculated contact angles by EQS and by the surface tension components (STC) were close to experimental values only for high polar liquids, while low polarity liquids differ greatly from them.

KARIM SAPAG, PhD

BIO

Prof. Sapag has a bachelor's degree in Physics from the National University of San Luis (UNSL), Argentina, and a Doctorate in Sciences degree from the Autonomous University of Madrid, Spain. In 2000 he founded the Porous Solids Laboratory (LabSoP) at UNSL and had been its director since. Since 2015 Prof. Sapag has been a Full Professor at the UNSL and PI at the National Council of Research in Argentina (CONICET). His research interests include studying and developing porous solids for different adsorption-based applications. He is the author of nearly 180 publications, where several involving adsorption processes mainly related to improvements in the methods and experiments used to determine textural properties from gas adsorption. In addition, Prof. Sapag delivered courses/tutorials about using gas adsorption as a characterization method in several universities and research centers. His expertise on this topic is widely recognized, mainly in Iberoamerica. He was the organizer of a series of symposia about "Adsorption, Adsorbents, and their applications" in Argentina (SAASA), starting an active network of about 100 researchers interested in Adsorption including researchers from other Ibero-American countries. In Argentina, Prof Sapag will chair the next Iberoamerican Symposium of Adsorption in 2023.

Adsorption and Nanoporous Materials for Energy, Environment and Health Applications

Solid materials with pores up to a few nanometers (nanoporous) are essential in Material Science owing to their diverse applications, mainly in the Energy, Environment, and Health fields. These applications involve surface process as adsorption, taking advantage of the nanoporous materials texture and chemical composition. The texture of a solid refers to its specific surface area, pore volume, and pore size distribution; being gas adsorption the most used process to characterize these properties. However, special care must take when using this technique, which faces specific difficulties mainly associated with the pores' size and surface groups' presence. This lecture will address some aspects of the gas adsorption technique using N2, Ar, and CO2 to characterize nanoporous materials. The selected materials are nanoporous solids: activated carbons, zeolites, carbon nanotubes, ordered mesopores materials, metal- organic-framework, and pillared clays. These materials will apply using adsorption to store H2 and CH4 (Energy) or capture CO2 (Environment) or release drugs (Health), discussing their properties; influence on the performance of the selected application.

MARIA LAURA SORIANO, PhD

BIO

M. Laura Soriano is currently Assistant Professor at the University of Córdoba. She obtained Ph.D. degree in Chemistry at Castilla La-Mancha University in 2007. After two postdoctoral stays at U.K. and Italy, she joined the FQM-215 research group at University of Cordoba funded by a FP7-EU project (INSTANT) developing new methods based on nanotechnology for analytical and pharmaceutical purposes. Up to date, she has directed one research project as IP co-financed by European Commission, and participated in numerous other projects (international, national, and regional ones). During this period, she has supervised two Doctoral Theses with European/international Mentions, three Master's Theses and three Final Degree Projects. Dr. Soriano has a multidisciplinary research profile focused on supramolecular chemistry and nanomaterials by virtue of the publication of an ebook, six book chapters (high-quality editorials), ca. of 50 articles with three front covers (in high impact factor international peer-reviewed journals) in diverse categories of material science, chemistry, and physics. Her research has been fully divulgated through several seminars and oral presentations in congresses along Europe. She participates in innovative teaching projects and other divulgation activities for teaching different aspects of “Nanoscience and Nanotechnology” to public community and introductory students.

Format of carbon based nanodots in sensing matters

A new class of fluorescent, colored, surfactant-free, water-soluble carbon-based nanodots emerged in the last decades as exceptional nanoemmitters owed to their fascinating and tunable optical properties [1]. Amongst them, graphene quantum dots (GQDs) and carbon quantum dots (CQDs) became the most explored in the field of Analytical Nanoscience and Nanotechnology to improve analytical methods at any step of the sample treatment or detection stage.

In this communication we take advantage of the fact that solid, gel and liquid nanoparticle formats affect to their properties and so to their ability to interact with certain (bio)molecules. In this sense, supramolecular interactions of nanoparticles in various media conditioned their applicability when they are dispersed in aqueous or organic media or even in a gel format. In this communication, various lines of research aiming at designing carbon-based nanodots as analytical tools are discussed, focusing on their excellent abilities as sensing probes for detecting (bio)molecules or nanosized structures in different environmental compartments. Regarding GQDs, it is highlighted the use of GQDs in liquid medium for determining specific drugs, GQDs in hydrogels for selective sensing explosives, and GQD aerogels for selective sorption and sensing of pesticides. On the other hand, we will briefly comment the use of GQDs for sensing and elucidating a food-colouring additive when found free or encapsulated into micelles.

THOMAS J. WEBSTER, PhD

BIO

Thomas J. Webster's (H index: 110; Google Scholar) degrees are in chemical engineering from the University of Pittsburgh (B.S., 1995; USA) and in biomedical engineering from RPI (Ph.D., 2000; USA). He has served as a professor at Purdue (2000-2005), Brown (2005-2012), and Northeastern (2012-2021; serving as Chemical Engineering Department Chair from 2012 - 2019) Universities and has formed over a dozen companies who have numerous FDA approved medical products currently improving human health. He has graduated over 200 Ph.D. students and has over 800 publications. Dr. Webster has numerous awards including: 2020, World Top 2% Scientist by Citations (PLOS); 2020, SCOPUS Highly Cited Research (Top 1% Materials Science and Mixed Fields); 2021, Clarivate Top 0.1% Most Influential Researchers (Pharmacology and Toxicology), and is a fellow of over 8 academic societies.

25 Years of Commercializing Nanomedicine: From Tissue Engineering to Fighting COVID-19

While advances in biomaterials have helped the lives of millions over the past century, it is clear that we are at a crossroads for the future of global healthcare. Considering the COVID-19 pandemic, constant struggles with cancer, and an emerging crisis in antibiotic resistant bacteria, to just name a few on-going healthcare problems, we need innovative ideas. Non-medical fields have advanced considerably in new material design, from using sensors to drive cars and touch screen pads for electronics. Innovation in biomaterials has been lagging behind. This presentation will cover some of the more innovative biomaterials than can meet today's challenges including the use of implantable sensors, 4D printed materials in which material shape can be controlled remotely after implantation, smart nanomaterials that can seek out and passivate viruses and bacteria, and so much more. This presentation will also lay the foundation for what is needed for future biomaterial design, especially obtaining regulatory approval for interactive biomaterials. This presentation will cover over 25 years of commercializing nanomaterials from an academic lab to real medical devices currently implanted into humans to aid in health. It will emphasize challenges and promises when trying to translate University based research into real medical products that can aid human health.

ATOMIC LAYER DEPOSITION

CHAIRMEN

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Dr. Pierre Giovanni Mani González: (UACJ),pierre.mani@uacj.mx
Dr. Hugo Tiznado:(CNYN-UNAM), tiznado@cnyn.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.

[ALD-193] Conformal deposition of conductive AZO on 3D-printed ZrO2 microstructures

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The atomic layer deposition of Al-doped ZnO (AZO) is studied over three-dimensional (3D) ZrO_2 microarchitectures printed using two-photon lithography. This work is unique because, for the first time, the deposition of AZO is investigated over complex 3D structures, which are other than polymer-based material. The influence of compound 3D sample morphology, surface roughness, and ZrO_2 crystallographic phase (tetragonal and monoclinic) on the quality and properties of the deposited AZO thin films is studied. Three different Al dopant concentrations (4.0 %, 4.5 %, and 5.0 %) are investigated and compared to undoped ZnO. The electronic properties of grown films are investigated using Hall effect measurements. The AZO witness film preserves low resistivity (ρ) values in the order of 1.1×10^{-3} Ω cm, which is expected to be similar to the AZO located over the 3D printed ZrO_2 structure. The presented results are a step toward dimensionally refined optoelectronic devices, in which the thin AZO films can serve a key enabling role, such as a transparent electrode.

Keywords: atomic layer deposition, transparent conductive oxides, two-photon lithography, thin films, AZO, ZrO_2
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[ALD-341] Deposition of titanium nitride (TiN) films and compatible high-k dielectrics via ALD processes.

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Titanium nitride (TiN) is a material with a Hardness Vickers of 1800-2100 kgf/mm², a superconducting critical temperature of Tc~6 K, an electron mobility for thin films of 5 — 20 cm²/V - s and a resistivity at 25 °C of < 300 μOhm - cm. Also, TiN is one of the highest known KI materials (Kinetic Inductance), which makes it suitable for quantum application junctions.
Then thermal and plasma-assisted processes employing atomic layer deposition (ALD) reactor were used to obtain TiN. Previously, it was performed the deposition via ALD of the insulator layers, i.e. TiO_2 (TDMAT and Oxygen) and MgO (Cp_2Mg and Oxygen or Cp_2Mg and deionized water) over Silicon n-type and SiO_2/Silicon between 80-250 °C, which are necessary to obtain better TiN electrical characteristics. Further, TiN layers were deposited at 300°C using tetrakis-dimethylamino titanium (TDMAT) varying Argon, Nitrogen and Hydrogen fluxes, and applying thermal treatments during the growth of the thin film of TiN, or after the growth process of the TiN film. Structural characterizations were determined by X-ray Diffraction (XRD), whereas morphological and compositional characterization were achieved by Scanning Electron Microscopy (SEM) and Energy Dispersive Spectroscopy (EDS). Finally, to analyze the electrical behavior we trace Current-Voltage curves (I-V). The results showed non stoichiometric layers of TiN with a minimal resistivity value of 5 kOhms.

Keywords: PEALD, ALD, TiN, TDMAT, Cp_2Mg.
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[ALD-231] Effect of Oxygen Source on the Various Properties of NiO Thin Films Deposited by Atomic Layer Deposition

Mario Alberto Hidrogo Rico (mario.hidrogo@cimav.edu.mx) [1] , María Isabel Mendívil Palma [1] , Francisco Servando Aguirre Tostado [1] , Eduardo Martínez Guerra [1]
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Nickel oxide has been widely used as hole transport layer (HTL) in perovskite solar cells (PSC), particularly in P-I-N structures. In terms of fabrication, PSCs with inorganics hole transporting layers are highly promising due to electrical and optical properties. In this study, atomic layer deposition (ALD) of 10 nm NiO films were performed using nickel (II) acetylacetonate ($Ni(acac)_2$) as nickel precursor combined with ozone (O_3) or water (H_2O) as co-reactant at different temperatures of substrates (250°C-300°C) on glass. Where, the growth per cycle (GPC) depends on the substrate and oxidant agent, respectively. At 300°C the GPC is favored using ozone as co-reactant with a GPC of 0.09 /c for all samples. Also, with H_2O as co-reactant, the GPC is lower, around 0.05 /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/Ni 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 NiO films was low (~x10^{-3} cm) for all films. Hall effect confirmed the resistivity of all films. Also, high carrier concentration was ~x$10^{-18}$$cm^{-3}$, and a high mobility (>0.1 $V^{-1}s^{-1}$) from all NiO films synthesized by ALD.

Keywords: Nickel oxide, atomic layer deposition, perovskite solar cells, inorganic hole transport layer.

[ALD-10] HfO2:Y2O3 ultrathin nanolaminate structures grown by ALD: bilayer thickness and annealing temperature effects on optical properties

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Ultrathin nanolaminate structures were prepared by sequential HfO_2:Y_2O_3 (*HY*) bilayer deposition at 250 °C on n-type (100) silicon wafers via thermal atomic layer deposition (ALD) method. Three sets of four samples were prepared, each sample with a total thickness of the nanolaminate of 54.5 ± 0.8 nm. The nominal thicknesses of the *HY* bilayers of the four samples were 0.5:0.5 nm, 1:1 nm, 2:2 nm, and 5:5 nm After the deposition, two of the sets were annealed in N_2 atmosphere for 1 hour at 500 °C and 750 °C, respectively. The third set was used as control samples. The optical behavior of the ultrathin nanolaminate structures was studied as a function of the *HY* bilayer thickness and annealing temperature. The thickness and optical parameters were analyzed via spectroscopic ellipsometry to gain information about the optical constants and bandgap values. An increase of the refractive index was found when the *HY* bilayer thickness decreased from 5:5 nm to 0.5:0.5 nm for both annealing temperatures as well as for the as-deposited sample, while the optical bandgap varied between 3.8 eV and 4.5 eV. The obtained results demonstrate the viability of *HY* ultrathin nanolaminate structures as a dielectric material for application in electronic and/or optoelectronic devices. Furthermore, the optical properties dependence on the bilayer thickness and annealing temperature could offer the possibility to design, fabricate, and improve samples with tunable optical properties at the nanoscale.

Keywords: Ultrathin nanolaminates; tunable optical properties; atomic layer deposition; thermal treatment.
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[ALD-51] ZnO thin films grown at low temperature by PE-ALD for application in electronic devices

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ZnO layers with thicknesses of 20, 40 and 60 nm were deposited by Plasma Enhanced Atomic Layer Deposition (PE-ALD) at 70 °C. Diethylzinc (DEZ) was used as organometallic precursor, O_2 and H_2O as oxidant agents and Ar as a purge gas. The deposition cycle consisted of 100 ms DEZ pulse, 10 s purge time, 6 s of plasma oxidation at 200 W and 10 s purge time. The optical constants and thicknesses of the grown layers were determined by spectroscopic ellipsometry, while the roughness was measured by atomic force microscopy. The average roughness was in the 0.20 – 0.22 nm range for films deposited under different conditions and having different thicknesses. The optical band gap of the films was 3.22 and 3.23 eV for H_2O and O_2 plasma, respectively. A high optical transmission (~90 %) was measured by UV-Vis spectroscopy. X-ray diffraction showed formation of polycrystalline patterns corresponding to (100) and (002) crystal planes. X-ray photoelectron spectroscopy revealed a high purity of the obtained ZnO films, no carbon was detected. The obtained excellent optical, morphological and compositional properties of the deposited films make them a promising candidate for electronic and optoelectronic applications, which require low temperature processes.

Keywords: ZnO, PE-ALD, thin films; low temperature, flexible electronic

Sesión Oral
[ALD-311] ALD for Advanced Logic, Memory, Sensing and Quantum Technologies

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This work resumes some of the most important results that have been obtained in our research group regarding the use of atomic-layer deposition (ALD) as the main thin-film deposition technique for metal oxides with high dielectric constant. ALD is routinely used as the *state-of-the-art* deposition technique for gate oxide development in advanced and deep-submicron FET architectures in all foundries worldwide. At INAOE, ALD has been applied for the development of several integrated electron devices with main application to logic, memory, sensing and quantum technologies and in which ultra-thin metal oxides (Al_2O_3, HfO_2 and TiO_2 with a physical thickness of less than 10nm), are the active part of the final devices under study.

Keywords: atomic-layer deposition, MOSFET, electron devices, high-dielectric constant.

[ALD-342] ATOMIC LAYER DEPOSITION OF TITANIUM DIOXIDE ANATASE-RUTILE PHASES HETEROJUNCTION FOR ENHANCED PHOTOCATALYTIC ACTIVITY

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ALD is a technique which allows the obtention of uniform thin films by using organometallic precursors. Titanium dioxide could be obtained by ALD for a biocompatible material with low toxicological risk. This research area is interest to photocatalysis field, as degrading micro viral agent's using the photogenerated electrons at the heterojunction interface. The heterojunction formed at the interface between anatase and rutile phases, promote the spatial charges separation which led to a rise in the photocatalytic activity. This photocatalytic activity is efficient at a wavelength range in UV-Light. This micro viral agent's degradation offers an alternative to stop the propagation of viruses and the time that this virus remains active in surfaces. This work is concerned with the creation and characterization of titanium dioxide phases heterojunction thin films with a ALD process using tetrakis (dimethyl amido) titanium (TDMAT) as precursor. Thin films of TiO2 were analysed with XRD to shows the characteristic signals of each phase. Electrical and optical characterization by I-V curves and spectrophotometry respectively were performed. XPS characterization also were performed for composition determination.

Keywords: ALD, XPS, Virus, Photocatalysis, thinfilms.
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One reference: N. Bono, F. Ponti, C. Punta, and G. Candiani, "Effect of UV irradiation and TiO2-photocatalysis on airborne bacteria and viruses: An overview," *Materials (Basel).*, vol. 14, no. 5, pp. 1–20, 2021, doi: 10.3390/ma14051075.
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[ALD-156] Effect of film thickness in TiOx slab waveguides prepared by atomic layer deposition

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Abstract: Optical waveguides are the basis for different types of photonic circuits, there are several important factors in the fabrication of these devices, such as the refractive index, roughness, transmittance. Titanium dioxide (TiO_2) was studied due to its high refractive index (>2.2), long-term stability, and commercial inexpensiveness, in the last decade an oxygen deficient with Ti^{3+} ions variant of TiO_2, so-called "Black TiO_2", has been studied. In this project, TiO_x waveguides of 244, 521, 770 and 1000 nm were fabricated by the atomic layer deposition technique. The physicochemical and optical properties of the core was measured by SEM, AFM, XRD, XPS, REELS, UV-Vis Transmittance, Ellipsometry, Impedance spectroscopy, four-point technique. The optical waveguide analysis was carried by prisma coupling technique, calculating the effective refractive index of the guide modes. The propagation losses were measured by the cutback method, obtaining losses of <1 dB/cm. This work is under review, available at SSRN: https://ssrn.com/abstract=4103690 or http://dx.doi.org/10.2139/ssrn.4103690

Keywords: Optical waveguides, atomic layer deposition, TiO_x, Black TiO_2.

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[ALD-195] Titanium nitride as a metallic contact by Atomic Layer Deposition

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Abstract: The improvement of MOS-type field effect transistors has focused on the choice of the gate material. The titanium nitride (TiN) has emerged as possible material with metallic behavior due to high stability and chemical compatibility with the underlying dielectric material. This work shows the synthesis of TiN thin films by ALD to study the effect of deposit parameters and post-synthesis annealing on film resistivity. TiN films were deposited on silicon (111) by atomic layer deposition (ALD) using titanium isopropoxide (TTIP) and ammonium gas (NH_3) as precursors varying the deposited cycles and annealing films under vacuum and ventilating these. The chemical analysis by XPS showed TiN as a surface layer and titanium oxynitride (TiOxNy) as an interface between the substrate and surface layer, which proposed a layer model: CO (adventitious) / TiN / TiOxNy / SiO_2 / Si (111) [2]. The layer model thickness shows that TiN layer increases with deposition number cycles (according ellipsometry thickness measurements as well). The low or high resistivity behavior in TiN films deposited between 25 and 120 cycles are strongly thickness-ratio dependent on the TiN/TiOxNy layers. In addition films presented a temperature dependence during annealing. Based on the analysis the film deposited at 25 cycles showed 5nm thickness and 284 μΩ-cm of resistivity, which suggests a metallic behavior, suitable for MOS-type devices. Ellipsometry analysis by dielectric – extinction coefficient supported a optical metallic tendency.

Keywords: *ALD, elipsometry, TiON, metallic, XPS*
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[ALD-28] TixHfyOz films growth by Atomic Partial Layer Deposition

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An innovative methodology that involves varying the doses of metal precursors that flow into the ALD reaction chamber by varying the pulse time to deposit two or more species in the same atomic layer is called atomic partial layer deposition (APLD) [1]. In this work, we present the methodology for the growth of $Ti_xHf_yO_z$ films by APLD. A series of films that vary Hf pulse times are compared with TiO_2, HfO_2 nanolaminates. Films were deposited on Si (100) wafers at a growth temperature of 250°C with a total of 100 cycles. One cycle consists of a complete oxygen layer, then in the next atomic layer a partial layer of Hf atoms is completed with Ti atoms. The films were obtained, and the thickness, density and roughness were determined by X ray reflectivity (XRR). The thickness varies from 9 to 39 nm. The density of APLD films varies from 7.4 to 4.6 g/cm^3. These values are intermediate values between the densities obtained in HfO_2 and TiO_2 of 9.1 and 4.5 g/cm^3, respectively. With this innovative methodology, it is possible to deposit thin films with two different atoms, in this work Hf and Ti, on the same atomic layer. This opens the possibility of exploring the different characteristics and properties of traditional nanolaminates.

Keywords: ALD-APLD, TixHfyOz films, XRR.
This work was supported by: CONACyT México - 2do año de continuidad de estancias posdoctorales por México modalidad 1 of M. I. Pérez-Valverde CVU 557501
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BIOMATERIALS AND POLYMERS

CHAIRMEN

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The XV International Conference on Surface Materials and Vacuum takes immense pleasure & feel honored in inviting the contributors across the globe to attend in the symposium on Biomaterials and Polymers during September 26-September 30th, 2022 at Puerto Vallarta, Mexico.

Conference will be organized on themes related with: 'Emerging Technologies and Scientific Advancements in polymers and Biomaterials Engineering.

The scientific event offers a best platform with its well organized scientific program to the audience which includes interactive panel discussions, plenary talks, short presentations, short courses, invited sessions and poster sessions on the topics that cover areas of:

- Polymer science,
- Engineering and technologies from the latest innovations in synthesis
- Processing and modeling to the advanced applications of polymers in health
- Advanced Biomaterials
- Biomaterials and Nanotechnology Applications in Biomedicine
- Use in Therapeutic and Investigative Delivery
- Biomaterials in Biological Engineering
- Biodegradable Biomaterials,
- Utility Based Biomaterials
- Energy and sustainability
- Future materials and devices

[BIO-52] Bionanocomposite of chitosan and ZnO and its functionality in the preservation of strawberries.

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The consumption of fresh fruits and vegetables has been associated with many health benefits due to the nutritional importance in human diet. However, their short shelf-life, associated with deterioration rate, is one of the most important issues that should be enhanced [Halonen, et. al., 2020; Ochoa-Velasco et. al., 2014]. Particularly, strawberry is one of the fruits with a very short shelf-life, mainly, because of fungal contamination and due its delicate tissue. Therefore, diminishing the rate of deterioration is one of the most important challenges to guarantee flavour, colour, and nutritional value. In this context, recently has been studied edible coatings to extend the shel-life and quality of fruits and vegetables. Some edible coatings like chitosan possess antimicrobial characteristics [TreviíƒÂ±o-Garza, et. al., 2015; Ziv, et. al., 2021]. The aim of this work was to evaluate the effect of chitosan-ZnO edible coating on the physicochemical, antioxidant, microbiological and sensorial properties of fresh strawberries. Strawberries were submerged into a chitosan-ZnO solution (dissolved in acetic acid) for 4 and 8 seconds. To evaluate the efficacy of the coating, the colour and humidity in coated and uncoauted samples were measured, firstly using only chitosan; where L indicates the bright red, a (chromatid) indicates the intensity in the red colour, and b (chroma) indicates the colour intensity. L values áre higher for coated strawberries. The mumidity at day 1 increased as the immersion time increased; after 10 days of applied the coating, this parameter decreased to 88.1% for 4 and 8 s of immersion. The uncoated strawberry diminished the humidity to 83.5% in the same time; it may be concluded that the coating helps to maintain the fruit freshness, which can be attractive to the consumer. Concerning the appearence, the samples coated with the chitosan solution look less damage at day 10, compared to those that were not coated; it is evident the damage of the uncoated samples, in which fungus has appeared. Experiments where the incorporation of 5% ZnO nanopartices into the chitosan solution are now conducted; results will be presented during the congress. It is expected that parameters like taste, colour and smell will not be affected.

[BIO-109] CELLULOSE EXTRACTION FROM ALOE VERA RIND FOR THE FORMULATION OF BIODEGRADABLE FILMS

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Nowadays, synthetic polymers are used in a massive way in the manufacture of packaging for food products, pharmaceuticals, among others. Howe ver, its excessive use has contributed to the deterioration of the environment. In addition to this, pollution caused by the emission of toxic gases, infertility of the soil and the generation of harmful fauna from the agro-industrial waste of *Aloe vera* has taken interest (Bachheti *et al.,* 2021); Therefore, the objective of this work is to extract cellulose from *Aloe vera* rind for the production of biofilms. The characterization of the biomass was carried out by percentage of humidity, ashes, infrared spectrophotometry (FTIR-ATR), scanning electron microscopy (SEM-EDS) and x-ray diffraction (DRX). Cellulose extraction was carried out by acid hydrolysis with 0.05 N HCl at 70 °C for 2 h, and subsequent delignification by alkaline method with 4% NaOH at 70 °C for 2 h. Subsequently, the extracted cellulose was subjected to a bleaching process with $NaClO_2$ at 80 °C for 8 h, washed with distilled water, filtered and dried. Biofilms were obtained using the solvent evaporation technique. The characterization of the biomass presented 89.54 ± 0.40% humidity and 1.85 ± 0.08% ash, in the FTIR-ATR spectra the characteristic vibrations to cellulose, hemicellulose and lignin molecules were identified, SEM-EDS analysis showed a morphology of irregular scales composed of K in 25.93%, Ca in 25.26% and Mg in 2.98% by mass. The crystalline structure analyzed by DRX gave rise to a diffraction spectrum with signals in 13.13°, 14.02° and 24.20° in 2θ, characteristic of cellulose. A series of biofilms were obtained with a thickness of 50 to 200 microns, homogeneous and free of imperfections.

Keywords: aloe vera, biofilms, biopolymer, cellulose.
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Reference: A. Bachheti, R. K. Bachheti, L. Abate and A. Husen, Current status of Aloe-based nanoparticle fabrication, characterization and their application in some cutting-edge areas, South African Journal of Botany. 147 (2022) 1058-1069. https://doi.org/10.1016/J.SAJB.2021.08.021

[BIO-104] CONTROL OF THE MELT SPINNING TECHNIQUE FOR MEDICAL APPLICATIONS

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The development of biocompatible materials is of great interest in the medical area. A technique that promises to generate structures for such applications is melt spinning, in which biocompatible materials like the polymer polycaprolactone (PCL), which has a melting point between 59 and 64 °C and a degradation period of two years can be used. In this work, a thyristor trigger control was used to control the temperature of the spinning technique. In addition, the temperature sensing and speed control of a stepper motor was employed to store the thread on a bobbin. On the contrary to the on-off control, the variation of the angle of the thyristor favors direct temperature control, since the voltage that feeds the thermal resistance is controlled. On the other hand, the LabVIEW program was used as the interface between the user and the control. Moreover, a pair of microcontrollers were used, one for zero crossing detection and SCR firing and another for temperature sensing and stepper motor speed control. Finally, the system was integrated into an optical plate for testing and adjustment, obtaining fibers of approximately 0.14 mm. This research aims to use this polymeric fiber melt spinning technique for the formation of carbon nanotubes and nanofibers for medical applications.

Keywords: LabVIEW, melt spinning, biocompatibility, PCL
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[BIO-211] Correlation of albumin and creatinine studied in photoacoustic spectroscopy

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Chronic kidney failure (CKF) is a long-term complication of different pathological entities such as cardiovascular, endocrine, and infectious diseases[1]. The evolution of CKF is uncertain due to difficulties to detect the beginning of renal damage[1]. According to KDIGO (Kidney Disease Improving Global Outcomes)[1] criteria, renal damage begins when total albuminuria in 24 h is above 30 mg and the glomerular filtration rate (GFR) is less than 90 ml/min. [2,3]. Measurement of creatinine is indispensable to quantify GFR. The problem is that two different techniques and samples are needed for the determination of albumin and creatinine[1,2]. It is necessary to implement a technology able to determine the levels of both substances in the same sample, which could reduce the time to collect the sample and will increase the precision in the evaluation of renal function. Photoacoustic spectroscopy (PAS) is a non-destructive technology that allows the determination of different substances in a 60 µl sample[4,5]. The goal of the study was to establish standards curves for albumin (0 to 64 mg/dL) and creatinine (0 mg/dL to 16 mg/dL) by PAS. Absorption spectra were detected from 250 to 650 nm. Maximum peaks were detected at 265 nm and 285 nm for albumin and creatinine, respectively. Standard curves were built measuring five times each of the 5 concentrations of albumin or creatinine. There was a positive correlation (maximum peak vs concentration) for albumin ($R=0.9762$, $p=0.0004$) and creatinine ($R=1.0$, $p<0.0001$). It is concluded that PAS is a suitable technology for the measurement of albumin and creatinine. The results open a possibility of applying an innovative technology for the evaluation of renal damage in patients with high risk of suffering acute or chronic renal failure.

Keywords: Kidney failure, Albumin, Creatinine, Photoacoustic spectroscopy
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[BIO-141] DESIGN OF MOLECULAR IMPRINTED POLYMER FOR LOCAL DRUG DELIVERY OF ANTIBIOTICS

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Molecularly imprinted polymers (MIPs), synthetic receptor like materials with specific recognition sites for template molecules, can be used for drug delivery in infected wounds due to their mechanical strength and biocompatibility. The aim of this proyect was to synthesize and functionally characterize MIPs for the local release of ciprofloxacin (CPX). 6 MIPs and 6 NIPs (without CPX) were synthesized by non-covalent methods using CPX as antibiotic and two different monomers (lactic acid LA and methacrylic acid MA); they were characterized by scanning electron microscopy, infrared spectroscopy and adsorption isotherms. In addition, the in vitro release kinetics were evaluated using a Franz cell apparatus, the cytotoxic effect against fibroblasts using alamarBlue and the minimum inhibitory concentration (MIC) was obtained in an ATCC strain of *Escherichia coli*. In micrographs the MIPs are observed with irregular and spherical morphologies. ATR-FTIR showed the presence of CPX, in the MIPs, with bands of higher intensity in stretching vibrations of the C=O, C=C, C-F and COO- groups. The interactions between monomer and CPX are given by hydrogen bonds (-COOH, -NH). The MIP performed with LA was adjusted to the Freundlich model, where adsorption occurs in multilayer, and that of MA to the Langmuir model, with adsorption in monolayer. The release kinetics for each of the polymers were performed from 0 to 24h, obtaining a first order best fit model, indicating that the drug release is due to a non-Fickian or anomalous diffusion mechanism, the release profile was above the MIC, which was verified by an assay in *E. coli* and finally, the MIPs did not present cytotoxicity in fibroblasts during the first 72h of exposure.

Keywords: Molecular Imprinted polymer, drug delivery.
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[BIO-38] Electrical response of Laser-Induced Graphene (LIG) in the presence of biological entities.

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The early detection of biological entities, such as fungi and bacteria that cause infectious diseases, has led to the need to design more efficient biosensors than those currently used, which require expensive equipment or controlled environments. In the last decade, the use of graphene has been chosen as a base material for the design of electronic devices such as transistors and sensors due to its electrical properties, its two-dimensional structure and as an adherent to biological entities, although the way it is obtained has made its commercial use difficult. Laser-Induced Graphene (LIG) has become an ideal candidate for the development of low cost and more efficient electronic devices. In the present work, from photothermal processes using CO_2 laser irradiation, polyamide films (Kapton) are converted into ultra-thin and porous sheets of Graphene. Carrying out a variation in the power of laser irradiation and making an analysis of the surface electrical properties of deposits of biological entities on the substrates of Laser-Induced Graphene, using the 4-point resistivity technique, a polynomial relationship is obtained between the irradiated power and the surface resistivity of the LIG, in order to obtain a quantifiable behavior given the electrical response of the LIG in the presence of biological entities.

Keywords: *Graphene, laser, irradiation, resistivity, biological.*
Acknowledgments: This work was supported by Instituto Politécnico Nacional (IPN), Secretaría de Investigación y Posgrado (SIP) through project numbers 20221310 & 20221437. JDCD is grateful to Consejo Nacional de Ciencia y Tecnología (CONACyT) for its financial support throughout my Master of Science Program. RGA and JOL are grateful to COFAA-IPN, EDD-IPN and EDI-IPN for support through academic fellowships.
Reference: Kaidarova, A., & Kosel, J. (2020). Physical sensors based on laser-induced graphene: A review. *IEEE Sensors Journal*, *21*(11), 12426-12443.

[BIO-54] Fabrication of Dielectric Phase Î² of Poly(vinylidene fluoride) Films by Phase Transformation and Solvent Casting Methods

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This study presents the experimental methodology and results of the fabrication of β phase in poly(vinylidene fluoride) (PVDF) films using dimethylsulfoxide (DMSO) as a solvent so that it can be used as a dielectric material. By both methods; phase transformation and solvent casting. The film prepared by phase transformation method was annealed at 90, 100, and 150 °C, during 5 hours at each temperature. Whereas in the preparation of the film by solvent casting method, the solvent evaporation rate was controlled at 0.04 MPa of vacuum pressure for 14 days. From X-Ray Diffraction (XRD) analysis of the film treated at different temperatures, the γ and β phases were identified coexisting between 90 °C and 100 °C. While, at the annealing temperature of 150 °C, the presence of α and γ phases was identified. On the other hand, it was observed that the low solvent evaporation rate favored formation of β phase at room temperature. Therefore, the results show that β phase can be produced by both methods. However, the solvent casting method presents better conditions for its production.

Keywords: DMSO, phase transformation, PVDF, solvent casting, XRD
Author for correspondence: dmejiad1500@alumno.ipn.mx
Reference: S. Satapathy, S. Pawar, P. K. Gupta, and K. B. R. Varma, Effect of annealing on phase transition in poly(vinylidene fluoride) films prepared using polar solvent, Bull Mater Sci 34, 727 (2011). https://doi.org/10.1007/s12034-011-0187-0
This work was supported by: The 20220377 and 20221423 SIP projects.

[BIO-252] Maghemite Nanoparticles Coated With Quercetin-Loaded Polyelectrolyte Multilayers And Their Cytotoxicity In Human Ovarian Carcinoma Cell Line

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We evaluated the cytotoxicity effect of polyelectrolyte–Quercetin (PMQ) coated iron oxide nanoparticles (Fe_2O_3) on a human ovarian carcinoma cell line (A2780). The γ-Fe_2O_3@shell (PMQ) was obtained by synthesizing magnetic nanoparticles (MNPs) by chemical co-precipitation and covering it through layer-by-layer (LbL) technique with two different systems of polyelectrolytes: (i) cationic polyallylamine hydrochloride (PAH) and anionic polystyrene sulfonate (PSS) as a synthetic system, and (ii) cationic chitosan (CHI) and anionic carboxymethylcellulose (CMC) as a biopolymer (natural) system. Before using the layer-by-layer technique, quercetin with a negative charge was added to the cationic polyelectrolyte (PAH or CHI) solution, leading to the formation of a positively charged complex. The nanoparticle size, morphology, and the structural, optical, and magnetic properties of the systems were analyzed by DLS, TEM, XRD, FTIR, and vibrating sample magnetometer, respectively. Otherwise, the experimental results of TGA and ζ-potential suggest that the layer-by-layer technique is a feasible way to encapsulate quercetin with high efficiency: 64.7% in the PSS/PAH (synthetic polyelectrolytes) and 87.7% in the CMC/CHI (natural polyelectrolytes). The MNPs@PSS/PAH and MNPs@CMC/CHI systems showed no cytotoxicity; however, when quercetin was loaded into the system, we have observed a statistically significant reduction in the viability of the human ovarian carcinoma cell line (A2780), though their cytotoxicity was less efficient compared with the high cytotoxicity showed with the quercetin alone. Our results indicated that the reduction in cell viability depends on the number of layers of polyelectrolytes. These systems have the potential to be possible drug carriers for targeted cancer chemotherapy.

[BIO-175] MOLECULAR IMPRINTED POLYMERS (MIPS) AND THEIR USEFULNESS IN EXTRACTION PROCESSES AND AS AN ADJUVANT IN THE DEGRADATION OF BISPHENOL A (BPA) BY THE O3/UV PROCESS.

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In this work, the synthesis, characterization and functionalization of molecular printing polymers (MIPs) on a bisphenol A (BPA) molecule was studied and evaluated. The synthesis was carried out by 3 different polymerization methods which were: mass, coprecipitation and emulsion, using sodium methacrylate as a functional monomer, bisphenol A as a template molecule, ethylene glycol dimethylacrylate (EDGMA) as a cross-linking agent, azobisisobutironitrile (AIBN) as initiator, and methanol and toluene as porogens. The retention capacity of the MIPs was evaluated using a concentration of 1 mg L-1 of BPA, demonstrating a retention capacity greater than 90% for the 3 synthesis methods. The MIPs were characterized through scanning electron microscopy, finding agglomerated and spherical pellet morphologies with a size range of between 80 and 100 nm. The nature of the external net load of the MIPs was analyzed where it was determined that the zero charge pH is 3.8; above this value the surface was negatively charged and below this value it will be positively charged. Through the study of adsorption isotherms, it was determined that this adsorption phenomenon was carried out in monolayer, where all the sites on the surface have the same probability of being occupied and that there is no interaction between adsorbed molecules. Similarly, the capacity of MIPs as an adjuvant in the process of degradation of BPA by O3/UV was determined, where it was demonstrated that MIPs have a high capacity for adsorption of BPA metabolites at a neutral pH and using 10 mg of polymer.

Keywords: Molecular Imprinting Polymer, Bisphenol A, Wastewater treatment
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[BIO-68] Nanocomposites based on polysulfone/carbon black for use in hemodialysis filters

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Chronic kidney disease is a big health problem in Mexico, due to the fact that 11 cities have high mortality rates, including Veracruz, which by 2020 had 551 people with hemodialysis treatment and 1,211 deaths from this disease. In this work, polymeric polysulfone compounds with carbon black nanoparticles obtained by ultrasound-assisted extrusion were developed to study their application as adsorbent materials for uremic toxins. Previously, the carbon black was chemically modified with citric acid using an ultrasonic tip with an output power of 750 W and variable frequency. The nanocomposite was synthesized by means of a twin-screw extruder assisted with an ultrasonic device using different concentrations of modified Carbon Black (0.25, 0.5 and 1%). The nanocomposites were characterized by FT-IR, TGA, XRD changes were observed in the polysulfone when incorporating the carbon black nanoparticles. The urea and creatinine adsorption study reveals that the sample with 1% nanoparticles obtained a 77% removal of urea and creatinine and the Freundlich isotherm was adjuste.

-Keywords: polysulfone, carbon black, creatinine, urea, chronic kidney disease.
-Corresponding autor: christian.cabello@ciqa.edu.mx.
-Reference: Andrade-Guel, M., Ávila-Orta, C. A., Cadenas-Pliego, G., Cabello-Alvarado, C. J., Pérez-Álvarez, M., Reyes-Rodríguez, P., ... & Quiñones-Jurado, Z. V. Synthesis of nylon 6/modified carbon black nanocomposites for application in uric acid adsorption. Materials (2020), 13(22), 5173. DOI: 10.3390/ma13225173
-This work was supported by: This research was financially supported by the Mexican Nacional Council of Science and Technology (CONACyT), specifically through the project 320802 CONACYT Convocatoria de Ciencia Básica y/o Ciencia de Frontera-Paradigmas 2022.

[BIO-256] Nanostructures in agriculture: the application of plastic waste

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In this work, nanofiber compounds of polyethylene terephthalate (PET) were developed from waste plastic bottles where zeolites were incorporated from the electrospinning technique for the development and growth of plants as well as the reuse of plastic waste which have been increasing in recent years. The obtained nanofibers were evaluated by scanning electron microscopy (SEM) and X-ray diffraction techniques to determine the optimal parameters for fiber generation. The evaluation of nanofibers in seed germination was designed based on different concentrations of PET/zeolites nanofibers, recording visual physiological changes (height and thickness of the stem, root, and seedling length) in lentil seeds (Lens culinaris), furthermore, the analysis of secondary metabolites by spectrophotometric techniques, obtaining a positive effect in concentrations between 0.5-1% of zeolite encapsulated in PET nanofiber, observing benefic results both in germination, foliar development, and protection against insects. Our results indicate that zeolite can be encapsulated in PET nanofibers from plastic waste to be useful as an agricultural source.

Keywords: PET, electrospinning, zeolites encapsulation, agriculture, nanofibers
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Reference: Thiruvengadam, M., Rajakumar, G., & Chung, I. M. (2018). Nanotechnology: current uses and future applications in the food industry. 3 Biotech, 8(1), 1–13. https://doi.org/10.1007/s13205-018-1104-7
This work was supported by CONCYTEQ, Nuevos Talentos 2022

[BIO-46] PET NANOFIBERS FABRICATED BY ELECTROSPINNING TECHNIQUE FROM A WATER BOTTLE

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The electrospinning technique allows to obtain fibers by coaxial stretching of a viscoelastic solution. These fibers have diameters ranging from sub microns to nanometers, dimensions where the material can achieve unique characteristics, such as a large surface area in relation to their volume (in the case of nanofibers is 1013 times more than a microfiber), high flexibility, high porosity, surface flexibility, and high mechanical strength compared to other forms of the material. Thus, nanofibers (NFs) are highly attractive for different uses, including special membranes, filtration media, tissue engineering, and medical applications, among others. The excessive use of polymer containers for food storage has generated a large amount of these wastes, so a second use is an important issue. In this research, PET nanofibers from a water bottle were electrospun using a mixture of trifluoroacetic acid (TFA) and chloroform as solvents, result in fibers with an average diameter of 500 nm. The fibers were analyzed morphologically by scanning electron microscopy analysis and thermogravimetrically. It was possible to obtain PET fibers giving an alternative use to PET bottles, obtaining a material with potential applications as membrane for electrodes and/or water filters.

Keywords: Reused PET, Nanofibers, Electrospinning Technique.
Author for correspondence: claudia.pergar@gmail.com
Reference: Teo W.E., Ramakrishna S. "A Review on Electrospinning Design and Nanofiber Assemblies", Nanotechnology, 17, R89 (2006).
This work was supported by: Proyecto Interno PI-22-15, del Centro de Investigación en Materiales Avanzados, titulado: “Desarrollo de membranas basadas en materiales nanocompuestos para su aplicación como electrodos flexibles en sistemas de almacenamiento de energía”.

[BIO-335] Properties of antibacterial agar films functionalized with Ag and TiO2 nanoparticles.

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Agar films with silver nanoparticles have the potential application in the transport of organic products since their antimicrobial properties would protect the transported product, which would allow greater flexibility and safety in the transfer and storage of products of rapid decomposition. In this work, agar films were synthesized as a polymer matrix using the standard microwave. After this process, different concentrations of Ag and TiO_2 nanoparticles were added. After the solidification of the agar, each of the gels obtained was subjected to a drying process for several hours on the drying stove resulting in the agar films with Ag and TiO_2nanoparticles. The nanoparticles in aqueous solution were characterized using scanning electron spectroscopy (SEM), dynamic light scattering (DLS), and ultraviolet to visible light spectroscopy (UV-vis), while agar films with different amounts of nanoparticles. Whereas characterized using UV-vis, Fourier transform infrared light spectroscopy with attenuated total reflectance (FTIR-ATR) and SEM.

Keywords: Biopolymer, agar film, antimicrobial, nanoparticles.
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[BIO-356] Silver Nanoparticles and Calendula Extract Embedded in Chitosan Dressings for Skin Regeneration in Diabetic Ulcers

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People suffering from diabetes can suffer from irreversible complications, such as diabetic ulcers, when they suffer an injury or scrape. In addition, 15 to 25% of patients with diabetes suffer from diabetic foot, of which 20% will suffer amputations and have an 80% probability of suffering a second amputation [1]. In this work, a composite material for the treatment of diabetic ulcers was made as a chitosan dressing with silver nanoparticles and marigold extract. By means of a colloidal solution and the use of a microwave oven, silver nanoparticles were synthesized as a microbial agent. The marigold extract was obtained by infusion with the flower petals, the extract was used as a healing agent and skin regenerator, the chitosan was acquired commercially and a chitosan dressing those functions as a scaffold to protect and integrate the active materials. Different tests were performed on the different materials, including crystalline structure, morphology and chemical composition, using UV-Vis spectra, XRD, SEM, EDS, TEM, as well as microbial and in-vivo tests. In-vivo tests were performed on 2 patients of advanced age, morbid obesity, type 2 diabetes and high risk of amputation (who gave their full consent to perform the treatment). By means of electronic microscopy it was observed that the nanoparticles not only presented a single spherical morphology but also presented cubic, pyramid and thread morphology, while in-vivo tests showed a complete recovery of the ulcer in a period of 2 to 4 months respectively in the patients.

Keywords: Chitosan, Nanoparticles, Clinical case, Diabetes, Wounds
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Reference: Borgnakke, W., 2021. IDF Diabetes Atlas. Diabetes Research and Clinical Practice, [online] 10. Available at: https://diabetesatlas.org/idfawp/resource-files/2021/07/IDF_Atlas_10th_Edition_2021.pdf.

[BIO-155] SOLID RAIN IRRIGATION SYSTEM USING POLYSTYRENE/POLY (POTASSIUM) ACRYLATE ELECTROSPUN NANOFIBERS

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The use of nanofibers in the agricultural industry has a promising approach both in the protection and growth of the plant through a prolonged release of nutrients and even safeguard elements of vital importance such as water. Implementing innovative technologies in the agriculture sector as an alternative solution represents a great challenge. In this work, we proposed the use of nanofibers by the electrospinning technique employing materials such as cellulose acetate and waste from polystyrene adding potassium polyacrylate which fulfills the function of capturing water. It was also studied how electrospinning parameters affect the morphological and absorption characteristics using a centered composite design to define optimal electrospinning conditions. The morphological characterization, as well as the surface tension (contact angle), porosity, strength, and absorption capacity, were used for the comparison with potassium polyacrylates mostly used as solid rain in crops which have the absorption ability, growing up to 500 times its normal size and its storage capacity for up to 8 years.

Keywords: PS nanofibers, solid rain, electrospinning, water absorption, polyacrylate, PS waste, experimental design
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REFERENCE: S. Meraz-Dávila, C. E. Pérez-García, and A. A. Feregrino-Perez, “Challenges and advantages of electrospun nanofibers in agriculture: A review,” *Materials Research Express*, vol. 8, no. 4, 2021, doi: 10.1088/2053-1591/abee55.
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[BIO-138] STUDY OF POLY(CAPROLACTONE) NANOFIBERS SCAFFOLDS USING A PHOTOACOUSTIC TECHNIQUE

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Electrospinig was used for production of poly(caprolactone) nanofibers scaffolds. Scanning electron microcopy (SEM) and optical microscopy were used in order to determine the diameter of the obtained fibers. A self-nomalization procedure is developed for measuring the thermal diffusivity of nanofibers scaffolds using a photoacoustic technique: considering the one-dimensional heat diffusion problem for a single layer, with harmonic heat source, and assuming the surface absorption model, we can use the ratio between the temperature fluctuations of both surfaces of the medium (nanofibers scaffold) and phase lag of the its complex signal [1]. From the phase difference of the temperature fluctuations we can evaluated the thermal diffusivity of nanofibers scaffolds.

Keywords: Electrospining, Photoacoustic Technique, Thermal Diffusivity

REFERENCE: J. A. Balderas-López, Self-normalized photoacoustic techniques for thermal diffusivity measurements in metals, *Rev. Mex. Fís.* **50** (2) (2004) 120–126.

[BIO-332] Synthesis and characterization of a gelatin-agar film polymer functionalized with sodium tripolyphosphate and loaded with silver nanoparticles for bacterial inhibition.

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The research and implementation of innovative and affordable biopolymers with various potential applications are becoming increasingly attractive due to the impact they represent in several industries; particularly, the use of gelatin and agar has had promising results in various studies that motivated the research of the present work. The synthesis of the film polymer was as a gelatin-based matrix with agar, both food-grade; the increase in the concentration of agar in the gelatin base with the use of sodium tripolyphosphate resulted in a modification of the mechanical properties of the matrix, at last, the silver nanoparticles were aggregated to lower the incidence of bacterial growth in the material. The addition of agar in the gelatin matrix was in a weight ratio between 100% gelatin and 75% and 25% of gelatin and agar, respectively, with a variation of 5%, 1ml solution in which were embedded the silver nanoparticles and 0.4 g of sodium tripolyphosphate (STPP) as a crosslinking agent, the polymer was left to solidify in room temperature until it reached a solid appearance. The characterization of samples was conducted employing scanning electron microscopy (SEM), attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR), optical microscopy, and tension characterization using ASTM D638 norm.

Keywords: Biopolymer, Composite material, Gelatin-Agar, Mechanical properties.
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[BIO-78] Synthesis of the I²-phase of PVDF using DMF and HMPA as solvents

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The use of polymeric composite, such as dielectric materials, has been of interest in recent years, due to the properties that they present, such as flexibility, high resistance to electrical breakdown and easy manufacturing process. Poly(vinylidene fluoride) (PVDF) is one of the most widely used polymers in these composite materials, due to its piezoelectric property, generated by the different crystalline structures formed in the polymer, such as the alpha phase (α) , gamma phase and the beta phase (β), which is the phase of interest and is the one with the maximum net dipole. The present work focuses on the manufacturing process of PVDF films based on the synthesis of the polymer using different types of solvents, hexamethylphosphoramide (HMPA) and dimethylformamide (DMF) over different conditions of pressure and temperature, with the objective to obtain the β phase. The synthesis was obtained at a concentration of 12% by weight of PVDF, at 90°C and 140°C with HMPA and DMF, respectively. The PVDF films were deposited in a spinner at 700 rpm for 30 seconds and drying at 50 °C for 24 hours at atmospheric pressure. A sample has a vacuum pressure of 0.04 MPa for 336 hours. From X-ray diffraction (XRD) analysis, it was observed relative peaks of greater intensity to 20.47° and 36.57°, corresponding to the β phase, as well as peaks of 18.60° and 20.16° related to the phases α and γ, respectively, for the synthesis of PVDF with DMF. PVDF sample with HMPA it was observe peaks at 15.58° and 17.65° corresponding to the α phase and 20.42° for the γ phase.

keywords: Synthesis, HMPA, DMF, β phase, PVDF.
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Reference: V. Sencadas, R. Gregorio Jr. and S. Lanceros-Méndez J. Macromol. Sci. Part B-Phys., 48 (2009), pp. 514-525, https://doi.org/10.1080/00222340902837527
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[BIO-421] ,Improving the corrosion resistance of Mg by the 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 TiO_2-based coatings through the PEO technique. Anatase-TiO_2 powders were incorporated into the electrolytic solution due to their good biocompatibility. Coatings were developed by varying the TiO_2 concentration from 0.08 g to 0.18 g, and the current density from 260 to 300 mA/cm^2. The distance between electrodes was set to 2 cm and the pH was 11.9.
The presence of TiO_2 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 TiO_2-based coatings have formed a porose 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 TiO_2-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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Sesión Oral

[BIO-172] ANTIBODY-FUNCTIONALIZED GOLD NANOPARTICLES SUPPORTED ON GRAPHENE OXIDE FOR THE DEVELOPMENT OF A BIOSENSOR FOR FAST DETECTION OF SARS-COV-2

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COVID-19 disease is generated by the identified SARS-CoV-2 coronavirus and has an incubation period of 2-10 days. Its manifestation in low-risk persons may present mainly as cold, dyspnea, fever, and fatigue. However, people over 60 years old or people with comorbid conditions such as hypertension, diabetes, and excess visceral fat, among others, may present severe symptoms including multi-organ failure, acute cardiac injury, and the development of severe acute respiratory syndrome (SARS), which can lead to death in a matter of days. In this regard, the development of a highly sensitive diagnostic in the early days and accurate detection of COVID-19 is vital. During this work, under the context of prevention, identification, and accurate diagnosis of SARS-CoV-2 and COVID-19, a biosensor based on gold nanoparticles (AuNPs) supported on graphene oxide (GO) functionalized with an antibody against the Spike protein of SARS-CoV-2 is developed. The Au-NPs are synthesized by photodeposition on graphene oxide sheets, afterwards, the nanocomposites (AuNPs-GO) are characterized by UV-Vis spectroscopy, FTIR, TEM, and Raman spectroscopy. The conjugation of AuNPs-GO with the IgG antibody specific for Spike protein is evaluated through UV-Vis spectroscopy. Finally, the AuNPs-GO-IgG system is evaluated in the detection of SARS-CoV-2 using virus-like particles (VLPs) that contain the Spike protein as a resemblance of the virus SARS-CoV-2. The VLPs are detected at very low concentrations by analyzing the variation in the UV-Vis spectrum of AuNPs-GO by the specific binding of the VLPs with the AuNPs-GO-IgG biosensor.

Keywords: virus-like particles (VLPs), gold nanoparticles, SARS-CoV-2, graphene oxide.
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[BIO-261] Depolymerized chitosan as a vehicle for the incorporation and release of anticancer active ingredients

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Cancer is one of the main causes of death in the world and nowadays biopolymer-based systems are being investigated for the transport of anticancer drugs with the aim of reducing the side effects of current therapies. Chitosan is a biodegradable and biocompatible polysaccharide, currently being investigated as a drug delivery vehicle. With lower values of molecular weight in chitosan, the appropriate particle sizes can be achieved to circulate in the body to reach the tumor site. Therefore, in this study the depolymerization of chitosan and the effect of incorporating and encapsulating curcumin, a natural phytochemical with antioxidant properties, is carried out. Starting from low molecular weight commercial grade chitosan and through oxidative degradation with $NaNO_2$, depolymerization is carried out by modifying the reaction time. The samples are characterized by Infrared Spectroscopy (FTIR-ATR) to demonstrate that there are no changes in the structure of chitosan when depolymerizing, in addition to estimating the percentages of the degree of deacetylation of the samples, thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) as indicative of the decrease in molecular weight due to weight drops at lower temperatures, indicating lower thermal stability. Subsequently, the fragmented samples are crosslinked with the aim of achieving higher percentages of curcumin incorporation and increasing the release time, indicating that the crosslinking agent has an effect on the incorporation of the drug in the material and on the release kinetics.

Keywords: Chitosan, depolymerization, curcumin
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[BIO-201] DEVELOPMENT AND EVALUATION OF A COLLAGEN/CHITOSAN NANOFIBER MEMBRANE FOR DELIVERY OF TRANEXAMIC ACID

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Biopolymeric nanofibers are a crucial part of tissue engineering that have shown important results in adherence, cell capacity and are a nutrient´s source. These membranes synthesized by electrospinning allow to apply to different wounds in tissues, one of them is the walls of the blood vessels that are of vital importance to care for and recover during an accident. In this work, a collagen and chitosan nanofiber membrane synthesized by electrospinning is used to promote an accelerated coagulation using tranexamic acid (TXA) as an antifibrinolytic as a first aid material. Collagen was extracted from bovine tendons by the alkaline hydrolysis with an extraction yield of 40% and Type I and Type V of collagen was covered by infrared spectroscopy. Subsequently, this collagen was dissolved in PBS:ethanol, while chitosan was dissolved in acetic acid to mix them; TXA was dissolved together with the collagen. The fibers of the polymers obtained have an average diameter of 265 ± 17 nm while the fibers with a concentration of 40 mg/ml TXA were around 413 ± 111 nm, meanwhile drug particles size was of 105 ± 21 nm and was distributed throughout the fibers. The infrared spectrum demonstrate electrostatic interactions between the amino and hydroxyl functional groups of the polymers without losing the triple helix structure of collagen, while TXA was assigned interacting through of hydroxyl group with the amino group; the swelling index of the membrane with drug increased 5% compared to purely membrane, and this is related to the type IV isotherms obtained by BET shows a mesoporous material with a pore of 32.40 nm and a surface area of 4.49 m^2/g, with an increase to 11.16 m^2/g when TXA was adding and the pore was of 29.18 nm. These characteristics and interaction of the polymers with the drug could allow controlled release in simulated blood flow and promote fibroblast cell adhesion.

Keywords: Chitosan, collagen, electrospining, tranexamic acid, nanofibers.
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[BIO-39] Implementation of ISFETs for glucose sensing

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In the last decade, a prominent rise in diabetic patients has been noted, according to the International Diabetes Federation (IDF), it is estimated that 14 million adults in Mexico live with diabetes, which represents an increase of 10% in the last two years. In order for patients to have better control of their disease, a non-invasive device for glucose sensing through sweat is proposed, using an ISFET (Ion Sensitive Field Effect Transistor) transistor for the detection of different concentrations (1, 2 , 4, 6 and 8 MM) of glucose. The ISFET transistor has a thin film architecture with the following material arrangement LIG/ITO/PDMS/P3HT/ITO. The sensing mechanism consists of depositing the different concentrations of glucose on the laser-induced graphene bioplatform, LIG (Gate contact), which will cause a change in the electrical resistance of the Gate, due to the latter, the gate voltage will be modulated, reflecting in a horizontal shift of the transferential response of the transistor compared to the transferential curve of the transistor without glucose in the device. Using this technique, it has been possible to appreciate current changes ranging from 1μA to 8μA with respect to the reference transistor signal. With this, we can conclude that this census technique is an auxiliary for monitoring glucose levels in low concentrations.

Keywords: *Sensor, ISFET, Glucose, LIG, Bioplatform*

Reference: Martinoia, S., Massobrio, G., & Lorenzelli, L. (2005). Modeling ISFET microsensor and ISFET-based microsystems: a review. *Sensors and Actuators B: chemical*, *105*(1), 14-27.

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[BIO-183] PHYSICAL PROPERTIES OF HYBRID COATINGS OF SIO2-RECYCLED PET UNSATURATED POLYESTER RESIN

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Abstract: Hybrid coatings generally consist of the combination of an organic and an inorganic phase that form a new material, with better properties than its original components. The aim of this work was measured the physical properties of hybrid coatings synthesized by sol-gel (hybrid system was SiO_2-unsaturated polyester resin from recycled polyethylene terephthalate, SiO_2-R_UPR). Methodology to elaborate the hybrid solution consisted in three alternated steps: 1) Synthesis of a SiO_2 solution by sol-gel from tetraethyl orthosilicate (TEOS). 2) Mechanical recycling of bottles of PET postconsumer to obtain PET flakes (1 cm^2) and chemical recycling of them (depolymerization by glycolysis) using propylene glycol and zinc acetate (ZnA) as catalyst, in a Vessel-type reactor (20-200 °C), to obtain bis(2-hydroxypropyl-terephthalate), then it was reacted with maleic anhydride to produce unsaturated polyester (UP) and then, was mixed with styrene (St) to obtain R_UPR. 3) Synthesis of hybrid solution (SiO_2- R_UPR) was synthesized by sol-gel at different molar ratios, R_UPR:TEOS:3-trimethoxysilylpropyl methacrylate (TMSPM), of 0:1:0 (T), 1:2:0.25 (HS1), 1:1:0.25 (HS2) and 1:0:0.25 (HS3), and from them hybrid coatings (HC) were made by dip coating. Molecular bonds in HS were identified by FT-IR and the physical properties of HC were measured by AFM (roughness), ASTM D-3359 (adherence), wettability (contact angle) and SEM (thickness). The coatings showed good physical properties, they were adhered perfectly to the substrate, with thicknesses of micrometer units, and flat surface (roughness average less than 1 nm), and hydrophilicity decreased as SiO_2 amount decreased (contact angle increased from 52° to 73°).

Keywords: Hybrid-coating; recycled PET; unsaturated polyester resin; SiO2; sol-gel process
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[BIO-442] Resistive Breath Sensor based on mesoporous silica and PEDOT:PSS

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Presently, sensors are used and demanded to develop various health monitor systems. Recently, breath sensors have been the most requested because of the COVID pandemia. In this work, we developed the mesoporous silica powder in an eco-friendly route and deposited it over a cloth with a spin-coater. Afterwards, PEDOT:PSS was also deposited over silica powder. Electrical characterizations demonstrate that using mesoporous silica improves the well-known PEDOT:PSS sensibility to humidity, allowing for the detection of the breath rhythm of a human body. Optical and morphological characterization of the synthesized mesoporous silica will be shown, as well as the fabricated sensor's response.

Keywords: mesoporous silica, eco-friendly synthesis, PEDOT:PSS, breath sensors

[BIO-63] SIMS ANALYSIS OF THIN POLIMER FILMS

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In recent years, there has been a growing interest in semiconducting polymers that can replace silicon in the production of chip but effective solar cells and other mass-produced electronic devices. With the advent of cluster ion sources, the possibility of depth profiling analysis of polymer films in time-of-flight mass spectrometers has appeared. Examples of depth profiling quantitative analysis of some typical polymers (Teflon, Kapton, PEN, PET) implanted with various ions, as well as of special thin polymer films (PEDOT, PEDOT-PSS, PFN, etc.) expressed on glass and on various conductive substrates, including multilayer solar cell structures, are presented in this work. All measurements were performed using a time of flight mass spectrometer TOF-SIMS-V from ION-TOF Co. (Germany). The analysis was performed by using a pulsing beam of Bi_3^+ ions with beam energy of 30 keV; the ion sputtering was performed with a beam of cesium ions with ion energies in the range of 500eV - 1 keV. In the report the process of polymer surface carbonization occuring due to ion irradiation, the mechanism of formation of secondary ions and the possibility of quantitative analysis by SIMS method of the specified materials are considered. The surface patterning of various polymer during the ion irradiation process is also considered.

Keywords: thin polymer film, TOF-SIMS, ion implantation, hybrid solar cells

[BIO-277] STUDY OF INFLAMMATORY AND OBESOGENIC BIOMARKERS WITH PHENOLIC EXTRACTS OF Cosmos bipinnatus Cav

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The purpose of this work was to determine the best method for extracting phenolic compounds and antioxidant capacity from *Cosmos bipinnatus Cav*., testing maceration for 24 h and ultrasound for 15 minutes at temperatures of 25 and 60 °C with 70% and 50% ethanol. Quantification of total phenols (TF), total flavonoids (FlavT) and the antioxidant capacity of the extract was carried out by means of the hydrogen peroxide test. The aerial part of the plant was dried in the shade, crushed and sieved through a No. 60 mesh (0.250 mm). For the extraction by maceration, 5g of sample were placed in each solvent, stirred for 24 h for each temperature. The sample was filtered and the resulting liquid was saved. For the ultrasound, the same temperatures and solvents were tested, only varying the form of extraction, which was with ultrasonic waves, emitted by the equipment with a power of 500 watts, 20 Khz frequency and 40% amplitude for 15 min with lapses 55 s and 5 s rest. The mixture was centrifuged for 10 min at a speed of 4000 rpm. The supernatant was filtered and the extract was saved. The ultrasound method at 60 °C with 50% and 70% EtOH showed the highest yield with 20.39% and 18.46%, respectively. The highest concentration of CF and FlavT was found in the ultrasound treatment at 60 °C with 70% ethanol, being 89.33 mgEAG/g of dry extract) and 68.73 mgEQ/g of dry extract, respectively. The amount of extract required to reduce the concentration of H2O2 by 50% was obtained with a lower concentration of the extract obtained by ultrasound, being 49.32 EC50.

Keywords: *Cosmos bipinnatus Cav, Biomarkers*
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[BIO-161] THE USE OF CARBON SPHERES TO ENHANCE THE ACTIVITY OF ENDOPHYTIC BACTERIA

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The use of nanoscale materials has increased in recent years, especially materials with carbon-based structures such as carbon nanotubes, graphene, graphite and fullerenes because they have exceptional physical, chemical and mechanical properties. Due to this, great developments have arisen in medicine, biotechnology, etc. One of the most important applications is the use of nanoparticles as carrier vehicles for the controlled release of drugs to improve stability, solubility and biodistribution. However, the effect of carbon spheres (CSs) on the phytohormonal activity of plant growth-promoting endophytic bacteria to enhance plant growth is little known. The objective of this work was to evaluate the effect of CSs at different concentrations with *Bacillus thuringiensis* and *Micromonospora echinospora* on germination of *Prosopis glandulosa*. The CSs were synthesized from rosin by the chemical vapor deposition method, then dispersed in a detergent solution and treated *P. glandulosa* seeds inoculated with the bacteria and sown in soil. The only response variable was germination percentage, experimental data were analyzed by ANOVA-Tukey ($P \leq 0.05$). The results indicated a positive effect on *P. glandulosa* seeds with *B. thuringiensis* and *M. echinospora* and presence of CSs, which registered 82% germination, a value statistically different from the 55% germination of *P. glandulosa* without CSs and bacteria fed. These facts support that the positive effect on seed germination was due to the hydrolysis of starch wich was reactivated when water was soaked, releasing organic compounds, which *B. thuringiensis* and *M. echinospora* transformed into phytohormones, which, potentiated with the CSs, stimulated a greater emergence of *P. glandulosa* seeds.

Keywords: carbon spheres, endophytic bacteria, phytohormonal activity, nanomaterial
Author for correspondence: ladamex@yahoo.es This work was supported by CIC of UMSNH and CONACYT

[BIO-66] THERMAL DIFFUSIVITY OF CHITOSAN-BIOACTIVE AGENTS EDIBLE NANOCOATINGS FOR HORTICULTURAL PRODUCTS PRESERVATION

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Edible films are of special interest for different applications in the agricultural field. They act as barriers to moisture and gas exchange and have antimicrobial activity. They are mainly prepared from starch and gelatin, among other biodegradable polymers. Chitosan is a biodegradable and non-toxic polymer with antimicrobial activity use in edible films that along with bioactive agents like essential oils and propolis can be used as coating for horticultural products. Moreover, chitosan can be added in the form of nanoparticles to increase its antimicrobial and thermal activity due to the higher surface area to volume ratio. On the other hand, edible films characterization is mainly based on physicochemical properties; however, thermal properties are still unexplored. In this work, edible films from a polymer matrix based on chitosan added with chitosan nanoparticles (CS) and chitosan added thyme essential oil (CS-EO) or chitosan added propolis (CS-P) were prepared using the nanoprecipitation method. Thermal diffusivity (*D*) of casting films was measured by the open photoacoustic cell technique at room temperature. From the results, the highest value of *D* was for the CS-EO ($1.9\pm0.04 \times 10^{-6}$ m^2/s) followed by the CS ($1.4\pm0.02 \times 10^{-6}$ m^2/s) and CS-P films ($1.1\pm0.01 \times 10^{-6}$ m^2/s) films, although values were similar. Therefore, for use in the preservation of horticultural products, the heat transfer through the edible films at room temperature is not a parameter influenced by the type of nanoparticles. Moreover, films showed lower thermal diffusivity due to the thermal properties of the polymer matrix used. It has been reported that chitosan confers thermal stability to composite films related to its structure and in the films due to the presence of agglomerations and degree of crystallinity [1]. Further studies are necessary to stablish these structure-properties relationship.

1. Polysaccharides Bioactivity and Biotechnology. 2015. K. Gopal Ramawat and Jean-Michel Mérillon (Eds.), Springer, Switzerland, https://doi.org/10.1007/978-3-319-16298-0
Keywords: thermal properties, biodegradable polymers, antimicrobial activity
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CHARACTERIZATION AND METROLOGY

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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

[CHM-435] Determination of the Damage Index of Diseases on the Upper Surface of Papaya Leaves Through Multispectral Images Using Machine Learning

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This work presents the development of a system for use in the agricultural sector through image processing. This system was applied for the detection and determination of the damage index (DI) caused by viral diseases in commercial papaya plots. Namely, papaya mosaic virus (PapMV) and papaya ringspot virus (PRSV), with initial signs of the disease on apical leaflet primordia and true leaves. Disease damage was recorded by taking photographs of the papaya (Carica papaya L.) tree canopy. The images were captured by means of a multispectral camera placed on an Unmanned Aerial Vehicle (UAV) in three crops selected by empirical experience with different levels of damage. Machine Learning (ML) methods were applied to the captured images to obtain the DI. Obtaining an unsupervised and adaptive algorithm capable of calculating the DI caused by the virus in the papaya crop canopy, as a complement to the use of molecular biology techniques for disease detection.

[CHM-432] ELECTROCHEMICAL DEPOSITION OF A NANOLAYERS OF FE2O3 ON SILICON

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We are interested in growing an ultrathin film of pure iron oxide on silicon with no other iron chemical species present. This is because the samples will be employed in synchrotron studies to learn about the physical origin of the Shirley background in photoemission spectra, and the presence of various species dramatically complicates the analysis. In previous studies using thermal oxidation of pure iron ultrathin films, we found that, as expected, Fe_2O_3 is the easiest to obtain and most stable oxide. However, a small amount of suboxide (Fe_3O_4) and pure metallic iron remains at low-temperature annealing, while higher-temperature annealing provokes a chemical reaction with silicon and the formation of protrusions. Here, it is proposed to overcome this problem by growing full hematite nanofilms on silicon using electrochemical deposition. This technique offers a facile synthesis route for controlling film thickness, large-area uniformity, and the possibility for room temperature deposition. The hematite films were characterized with XPS to corroborate the thickness, composition, and purity. We will present the optimized processing conditions and the thickness and composition obtained through detailed XPS analysis.

Keywords Hematite, ultrathin-film, cyclic-voltammetry, XPS, synchrotron.
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[CHM-206] EVALUATION OF THE THERMOCHEMICAL TREATMENT IN STEEL SURFACES

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In present times, surface engineering has become a highly attractive and economically viable technology aimed at improving the properties of the surface of a material. Since the surface of a material highly dictates its total service life, the aim is to develop surfaces with ideal properties that are different from its base predecessors, including physical, chemical, mechanical, magnetic, or electrical. The surface in steel materials is of great interest for its different applications, the development of stainless-steel surfaces is needed for heat exchangers, valves, boilers, mainstream lines as well as aeronautical applications. Thermochemical treatment is a type of material engineering, that employs metal atoms through thermal diffusion to incorporate them in a material surface to modify its chemical composition and microstructure. The aim of this study is to evaluate steel surfaces that have been thermochemically treated to improve its performance properties.

Keywords: Steel, Thermochemical treatment, Structural evaluation.

[CHM-437] Glass-forming zone of the CrO3-V2O5-TeO2 system: a Raman spectroscopy study

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CrO_3-V_2O_5-TeO_2 system glasses were prepared by the melt quenching technique, at 900 °C, in a Coor brand high-alumina crucible, glass-forming zone of the system was determined. Two types of glass were obtained: opaque and transparent (visually), glass color is greenish black. Raman spectra present vibrational modes related with bond kinds: V-O-V or V-O-Te (315-344 cm^{-1}), Te-O-Te (453-501 cm^{-1}), O-V-O (557-563 cm^{-1}), TeO_4 (639 -696 cm^{-1}), TeO_3, TeO_{3+1} (736-802 cm^{-1}), V-O-V at VO4 (829-905 cm^{-1}) and V=O (930-982 cm^{-1}). X-ray diffraction patterns show two types of diffractograms. One type is related to crystalline phase and the other type to amorphous phase with crystals embedded in the glassy matrix. Scanning electron microscopy detects the formation of hexagonal-shaped crystals that could be related to Cr_2O_3. The optical band gap of the glass samples was determined by optical absorption spectroscopy using the Tauc method.
A TeO_4 groups transformation (trigonal bipyramids) to TeO_3 groups (trigonal pyramids) is observed. On one hand, VO_4 and VO_5 groups are detected, as well CrO_6. On the other hand, chromium oxide remains constant for all glasses, while TeO_2 and V_2O_5 vary as TeO_2 increases and V_2O_5 decreases. These variations allow the formation of bridge bonds of the Te_{ax}-O_{ec}-Te type that, because of CrO_3, form non-bridging oxygens.

References: [1] Alvarado Rivera, J., Pérez Hernández, C. G., Zayas, M. E. and Álvarez, E., Nanocrystallization of the Cd_3Al_2 Ge_3O_{12} Garnet in Glasses of the CdO-TeO_2-GeO_2 System. in Advances in Glass Science and Technology 39–59 (IntechOpen, 2018). doi:http://dx.doi.org/10.5772/intechopen.73295
[2] Pérez Hernández, C. G. Síntesis de Nanoestructuras de $Cd_3Al_2Ge_3O_{12}$ por la Técnica de Fusión de Polvos en Materiales Vítreos de la Matriz CdO-TeO_2-GeO_2 Con Propiedades Luminiscentes. (Universidad de Sonora, 2016).

[CHM-426] Insight into the physical origin of the Shirley background and the peak asymmetric through the analysis of the 3d core level of the 5th-period elements

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Peak-fitting of the 3*d* core level from the 5th-period elements is challenging due to the high asymmetry of the main peak, the complex multiplet structure including plasmon and satellite peaks, and the intense Shirley-type background. This work presents 3*d* X-ray photoelectron spectra from pure elements ranging from Sr(Z=38) to Te(Z=52). These were analyzed using the DoubléLorentzian lineshape to account for the asymmetry of the main photoemission line, the branching ratio was forced to the theoretically expected value from the Scofield tables. It was possible to quantify the modulation with Z of the asymmetry of the $3d_{3/2}$ and $3d_{5/2}$ main peaks. It is remarkable that, for elements with completely filled 4*d* orbitals, the Double-Lorentzian asymmetry tends to be roughly equal between the two 3*d* branches. The background was modeled as a combination of a Shirley-type background, SVSC, a baseline, and, in some cases, a Slope background. The Shirley parameter decreases from a high value for Sr to a local minimum for Mo, to a local maximum for Rh. How this behavior sheds light on the physical origin of Shirley's background will be discussed. The fitting parameters employed in the analysis has been published in https://xpsoasis.org/

Keywords: asymmetry, Double-Lorentzian line-shape, Shirley background, plasmon and satellite peaks, 5th-period elements.
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Reference: Kaga, Y., Abe, Y., Yanagisawa, H., Kawamura, M., and Sasaki, K. Ru and RuO2 Thin Films by XPS. *Surf. Sci. Spectra* **6**(1999) 68-74. https://doi.org/10.1116/1.1247890

[CHM-166] MECHANICAL PROPERTIES OF GRAPHENE OXIDE WITH DIFFERENT OXIDATION DEGREES: AN APPROACH BY AFM.

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Two dimensional materials, have drawn attention due to their unique electrical, optical and mechanical properties. Moreover, graphene has become the most promising two-dimensional (2D) material for several applications comprising electronics, optoelectronics, energy storage, energy harvesting, among others. Graphene properties are related to its structure, crystallinity and oxidation degree. In this work, graphene oxide (GO) samples were prepared at different oxidation degrees using a modified Hummers' method. The degree of oxidation is directly related to the C/O atomic ratio based on the carbon and oxygen contents. The C/O ratio of GO, rGO and SOG was calculated to be ~2, >80, 4-5, respectively. The samples were suspended by drop casting on membranes with an array of circular holes. The mechanical response of these free-suspended few layers of GO with different oxidation degree were evaluated by classical force – displacement curve indentations using an MFP3D-SA AFM. The mechanistic approach of the data will allow determining the relationship between the mechanical response and the degree of oxidation of the samples and thus propose future potential applications.

This work was supported by the Internal project No. PI-22-15 granted by Centro de Investigación en Materiales Avanzados S.C. and entitled " Desarrollo de membranas basadas en materiales nanocompuestos para su aplicación como electrodos flexibles en sistemas de almacenamiento de energía"

[CHM-224] Morphology study of MoO3 by thermal treatment and chemical attack for 3D nanostructured arrays.

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Nowadays, morphology and crystallinity control is important due to the close relationship between them and the properties of nanostructured materials. In molybdenum oxides there have been extensive reports on the synthesis of MoO_x in multi dimensions, to mention a few zero dimensional, quantum dots, nanosheets, and 3D materials. The properties decide the structures and therefore their applications such as use for photodevices, energy storage, drug delivery, ion batteries, and gas sensors, among others. Molybdenum oxide (MoO_3) is a relatively inexpensive semiconductor material, n-type semiconductor and can be used as a catalyst, solid lubricant, electrochromic applications, etc. It has been demonstrate that different synthesis methods at different conditions result in nanowires of different structure. For example, microwave-assited hydrothermal synthesis results in hexagonal nanowires while conventional hydrothermal results in nanobelts. It is worth to mention that in conventional hydrothermal synthesis the usage of acidifying agents results on thinner and longer for HNO_3 and shorter and irregular belts for HCl. In this work, molybdenum oxide nanowires were synthetized by chemical attack and thermal treatment. First, a commercially obtained Mo foil (99 % purity) was mechanically polished until a mirror-surface was obtained, then ultrasonically clean in milli Q water. The obtained polished foil was then deposit in HCl at different concentrations (10 M, 5 M, 2 M and 0.5 M) for 3 minutes and then dried at room temperature. The MoOx foil is then taken for thermal treatment at different temperatures (600 °C and 700 °C) and time exploration (1, 3 and 5 h) was conducted. XRD confirms MoO_3 orthorhombic structures in the obtained substrate that shows growth of certain crystalline planes and decrease in others due to changes on the crystallinity. Morphology characterization by SEM and TEM analysis demonstrates the obtained nanowires array and the changes in the morphology form irregular nanowires at lower temperatures to well defined and longer nanostructures at higher temperatures making the basis for the optimal conditions for MoO_3 nanowires array synthesis. The effect of chemical etching on the surface properties of MoO_3 structures is discussed.

Keywords: MoO_3 nanowires, thermal treatment, chemical attack.
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[CHM-348] NANOMATERIALS AND BIOLOGICAL SAMPLES PREPARATION FOR CHARACTERIZATION WITH TRANSMISSION ELECTRON MICROSCOPY (TEM)

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The development of science and technology require techniques for following up the progress and conclusion of projects. The study of nanomaterials with properties attributed to size and shape is increasing. Therefore, characterization techniques that have the required resolution to observe and interpret the properties of nanomaterials are needed. Due to the nano scale, the use of transmission electron microscopes (TEM) with high resolution have become indispensable and, in some cases, special sample preparation is needed. TEM allow us to study the morphology, crystallinity, surface details, and more of nanomaterials, to the point of becoming a rutinary characterization technique. In this work we present the versatility of the characterization and support that TEM can offer. We show the images acquired and the preparation protocols from a variety of samples that were used to complete and publish the work of several projects. The idea is to generate confidence in the results that can be endorsed using this technique. The presented examples include monitoring the size and shape of nanoparticles during the synthesis process using green methods. Monitoring viral nanoparticles during the encapsulation of drugs and the changes produced by using different buffers to see their stability for application in medicine and agriculture. Also, in cytotoxic studies it is necessary to determine nanoparticles internalization to see how deep they penetrate in cells. Additionally, it becomes important to let know users, that organic samples (nanogels, cells, virus, bacteria, and fungi) need special preparation protocols because the technique involves high vacuum and high energy impact of electrons on samples, that are important features to consider when working with organic or responsive materials. Nonetheless, there are several projects in all levels that can be highly beneficiated by TEM.

Keywords: TEM, electron microscopy, nanomaterials, characterization, biological sample preparation.
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[CHM-365] Overcoming the difficulties of assessing the Cu1+-Cu0 ratio from XPS data

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In recent years, a series of very high-quality peak-fitting analyses of X-ray photoelectron spectroscopy (XPS) data have been reported [1]. These works, which were especially focused on the accurate fitting of complex structures of the 2p photoelectron spectra of the 4th period transition metals, also showed the need to use physical parameters in the fitting process, adequate line shapes, the consideration of both photoemission lines, and especially a proper modeling of the background. The reports also showed the robustness of the proposed fits by successfully assessing the chemical composition. For the special case of the Cu2p photoelectron spectra, there is no direct way to differentiate between the signal contribution of Cu0 and Cu1+ since the shape of the spectra are almost identical. Some works use the Auger parameter to determine this difference in chemical species, however, in thin films, the shape and the Auger parameter cannot properly be used, because as it happens in the Cu2p spectra, the Cu1+ Auger signal is also identical to metallic copper Auger signal. Ultra-pure copper films were deposited by sublimation in ultrahigh vacuum, which guaranteed films were free of carbon and oxygen. Subsequently, exposures were made in a controlled atmosphere of ultra-pure oxygen for 10, 100, 1000 and 10,000 mega Langmuir (ML), obtaining high-resolution spectra of Cu for the first stages of oxidation. For the spectrum of metallic copper, it was possible to assess the Lorentzian width of both branches as a function of oxygen exposure. We found that, while the width of the 3/2 branch is the same for the Cu^0 and Cu^{1+} cases, the Lorentzian width of the 1/2 branch evolves from 1.34 eV (for Cu^0) to 1.01 eV for Cu1+. This modulation allows, employing XPS data, for the quantification of the Cu^{1+} when both Cu^0 and Cu^{1+} are present.

This work was partially financed by Proyecto Fronteras 58518, Conacyt, Mexico.

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[CHM-302] PATTERN ANALYSIS OF LASER LIGHT SCATTERED BY WEAR SCARS PRODUCED IN A PIN-ON-DISK TRIBOMETER

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Unidirectional surface finishing is ideal for laser light-scattering analysis since, under some conditions in the plane of incidence, the scattering pattern exhibits likewise variations along its width. In this work, we describe a laser light-scattering apparatus comprised of a 650 nm wavelength, 3 mW laser beam, and a CMOS camera that registers the scattering pattern. The laser beam is normal to the surface. The mechanical structure to support the optical elements was designed with Solid Works™, image acquisition and processing was performed in Visual Studio and C++ platforms. The system was calibrated using 304 stainless steel surfaces with average roughness 0.152 to 1.124 micrometers, produced with sandpaper, characterizing the effect of surface roughness and angular speed on the laser light-scattering pattern. Angular speed between 0 and 500 rpm, has no significant effect on the width of the scattering pattern for surface roughness between 0.152 and 0.802 micrometers. Then, wear scars were produced in a pin-on-disc set up, keeping average roughness within the interval previously determined. Finally, comparing the experimental results, we determined that for sanded surfaces the width of the scattering pattern increases with average roughness, while for wear scars, the relationship is quadratic.

Keywords: Laser light scattering, Roughness, Pin-on-Disk, Wear scar.
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[CHM-90] PHOTOPYROELECTRIC TECHNIQUE FOR OPTICAL CHARACTERIZATION OF PURE LIQUIDS

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Photopyroelectric technique, in the transmission configuration, was shown adequate for the measurement of the optical properties of pure liquids. The analytical scheme involves the scanning of the photopyroelectric signal as a function of the sample´s thickness. Optical absorption coefficients, at four wavelengths in the near infrared region (904 nm, 980 nm, 1310 nm and 1550 nm), were measured for eight pure substances, distilled water and glycerol, among them. Strong optical absorption was observed, especially for pure liquids with a hydroxyl group in their molecular´s structure.

Keywords: Photopyroelectric Technique, Optical Properties, Pure Fluids
Reference: J. A. Balderas-López, Generalized 1-D Photopyroelectric technique for optical and thermal characterization of liquids, Meas. Sci. Technol., num 6, vol. 23 (2012), 065501, 10pp.https://doi.org/10.1088/0957-0233/23/6/065501

[CHM-286] PHOTOTHERMIC INFRARED EMISSION OF SPUTTERING TARGETS FOR REACTIVITY INDICATIONS

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In sputtering deposition systems, several factors are commonly varied in order to be produce a coating or thin film, such as working gas, reactive gas, DC/RF power and even in some cases heating of the substrate to obtain a certain crystallinity or biasing of the substrate to improve certain properties of the deposited materials. Some characteristics of the sputtering techniques are usually left for granted, as for example, the intensity or shape of the magnetic field of the magnetron, or the cathode/target temperature as “room temperature”. The latter is not entirely a stable or constant during most of the sputtering processes, and in most cases, this can greatly affect the physical and chemical surface properties of the cathode/target and the resulting film. Furthermore, if a reactive atmosphere is used, the bombardment of excited species towards the cathode/target, will increase its temperature, and for higher powers this may rise significantly up to a point that can induce chemical reactions, thus changing the electric properties and also the sputtering yield.

In this work we present the results of studies of the photothermic emission in the infrared (IR) of several commonly used sputtering targets: Ti, Ti-O, Al, Al-O, Cr, Ag, graphite, Si and Si-O; via thermal imaging using an IR camera. Each of these materials have a unique thermal emissivity, thus we had to perform individual measurements to adjust each emissivity to match the temperature reading from an electric thermocouple. The results are expected to give information for in-situ measurements of the sputtering targets, and its possible reactivity during the bombardment processes throughout the coating deposition.

Keywords: IR imagery, magnetron sputtering, emissivity.
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CHM-244] SULFUR DISTRIBUTION OBSERVATION OPTIMIZATION THROUGH BACKSCATERED ELECTRONS IN CIS-1-4-POLYISOPRENE/CARBON NANOSTRUCTURE COMPOSITES

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Characterization through electron microscopy is a versatile technique to analyze material surfaces. Composites formed by cis-1,4-polyisoprene, as matrix, and carbon nanostructures, as filler, without the use of vulcanize agents were extensive examined. The Backscattered Electron Microscopy characterization enable to distinguish atoms with different atomic number due to a brightness difference. This technique was used to analyze the sulfur distribution into the composites due to, according with other spectral analysis, the linkage contribution between the polymer was given by the carbon nanostructures. The sulfur weight percentage in composites only represents the 0.3 % and its dispersion is fundamental to understand the polymer mechanic properties improvement, as the four times Vickers hardness increment. In order to ameliorate the sulfur observation through backscattered electron microscopy, a work distance between 10 and 11 mm was used with a voltage range of 10 to 20 keV. The composite was coated with gold and carbon, 15 nm thickness, to ensure the high current utilization. The variables voltage, thickness, and materials were simulated to analyze the electron penetration and backscattering coefficient. A better understanding of electron interaction, volume penetration, with the material, entails a more favorable characterization of sulfur distribution within the composite.

Keywords: backscattered electron microscopy, polymer composite, SEM, carbon nanostructure
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[CHM-25] Thickness dependence of optical properties of silver and aluminum ultrathin films

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Metal-based transparent films play an important role in modern optoelectronic devices and as radiative heat-reflectors in energy saving applications [1,2,3]. In this work, a study of transparent ultra-thin silver (Ag) and aluminum (Al) films is presented, where protection layers of titanium (Ti) and alumina (Al_2O_3) are added on the surface. This protection makes isolation of ultra-thin metal films from environmental media to avoid the corrosion. The thin films were synthesized by the magnetron sputtering technique and optically characterized by ellipsometry and spectrophotometry. Furthermore, surface morphologies of the samples were investigated using AFM and the chemical state using XPS technique.

Keywords: Thin-Metal-Film, Optical-Filter, Sputtering
Acknowledgments: This work was supported by the National Council of Science and Technology of Mexico, CONACyT (CB-2015-254494, PAPIIT-UNAM IT101017).
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Sesión Oral

[CHM-215] ANALYTICAL MODEL FOR THE SPECTRAL INTERPRETATION OF ATTENUATED TOTAL REFLECTION DATA FROM LOSSY SAMPLES: APPLICATION TO BULK AND THIN-FILM WATER AT TERAHERTZ FREQUENCIES

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Spectroscopy of biological samples at the mid-Infrared and terahertz (THz) frequency ranges for biological and medical purposes has acquired particular importance in recent years. Attenuated Total Reflection (ATR) is one of the most promising techniques for THz spectroscopy because the sample interacts with only the evanescent field, and minimal sample preparation is required. THz-ATR spectroscopy has become a powerful tool in the study of biological samples as well as in material science research. For these reasons, it is crucial to ensure a good understanding and interpretation of ATR spectra, especially since the water content of biological samples plays an essential role in their spectral response. This work reports an analytical and numerical interpretation of ATR spectra for highly absorbent liquids. Water in the terahertz range provides a good case of study, where both the real and imaginary parts of the complex refractive index increase with the wavelength to a point where losses are not negligible. Indeed, beyond the low-loss limit, the conventional definition of low absorbance, commonly accepted in ATR data interpretation does not apply anymore. Here, we present a systematic study including experimental spectra and finite element method simulations of bulk water and water films (thicknesses in the range 0.5-18 mm) to discuss the physical implications of the analytical model. One of the most important conclusions for the ATR spectroscopy community at any frequency range is that the condition for total internal reflection can never be satisfied for highly absorbent samples. However, it is possible to estimate the relevant parameters such as absorption coefficient and penetration depth from the signal retrieved in reflection after the ATR accessory. In conclusion, our results suggest that the community should be aware of the proposed analytical model for interpreting ATR spectra in general and particularly for terahertz spectroscopy of biological samples.

Keywords: terahertz, ATR, spectroscopy, water
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[CHM-294] Measuring non-conductive surface with Contact Kelvin Probe Force Microscopy

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In this work I present some details of the implementation in our microscope of the Kelvin Probe Force Microscopy technique in contact mode. The technique is useful to determine the junction potential difference between a non-conducting surface and the conducting probe of an atomic force microscope. It is observed that non-ferroelectric surfaces show a strong electromechanical hysteretic response in the loops obtained with write voltage, but in the read voltage the loop hysteresis is absent. The junction potential can be determined at zero bias and results indicate that there are considerable surface charge states on the non-conducting surfaces. To improve the sensitivity of the technique, in our implementation we take advantage of contact resonance tracking, in contrast to the original conception of Balke et. al. [1], which use a band of frequencies.

Keywords: AFM, junction potential, cKPFM.
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[1] N. Balke et. al., Exploring Local Electrostatic Effects with Scanning Probe Microscopy: Implications for Piezoresponse Force Microscopy and Triboelectricity, *ACS Nano* 2014, 8, 10, 10229–10236. https://doi.org/10.1021/nn505176a.+
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[CHM-140] OPTICAL PROPERTIES OF KNN FERROELECTRICS LEAD FREE OBTAINED BY HIGH ENERGY MILLING

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$K_{0.5}Na_{0.5}NbO_3$ (KNN) is a lead-free material with good ferroelectric, dielectric, and interesting optical properties. In this investigation, we synthesized KNN ferroelectric ceramics doped with La^{3+} (0.25% and 0.75% mol), Li^{1+} (0.9% mol) and Ti^{4+} (0.5% mol) individual and combined way to study their structural, ferroelectric, and optical properties. The synthesize process was made by mechano-chemical activation of the combination of oxides and carbonates powders. The chemical precursors for KNN system were K_2CO_3, Na_2CO_3, Nb_2O_5 and the dopants were Li_2CO_3, La_2O_3, TiO_2. The milling was made in a nylamid container with zirconium balls in a relation weight: balls 1:10 in an 8000 spex mixer mill for 2.5 hrs. after that the powders were pressed in circular disks and calcined at 800 °C. Finally, the samples were sintered at 1080 °C for KNN + Li1+, 1100 °C for KNN, 1060-1070 °C for KNN + La^{3+} Ti^{4+} and finally 1060-1070 °C for KNN + La^{3+}. The XRD analysis showed that the samples KNN and KNN + La^{3+} Ti^{4+} crystallize in the monoclinic phase, but the samples KNN + Li^+ crystallize in the orthorhombic phase. Uv-vis spectroscopy (380-780 nm) showed that the ceramic samples are transparent below the wavelength corresponding to 249 nm, where the samples do not absorb enough energy for electronic state transitions. The bandgap energy of all samples is in a range of 3.20-3.02 eV. In the fluorescence spectroscopy, we used excitation energy of 325 and 457 nm, and we can see the typical bands associated with oxygen vacancies.

Keywords: Optical, ceramic, Lead-free, milling, fluorescence, ferroelectric.
Acknowledgment: This work was supported by CONACYT. I also thank the CINVESTAV, Queretaro and LIDTRA team for allowing us the use of the laboratories for the characterization of the materials.

[CHM-314] Periodic Table's column modulation of the Shirley background of photoemission spectra of pure metals

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The 2*p* photoemission spectra of the third-period pure metals are similar enough to each other to display a meaningful progression of the characteristics of the peaks and background [1]. The same goes for the 3*d* spectra of the fourth row [2] and the 4*f* spectra of the fifth row [3] pure metals. In addition, there are similarities between the behavior, as a function of the column, of the peak and background parameters of these three rows, such as the intensity of the Shirley background. The Shirley background is largest for the first column (2B), decreases to a local minimum then rises again to a local maximum in the seventh column (8B). The large value of the Shirley background for the first column elements is correlated with the large asymmetry of the main peak and the presence of strong intrinsic plasmons. This correlation might be due to a similar physical origin [4] The local maximum in the 8B column coincides with the maximum of permutations of the valence band, as previously pointed out by Castle and Salvi [5]. The physical mechanism of these phenomena will be discussed.

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[CHM-220] Photoacoustic imaging using the Single-Sensor Scanning Synthetic Aperture Focusing Technique

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The photoacoustic imaging is proposed as a non-invasive biomedical detection technique that combines the high contrast of the optical excitation with the high spatial resolution of the ultrasonic detection. Investigations and proposals on the physical foundations as well as the reconstruction algorithms can improve the quality of the image. This work aims to present the results obtained with a proposed measurement technique and our reconstruction algorithm for photoacoustic imaging. The proposed experimental technique consists of a homemade photoacoustic tomograph in which both the light source and the detector are fixed, while the sample is rotating around a fixed axis. The photoacoustic wave is detected by the acoustic sensor in the plane defined by the sample cross section and the height at which the laser light strikes. The acquired electrical signals for the different positions of rotation are the entry data for the proposed reconstruction algorithm, which consists of a segmentation of the reconstruction sections in the computational grid using the synthetic aperture focusing technique. The images obtained from *ex-vivo* Sprague-Dawley rat heart and kidney, are shown, as well as a quantitative analysis of the image quality parameters. Demonstrating that the proposed detection and reconstruction method is suitable for tomographic detections systems providing high-quality photoacoustic images. The proposed measurement and reconstruction technique avoids the need of multiple characterized sensors and the multiplexing in acquisition, resulting in a low-cost experimental system to obtain photoacoustic images and to study its capabilities, reducing the computational cost and improving the quantitative quality parameters of the photoacoustic images.

Keywords: Laser-Induced Ultrasound, Delay-and-Sum beamforming, Synthetic aperture, Photoacoustic imaging.
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[CHM-275] Study of the 1D-laser-induced ultrasound longitudinal waves for multilayers solid-systems

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When thermal and stress confinement conditions are satisfied, the generation and propagation of laser-induced ultrasound (LIU) is governed by an inhomogeneous wave equation for pressure. These waves are longitudinal, and it has been shown that allows the thickness detection of a metal slabs [1]. In order to use the longitudinal waves to detect the thickness of two layered-systems, we explore the solutions of a proposed 1D-Cauchy boundary value problem for the LIU inhomogeneous wave equation. In the proposed mathematical solution, as well as, in the experimental arrangement, the Aluminum slabs are submerged in water. These samples with three different thicknesses (12, 6, and 3 mm) were exchanged to obtain all the possible combinations for the two-layered systems. In the first layered system, where there is a finite and a semifinite slab, the distance between the finite sample and the PDVF film sensor is fixed. While the distance between the finite and semifinite slab is adjusted for the data sweeping. Meanwhile, the second layered system, has two finite samples in which the distance between one of the finite slabs and the PDVF film sensor is fixed. The other slab is movable so we can vary the gap among them and recollect the data. The 1D-Cauchy boundary value problem for the LIU-inhomogeneous wave equation was solved in the frequency domain, considering a 532nm pulse laser with Gaussian finite time-width. The source term in the inhomogeneous wave equation was assumed to be proportional to the optical energy absorbed by the samples. A comparation between the experimental and theoretical data provided information about the layer's thicknesses, which suggest that the proposal can be applied to detect sub-superficial defects in manufactured objects.

[1] J. Appl. Phys. **130**, 025104 (2021); https://doi.org/10.1063/5.0050895

[CHM-268] Synthesis of inhomogeneous optical filters by Fourier Transform

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A rugate or inhomogeneous filter is a kind of optical filter whose optical thickness is denoted as the index profile continuously varies its refractive index perpendicularly to the substrate. In 1976, J. A. Dobrowolski et al. [1] used the equation developed by Sossi [2] to create a computation algorithm, which proved the potential of the Fourier Transform method for the synthesis of inhomogeneous filters. Since then, many applications have been proposed, some of them made in practical filters. According to the Fourier transform theory, there is a relationship between two different domains denoted as transform pairs. According to the Fourier transform principles, for the rugate filter synthesis method, more optical thickness (high frequencies) added to the filter, implies finer details in the desired spectral response (transmittance) can be achieved. These are the fundamental concepts for the present work and the obtained results.
This work demonstrates that the spectral response of a rugate filter can be improved as more optical thickness is added to the filter, also showing that Fourier theory statements can be applied to the rugate filters theory. The second point of the study is how thin the rugate filters can be built without compromising the spectral response, and also maintaining a viable optical thickness for experimental growing conditions.

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Keywords: Inhomogeneous filters, rugate filters, Fourier Transform

[CHM-271] Systematic Shirley background intensity assessment for the 2p spectra of the first-row transition metals

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In recent years the use of X-ray photoelectron spectroscopy as a characterization technique at the nanoscale has received widespread attention, and nowadays increasing works are published employing it as a powerful tool for chemical state determination. However, there are many contributions to the photoelectron spectra of many materials, which are complex with not so clearly defined natures, tampering with the quality of the analyses. This issue is far greater enhanced when transition metals are present, not allowing for a proper quantitative analysis of the experimental data. To solve the issue accurate background determination is paramount where theoretical and empirical approaches have been previously employed, where the empirical Shirley background used to reproduce the step-shaped nature of the photoelectron background remains the most accurate approach. Due to the satisfactory results in quantitation, the so-called empirical Shirley background may also have a physical origin as a previous report [1] has shown. Therefore, we present a systematic approach employing a well-established peak-fitting methodology to assess the Shirley intensity of the 2*p* photoemission spectra for the first-row transition metals. The results show that the Shirley background intensity is consistent and reproducible over many types of samples irrespective of the synthesis method and measuring conditions. Outstandingly, our results suggest that the Shirley intensity varies upon increasing atomic number, which might suggest that the Shirley intensity may be an intrinsic periodic property of the atoms. The Shirley intensity appears to be the largest possible when the *d*-band is almost empty or half empty, indicating the Shirley intensity might be related to many possible relaxation channels coupled to the available states in the *d*-band. Irrespective of the latter, we present an interesting trend that has not been before analyzed with the present degree of detail.

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[CHM-423] The 4f photoemission spectra deconvolution for Pt78 to Bi83

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The resulting peak fitting parameters obtained from analyzing the 4f and 4d core levels of the 6th period, from Pt (78) to Bi (83) of the transition metals and other metals by periodic table definition, have a well-defining behavior as a function of the atomic number. Assessing this dependence is a difficult task that requires state-of-the-art fitting methods because the spectra show complex asymmetry shapes, multiplet structure, plasmons, and also satellites. Through the use of the empirical double-Lorentzian lineshape, it is an approach to reproduce the asymmetry for all the elements (Pt, Au, Hg, Tl, Pb, Bi), suggesting that it could bear a fundamental basis. A combination of Shirley-type (SVSC) and Tougaard-type backgrounds was necessary to reproduce the data. The SVSC parameter has different improvements trying to understand the shape and correlate with an understudied physics. This resembles the behavior of the 2p spectra for the fourth-period and the 3d spectra for the fifth-period elements for the corresponding group elements. The fitting parameters employed in the analysis has been published in https://xpsoasis.org/.

Keywords: XPS, Photoemission Spectra, Tougaard Background, Shirley SVSC Background, Transition Metals.
This work was partially financed by Proyecto Fronteras 58518, Conacyt, Mexico.

[CHM-279] Uncertainty calculations in the photoemission process in X-ray photoelectron spectroscopy on soft and hard energies

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In the present work the methods for the calculation of uncertainties for spectra obtained by ARHAXPES and ARXPS are shown. The specimens correspond systems Zr-P4VP and Hf-P4VP deposited by spin coating with and without heat treatments, and deposition via PEALD. Results can be divided in binding energy of chemical states and intrinsic parameter values of the samples. As both are stablished as continuous data obtained from signal adjustments, the possibilities are open for determining uncertainty with levels of confidence (95% as commonly used. For binding energy, it was applied and ANOVA in two directions with a secondary evaluation using Welch's test for the ranges of Gaussian and Lorentzian values. The uncertainty of the variables such as elastic attenuation length and cross section which are related to the material and source energy of the x-ray beam were calculated in dependance of the incidence angles utilized for each sample with uncertainty relative to the mean. Overall results are presented under Beer-Lambert's law for multilayer samples.

[CHM-70] UNDERSTANDING THE CONDUCTIVE, PIEZOELECTRIC AND FERROELECTRIC BEHAVIOR OF ONE LAYER SOL-GEL BiFeO3 THIN FILMS

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Regularly, sol-gel $BiFeO_3$ films are deposited by nth layers (nL) until they reach a thickness that allows characterizing their macroscopic ferroelectric properties. However, the overall performance of the multilayer resulting in a $BiFeO_3$ film will be largely determined by properties of the first layer, but this has received little attention, even though defects of this layer can accumulate as the number of layers increases. Defects as cracks, leakage currents, or morphological may depend on the sol-gel synthesis method and can be examined in advance from the first layer. Here, we perform and electrical and ferroelectric study of one layer (1L) dip-coating sol-gel $BiFeO_3$ films throught two of the main reported sol-gel solutions that give rise to well-defined ferroelectric-loops when they are deposited with nL. The main variation in the two identified routes is the dissolvent, the first route being based on the toxic *2-methoxyethanol* (ME), and the second one on the relative safe *acetic acid* (AA) with some 2-*methoxyethanol.* We perform the study at the nanoscale using advanced atomic force microscopy (AFM) techniques to identify the fine features or defects of the 1L $BiFeO_3$ films. Our results reveal the occurrence of a dielectric breakdown at lower voltage for the ME films than for AA films, which agree with the observed in the conductive maps. The piezoelectric coefficient for ME films was found to be 20% higher than for AA films. Both deposition methods give ferroelectric films with an electromechanical strain controlled by the piezoelectric effect, while that of electrostriction one was minimal. An optimization for AA route in one of the deposition parameters, namely the immersion speed, results in a significant reduction of the dielectric breakdown and a more than twofold increase in the piezoelectric coefficient. Our results broaden the understanding of electric and piezoelectric behavior of 1L $BiFeO_3$ films.

Keywords: Perovskite films, $BiFeO_3$, PFM.
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[CHM-315] XPSOasis: the XPS Peak-Fitting Network

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The XPSOasis Web platform (https://xpsoasis.org/) aims to make available to the XPS community, free of charge, tools that facilitate communication between XPS users; this includes discussion forums and peak-fitting databases (one for each core-level), dynamic communication between users, and free data analysis software. The web platform allows users of different fitting software to easily upload posts to ask questions with images of the fitting that concern them. To answer the questions, the posts contain the data, allowing knowledgeable users to download and work on the recommendations. Novice users can consult expert users in direct conversations. Technical discussions on the analysis of XPS data can also be held.

To hook expert (and non-expert) users, the participation is rewarded with *Spicer* points, which are accumulated through *likes* in their posts (given by other users) and when one of their posts reaches the peak-fitting database (which is a decision of the corresponding moderator). Categories are defined in terms of the points. Users belonging to certain categories can compete to become moderators of a certain core-level forum and database. They could also offer courses. Another advantage of having posts in the database is that they become the norm and could be cited.

The usefulness of XPSOasis.org is a function of the availability of peak-fitting parameters for each core level for each element under a variety of chemical environments. Since it is a user-based platform, it becomes more useful as the number of user posts increases. This is a possible solution (which will, in fact, be provided by the XPS community itself) for the erroneous XPS analyses all too common in the scientific literature.

[CHM-448] Raman spectroscopy in Agave leaves powder for sugar quantification; pH-dependent optical properties of agave fluorescent compounds

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The efficient use of resources is vital for sustainable development. In particular, the production of second-generation biofuels obtained from organic material not used by the agroindustry is an area of opportunity for new development and research. In the production of biofuels, the ideal raw material is reducing sugars, corresponding to the energy storage of plants. Currently, the conversion into bioethanol from the leaves of Agave tequilana is being studied.The objective of the present work is to characterize the pH-dependent fluorescent properties and improve the quantification of sugars using Raman spectroscopy in aqueous extracts of agave leaves powder. The sequence of the work was as follows: the absorption wavelengths were identified using UV/Vis spectroscopy, the fluorescence spectrum of the samples was obtained by fluorescence spectroscopy, and the relationship between fluorescence and pH was studied by analyzing the Raman spectra performed at different pH values, and finally, the reducing sugars were identified in the Raman spectra. We found that the samples presented a strong fluorescence centered at 500 nm and 680 nm, to deal with the fluorescence present in the Raman spectra, the pH of the samples was modified from 4 to 12. It was found that at pH 9 the Raman signal presents a significant reduction in fluorescence and the damage caused by higher pH is avoided, when comparing the Raman spectra at different pHs it remains undisturbed, expanding the detection limits of reducing sugars. It is important to mention that this work focused on studying the reduction of fluorescence in the Raman signal, for future investigations of carbohydrates and other compounds of interest present in agave leaves samples. It is the first step and makes possible the study of different processes that involve the use of agave leaves and their study with Raman spectroscopy.

Keywords: Raman Spectroscopy, Agave, Biofuels, Fluorescence
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LUMINESCENCE PHENOMENA: MATERIALS AND APPLICATIONS

CHAIRMEN

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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
- Displays
- Solar cells

[LPM-127] Characterization of Cobalt Wolframate doped with Erbium

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Nanoparticles of Cobalt Wolframate doped with Erbium were made by the Solvothermal method assisted by microwave, the material comes naturally the Wolframite mineral and was synthesized using the precursors of Sodium Wolframate and Cobalt Chloride with Erbium doping concentrations of 0.5%,1 %,1.5%,3%,4.5% and 6%. Cobalt tungstate has a wide range of uses due to its optical and electronic properties, such as solar cells, transistors, UV lasers, sensor design, photoluminescent materials, etc.
X-ray diffraction (XRD) and scanning electron spectroscopy (SEM) were performed to characterize the structures and morphology of the nanophosphors, and their optical properties were determined by FTIR methods.
Through reported data, it is expected to observe spectral emissions in a range 410nm to 420nm with an excitation wavelength of 300nm, which corresponds to cobalt tungstate with an excitation wavelength of 488nm. Emissions are expected to be observed in 976, 847 , 668 and 550 nm, corresponding to the transitions of the Erbium ions.

[LPM-94] Eu(III) doped zinc vanadate nanoparticles, hydrothermal synthesis.

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This work reports the structural and optical properties of zinc vanadate powders doped with Eu (III) its synthesis was carried out by a double replacement chemical reaction supported by the microwave assisted hydrothermal method. For this material, luminescence spectra present bands associated with inter level transitions within the electronic energy states of Eu (III) ions, particularly those associated with transitions levels $^5D_0$ to $^7F_1$, $^7F_2$, $^7F_3$ and $^7F_4$, located at 590, 612, 650, and 697 nm, respectively. PL spectra show the characteristics emission displaying a dominant peak associated with the transition $^5D_0$ to $^7F_2$ at 612 nm, so that the light emission is predominantly red. SEM and XRD measurements for these phosphors will be presented as well.

[LPM-97] Formation and characterization of Calcium Wolframate activated with Europium synthesized by the Solvothermal technique assisted by microwaves

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Nanoparticles of calcium tungstate phosphors activated with Europium were synthesized by the microwave-assisted solvothermal method, which allows us to control different synthesis parameters, such as pressure, temperature, time, volume, etc. Allowing reproducibility of samples.
Calcium tungstate is a luminescent material that acts as a host for a variety of rare earth ions, the structural units of the tungstate ion absorb light in the short and medium wave UV range through charge transfer of oxygen ions to tungsten ions and the absorbed energy is transferred to rare earth ions, which subsequently undergo ff transitions and produce sharp emission peaks.
X-ray diffraction (XRD) and scanning electron spectroscopy (SEM) were performed to characterize the structures and morphology of the nanophosphors, and their optical properties were determined by FTIR methods.
The nanophosphors present emission peaks when excited with a wavelength of 265 nm and 395 nm, which correspond to the emissions of the matrix and europium, the emission wavelength of the matrix is between 350 mn and 500 nm, Peaks are also observed at wavelengths of 580 nm, 592 nm, 615 nm and 702 nm, which are associated with transitions corresponding to Europium, ranging $^5D_0$ to $^7F_0$, $^7F_1$, $^7F_2$, $^7F_3$ and $^7F_4$, respectively, where the emission most intense corresponds to 615 nm.

[LPM-182] Ionoluminiscence analysis of ZnO thin films.

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The focus of this work is to present the analysis of point defects in ZnO thin films using ion beam induced luminescence analysis or ionoluminiscence (IL). As some ZnO applications are related to oxygen vacancy densities, special emphasis was given to the effects on the luminescent spectra due to these punctual defect concentrations. The ZnO samples were made by thermal oxidation of metallic Zn thin films at 400ºC in air atmosphere for 1 hour. The Zn films varying their thicknesses were deposited on top of sodalime glass substrates by thermal evaporation using a basket filament under vacuum. The IL was performed by bombarding the samples by 2 MeV 4 He^{++} beam using the 3MV Pelletron Accelerator at the IF-UNAM. Part of the luminescent emission was captured by an optical fiber and registered with a spectrometer in the UV-VIS range. The ionoluminiscent spectra were analyzed by the deconvolution of Gaussian peaks, each one associated with a different punctual defect emission [1]. The decrease in luminescent emission intensity during the time that samples are being exposed to the ions, known as quenching, was also considered in the analysis. For samples subjected to a second heat treatment an increase in the intensity of the violet color center emission was observed.

Keywords: ZnO, thin films, ionoluminescence, punctual defects, oxygen vacancies
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Reference: Bertoni Álvarez, A..Análisis por ionoluminiscencia de defectos puntuales en películas delgadas de Zn0 creadas por medio de la oxidación térmica de Zn. (2022) [Tesis que para obtener el título de Licenciado en Física, Facultad de ciencias, UNAM] http://132.248.9.195/ptd2022/enero/0821800/Index.html

[LPM-147] Luminescence properties of Ag_m^(n+) clusters and Tb^(3+) doped ZnO-P2O5 glasses for solid state green laser and color tunable phosphor applications

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In recent years, several glass phosphors have been subject of studying for white light emitting diodes (WLEDs) applications. In this direction, the present work aims to analyse the structural and photoluminescence properties of zinc phosphate glasses activated with silver clusters (Ag_m^{n+}) and Tb^{3+} synthesized the by melt-quenching method. X-Ray diffraction (XRD) patterns showed an amorphous structure up to doping content of 3.0 and 1.0 mol% of Ag and Tb_4O_7, respectively. Raman spectroscopy indicated the existence of (P-O-P), (P-O-P), (PO_2), Q^2 and (PO_2), Q^2 vibrational modes, characteristics of zinc phosphate glasses. The optical properties evaluated by UV-Vis absorption spectra, revealed the absorption related band, which is attenuated as the Tb^{3+}:$^7F_6 \rightarrow {}^5H_7$, $^5L_{7,8}$, $^5D_2$, $^5L_9$+$^5G_6$, $^5L_{10}$, $^5D_3$+$^5G_6$ y $^6D_4$ bands grow. The emission spectra recorded under 325 and 351 nm excitation, displayed the wide : S_1, $T_{1,2} \rightarrow S_0$ band along with the terbium narrow $^5D_3 \rightarrow {}^7F_{5,4,3,2}$ and $^5D_4 \rightarrow {}^7F_{6,5,4,3}$ transitions. The intensity of such bands was modulated depending on the wavelength excitation and Tb_4O_7 doping content. This fact led to emission tonalities from bluish-white, neutral white to the green region, with correlated color temperature values in the 11631-6127 K range. The overall emission properties suggested that the zinc phosphate glasses activated with Ag_m^{n+} and Tb^{3+} might be suitable for green laser and color modulable phosphors.

[LPM-60] Luminescent properties in the vitreous zinc phosphate system coactivated with Ag_m^(n+) clusters and Pr^(3+).

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The research for sustainable energy sources has allowed the development of a wide range of solar cells. Particularly for Si cells, the absorption in the ultraviolet region is not very efficient due to thermalization processes. In this direction, zinc phosphate glass activated with Ag_m^{n+} and Pr^{3+} were prepared by melt-quenching method. The X-Ray diffraction patterns showed amorphous phases for doping contents up to 3.0 and 1.0 mol% of Ag^+ and Pr^{3+}, respectively. Raman spectroscopy revealed the existence of functional groups of tetrahedral phosphate chains: D(P-O-P), V_s(P-O-P), $V_s(PO_2)$,Q^2 and $V_{as}(PO_2)$,Q^2. The absorption spectra displayed the typical absorption band of associated with the Ag_m^{n+}:$S_0 \rightarrow S_1$ and Pr^3:$^3H_4 \rightarrow {}^3P_2$+$^1I_6$, $^3P_1$, $^3P_0$, $^1D_2$, $^3F_4$, $^3F_3$ and $^3F_2$. The visible emission spectra upon Ag_m^{n+} cluster excitation at 350 nm exhibited the characteristic cluster: S_1, T_2, $T_1 \rightarrow S_0$ broad bands, which presented the creation of sinks as the Pr^{3+} content increases, while the near infrared region displayed the Pr^{3+}:$^1D_2 \rightarrow {}^3F_{3,4}$ emission, as consequence of energy transfer from clusters. The presence of sinks on the Ag_m^{n+} cluster emission band revealed the existence of radiative energy transfer. Under Pr^{3+} excitation at 444 nm, the visible emission spectra showed the Pr^{3+}: $^3P_0 \rightarrow {}^3H_{3,4,5,6}$, $^3P_0 \rightarrow {}^3F_{2,3,4}$ and $^3P_0 \rightarrow {}^1G_4$ transitions, whilst the near infrared region displayed the Pr^{3+}: $^1D_2 \rightarrow {}^3H_6$,$^3F_{2,3,4}$ and $^1D_2 \rightarrow {}^1G_4$ transitions. The Ag_m^{n+} cluster emission decay profiles were shortened as the Pr^{3+} content increases, which was attributed to non-radiative energy transfer. Finally, the overall emission properties suggested that the zinc phosphate system coactivated with Ag_m^{n+} clusters and Pr^{3+} could be promissory for Si-C solar cell applications.

[LPM-123] Optical characterization of Er3+-doped CdO-B2O3-ZnO-V2O5 invert glasses

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Er^{3+}-doped $CdO-B_2O_3-ZnO-V_2O_5$ invert glasses were synthesized by the melt quenching technique, using starting proportions of 80, 12.5, 2.5 and 5.0 mol% of CdO, B_2O_3, ZnO and V_2O_5, respectively. The XRD patterns showed that the glass system is predominantly amorphous, with a segregation of a crystalline phase related to CdO species. The effect of Er^{3+} doping on the optical transparency was evaluated by plotting $(\alpha h\nu)^2$ and versus $h\nu$, for allowed direct transitions, showing that the Er^{3+} content increment did not modify the bandgap energy, keeping values around 2.75 and 2.50 eV, respectively. By using the Dimitrov-Sakka approximation, a refractive index value of 2.51 was found. The excitation spectra monitoring the emission at 1533 nm, exhibited excitation peaks corresponding to Er^{3+} transitions from the ground state $^4I_{15/2}$ to the excited $^4G_{11/2}$, $^2G_{9/2}$+$^4F_{9/2}$, $^4F_{5/2}$, $^4F_{7/2}$, $^2H_{11/2}$, $^4S_{3/2}$, $^4I_{9/2}$ and $^4I_{11/2}$ ones. The emission spectra in the infrared region, exciting at 521 nm, showed the characteristic Er^{3+}:$^4I_{13/2} \rightarrow {}^4I_{15/2}$ emission band centered at 1533 nm. Up-Convertion (UC) emission spectra recorded under 980 nm laser excitation, displayed the Er^{3+}green ($^2H_{11/2} \rightarrow {}^4I_{15/2}$ and $^4S_{3/2} \rightarrow {}^4I_{15/2}$) and red ($^4F_{9/2} \rightarrow {}^4I_{15/2}$) emissions. Such spectra were also monitored as a function of excitation power to recognize the mechanism involved in the UC process. Finally, from the experimental and theoretical oscillator strengths, the Judd Ofelt intensity parameters (Ω_2, Ω_4, Ω_6) were determined to evaluate potential laser applications.

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[LPM-327] Optical studies of ZnWO4: xHo-xYb crystal

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In the present work $ZnWO_4$: xHo^{3+} - xYb^{3+} phosphors synthesis using a double replacement chemical reaction by simple evaporation technique (SET) are reported. The resulting materials were washed using deionized water three times and ethyl alcohol once and then annealed in an electric furnace at 500 °C for 2 h. The X-ray diffraction results show an expected $ZnWO_4$ sanmartinite structure. Raman spectra displayed vibration modes mainly constitute by wolframite groups. As to their luminescent properties, phosphors under 980 nm laser excitation displayed two emission bands located at 541 and 670 nm associated with the transitions $^5F_4$, $^5S2 \rightarrow {}^5I_8$ and $^5F_5 \rightarrow {}^5I_8$ respectively, which are associated with inter-level transitions within the electronic energy states of Ho^{3+} ions revealing an up-conversion luminescence type. Although Ho^{3+} bands are clearly observed, it could not be possible without Yb^{3+} presence because an energy transfer Yb^{3+} to Ho^{3+} is observed, this topic will be fully discussed.

[LPM-438] OPTIMIZATION OF LUMINESCENCE OF CsCl:PbBr2 PEROVSKITES SYNTHETIZED BY AACVD.

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In recent years, the study of perovskites has grown considerably due to their optoelectronic properties that are well suited for devices such as solar cells, lasers, and light-emitting diodes, among others. In this work we report a study of the synthesis and characterization of the family of photoluminescent perovskites $Cs_xPbBr_{3-x}Cl_x$ on SiO_2, varying the nominal ratio CsCl:$PbBr_2$, by the technique of aerosol-assisted chemical vapor deposition (AACVD). The films were synthesized with thickness up to 700 nm at a substrate's deposition temperature of 132°. The morphology and chemical composition were studied by AFM, SEM, XRD and XPS. The optical properties were studied by UV-Vis transmittance and Photoluminescence. Emphasis is placed on finding the ratio of CsCl:PbBr2 for which the luminescence is maximized. The structural and optical characterization were correlated in order to find the emission mechanism responsible for the luminescence. For the perovskite family studied the emissions are centered at o2.55 eV, which corresponds to the blue-cyan color, and a luminescence maximum is found with a nominal ratio of CsCl/PbBr2=2/12.

Keywords: perovskite, luminescence, aerosol-assisted chemical vapor deposition.
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[LPM-74] PHOSPHORS SYNTHESIS BY DOUBLE REPLACEMENT CHEMICAL REACTION

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Double replacement reaction is considered an easy and non-expensive method to synthesize many compounds, because commonly factors as electronegativity values and solvents are responsible of the synthesis success. Some phosphors can be also obtained using this path, such as tungstates, silicates and vanadates, In the present work $CaWO_4:Eu^{3+}$, $ZnWO_4:Ho^{3+}$: Yb^{3+}, $Zn_3(VO_4)_2$ and $Zn_2SiO_4:Mn^{2+}$ synthesis will be discussed. Morphological and luminescent properties will be addressed also.

[LPM-190] Photoluminescent properties of hydroxyapatite with different amounts of functionalized multi-walled carbon nanotube

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The interest in studying the mechanical and structural properties of materials like hydroxyapatite (HAp) and multi-walled carbon nanotube (MWCNTs) arises because they have great biocompatibility with the human body and can be used to heal it. However, the photoluminescent properties of the HAp/MWCNTs composites have not been studied, and they can increase the applications of the composites in the medical areas as well in other science fields. In this research, hydroxyapatite and hydroxyapatite/functionalized multi-walled carbon nanotube (OMWCNTs) composites were obtained by co-precipitation method, followed by ultrasonic radiation and thermal treatment at 250 and 400 °C. X-ray diffraction (XRD) confirmed the presence of a hexagonal phase and showed changes in the crystallite size of all the samples, related to the heat treatment temperatures and the diverse concentration of OMWCNTs. The photoluminescent technique revealed that the influence of the two different thermal treatment temperatures shifted the maximum emission of HAp to higher wavelengths. The addition of the three different amounts of OMWCNTs (15, 25, and 35 mg) changed the maximum emission and intensity of each sample. These results allow presenting a proposal where the heat treatment on the composites with 15 mg of OMWCNTs help to modify the photoluminescent properties that one desires for different applications such as optoelectronic and medical ones.

Keywords: hydroxyapatite; functionalized multi-walled carbon nanotube; composites; photoluminescence
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[LPM-216] Structural and luminescent properties of ZnGa2O4 obtained by co-precipitation synthesis

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Spinels have attracted attention due to their potential applications *in vivo* imaging systems, identification markers, photocatalysis, and a wide variety of optoelectronic devices: solar cells, optical memories, and photovoltaics and sensing systems; as result of structural, optical and luminescent properties. Particularly the zinc gallium oxide ($ZnGa_2O_4$) a wide band-gap (4.4 to 5.0 eV) semiconductor has high chemical and thermal stability, stability under vacuum, emits in the blue region when it is irradiated with UV light, high transmittance against the UV region and photocatalytic activity [1]. Its properties can be influenced by the conditions of the synthesis method. In this work, $ZnGa_2O_4$ was obtained by co-precipitation synthesis at a molar ratio of 0.5 and a pHs interval of 6 to 12. In order to observe the pH effect and molar ratio on its properties. X-ray diffraction and reflectance data showed the pH effect on resultant phases as zinc oxide and Zn-Ga layered double hydroxides (LDH). The PL measurements showed the self-activated emission of $ZnGa_2O_4$ and its peak changes are attributed to a variation of cations incorporation into the lattice. The samples were subject to thermal treatment at 800 °C and the DRX results indicate the obtaining of highly crystalline spinels, however, the ZnO remained as a secondary phase at the highest pH. Band gap estimation confirmed the DRX results. The results of those characterizations promise to be reliable to continue research on the pH effect on the mechanism of formation of these materials.

Keywords: spinels, zinc gallate, pH effect, co-precipitation, photoluminescence
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[1] Y. Zhuang, J. Ueda, S. Tanabe, and P. Dorenbos, Band-gap variation and a self-redox effect induced by compositional deviation in $Zn_xGa_2O_{3+x}$: Cr^{3+} persistent phosphors, J. Mater. Chem. C, 2(28), (2014) 5502–5509. doi:10.1039/C4TC00369A.

[LPM-80] STUDY OF THE PHOTOLUMINESCENCE OF METALLURGICAL POROUS SILICON WITH OXIDIZING AGENTS

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Electroless etching of silicon in the presence of HF and strong oxidants is an emerging technique used to produce porous nanostructured structures, which could be used in semiconductor devices. This type of electroless etching to form porous silicon is well known as stain etching. Porous silicon powder (PSP) has attracted much attention due to its characteristic photoluminescence, large specific surface area, and controllable physical and chemical properties (with the porosity) for its application in many fields, particularly in optical/chemical/biological sensors and other devices[1]. In the present work, stain etching was used to prepare PSP metallurgical silicon powder. For stain etching it is usually necessary to add a metal salt (iron salts, for example), which at the end of the process leaves a stain mark in a porous layer. However, in this work the addition of the salt was not necessary since metallurgical grade silicon already contains high levels of iron impurities. The photoluminescence of the produced PSP exhibits a characteristic spectrum, given by surface defects and metallic impurities. In order to see if some of the defects of PSP are non-radiative, it was chemically oxidized with oxidants of different nature (acetic acid, nitric acid and hydrogen peroxide). Each oxidant had a different effect on the photoluminescence. The photoluminescence intensity is greatly reduced when applying hydrogen peroxide, which passivates the dangling bonds of the porosified surface producing silicon oxides. On the other hand, the interaction between PSP and nitritic acid or acetic acid enhances the intensity by removing impurities the material, which act as recombination centers. By these chemical treatments, it was then possible to tune the shape of the emission spectra, and to maximize their intensity. Large quantities of PSP with optimized photoluminescence could be obtained by stain etching followed by chemical oxidation, which represent a simple and economic process. The powders could be used for sensors of oxidative substances.

Keywords: porous silicon, photoluminescence quenching, photoluminescence enhancement
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Reference: [1]Vázsonyi, É., et al. "Porous silicon formation by stain etching." *Thin Solid Films* 388.1-2 (2001): 295-302.
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[LPM-49] SYNTHESIS AND PRELIMINARY STUDIES OF NOVEL Na2-xCsxZrO3 PEROVSKITE NANOPARTICLES

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The influence of Cesium doping on structural and optical characteristics of sodium zirconate has been investigated. The undoped and Cs^+ ion-doped Na_2ZrO_3 nanoparticles were synthesized via the citrate-ethylene glycol sol-gel route. All the obtained samples crystallize and are indexed to the monoclinic phase. The average crystallite sizes from the XRD analysis were 20 nm. Incorporation of Cs^+ ion enhances the stability of the perovskite tolerance factor (t = 0.916) which tend to be unity as against the undoped (t = 0.807); Cesium content reduced the rate of decomposition and weight loss from the TGA results. The energy band gap shows a decreasing trend with a red shift toward the visible wavelength, implying $Na_{2-x}Cs_xZrO_3$ semiconductor is a good host for photocatalysis, optical, and luminescence application.

[LPM-269] Ytterbium-Doped CsPbCl3-CsPb2Cl5 thin films deposited by AA-CVD with green synthesis approach and analysis of antisolvent use effect

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Inorganic cesium lead halide $CsPbX_3$ (X=Cl, Br, I) perovskites have recently received significant attention as luminophores in optoelectronic applications. Specifically, the $CsPbCl_3$ structure has the largest exciton binding energy and has been reported as an extremely sensitizer Yb^{3+} luminescence in nanocrystals, achieving photoluminescence quantum yields greater than 100%, a consequence of the quantum cutting effect. However, little has been reported about the reproducibility of this effect in thin films. The present work uses the Aerosol Assisted Chemical Vapor Deposition (AA-CVD) technique for depositing $CsPbCl_3$-Yb^{3+} perovskite films, resulting in a cost-effective alternative that allows antisolvent use in situ for assisted crystallization. Continuing in this green route, we analyzed the non-toxic antisolvent effects in the film morphology and stoichiometry and how these can contribute to the effective doping mechanism model, in which 2 Yb^{3+} ions replace 3 Pb^{2+} ions in the crystal lattice of $CsPbCl_3$, generating a bidimensional perovskite phase $CsPb_2Cl_5$. Results show that H_20 is an alternative green solvent that reproduces the sensitization of Yb_{3+} in CsPbCl3 films deposited by AA-CVD and how the generation of the $CsPb_2Cl_5$ phase is an indicator of this adequate sensitization. Moreover, we can control crystal size using green antisolvent that impacts the luminescence properties at a different wavelength.

Sesión Oral

[LPM-313] Antenna effect in CaF2: Nd/Yb/Li phosphors when are paired with 2-thenoyltrifluoroacetone (TTA)

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Luminescent materials based on lanthanides have a wide range of applications. Therefore, different precursors, synthesis processes, and junctions with other materials have been investigated in order to improve the luminescence of these compounds. An approach to improve the absorption range of lanthanide-based luminescent materials involves the use of organic ligands. It is well known that the absorption peaks of lanthanides ions are narrow because of their intrinsic electric properties. In this way, chromophores or organic ligands, with higher absorption capacities, serve as antennas when bound to lanthanides. In this work, CaF_2: Nd/Yb/Li phosphors were coupled with 2-thenoyltrifluoroacetate (TTA) to increase their luminescence in the near-infrared region upon UV excitation region.

[LPM-176] Carbon luminescent nanoparticles for diagnostics and treatment of cancer

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In the present work, carbon nanoparticles (CNP) were synthesized by microwave-assisted hydrothermal and ultrasonic agitation methods, and differences in luminescent properties as a function of synthesis parameters were explored. In the case of the microwave-assisted solvothermal method, the reaction time and temperature were modified. While in the case of ultrasonic agitation, a basic or acid medium was explored as well as different concentrations of precursors. All of them cases present luminescent emission in the visible region, but only the samples synthesized by ultrasonic agitation emitting in the red region of the spectrum. Since these samples have these kind of emission wavelengths (in the red region), they can be used in distinguishing, monitoring, and coupling with drug delivery vehicles commonly used for cancer treatment *in vivo*.

[LPM-243] Enhancing the luminescent properties of CVD synthetized SiO2/K2CuCl3 composites via manganese doping

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White light emission diodes (WLEDs) should have high luminescence efficiency and brightness, long lifetimes, low power consumption, and excellent stability. Phosphor converted WLEDs are the most common, however the color rendering index (<85) is less than expected for high quality general illumination. Recently, emission-tunable phosphors have been developed to avoid this disadvantage. Metal halides such as K_2CuCl_3 emit light with high efficiency due to their low dimensional structure and self-trapped exciton phenomenon[1]. In this work, SiO_2/K_2CuCl_3 Mn-doped composite material with a broad emission spectrum (350-550 nm) is proposed. We conducted the synthesis of this materials by Chemical Vapor Deposition, where precursors solutions and TEOS were ultrasonically nebulized and transported in N_2 to a tube furnace at 680 °C. The doping of manganese was controlled by varying the percent present in precursor solutions, ranging from 1.5% to 10% mol. To enhance their morphology and eliminate reaction by-products, we annealed the powders at 800°C and 1000°C for two hours. Structure, morphology, chemical composition, and optical properties of the composites were characterized using X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), Photoluminescence spectroscopy (PL) and UV-Visible spectroscopy (UV-Vis). Doping the photoluminescent material to promote energy transfer can produce novel luminescent materials for high-performance pc-WLED devices.

[1]Creason, Tielyr D., Timothy M. McWhorter, Zane Bell, Mao Hua Du, and Bayrammurad Saparov. 2020. K_2CuX_3(X = Cl, Br): All-Inorganic Lead-Free Blue Emitters with Near-Unity Photoluminescence Quantum Yield. Chemistry of Materials 32 (2020) 6197–6205. https://doi.org/10.1021/acs.chemmater.0c02098.

[LPM-238] Fluoride based luminescent material synthesized by Microwave-assisted Fluorolytic sol-gel route

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In the sol-gel synthesis, the first reaction is the hydrolysis of the metal alkoxide bond and then it may be named as hydrolytic sol gel synthesis, when the H_2O replaced by HF then we have Fluorolytic sol-gel synthesis. This latest synthesis has proven to be an excellent and versatile way to obtain different types of transition metal fluoride materials. Usually, this approach is based on the dissolution of metal alkoxides in an organic solvent. In this research work, we show a novel microwave assisted fluorolytic sol gel synthesis of microcrystalline K_2TiF_6 in 20 minutes at 150 °C. Ammonium fluoride (NH_4F) was used as a fluorination source instead of highly toxic hydrofluoric acid. K_2TiF_6 microcrystals were doped with Mn^{4+} ions by means of cation exchange reactions with K_2MnF_6 under acidic conditions. Photoluminescence spectra of Mn^{4+} doped K_2TiF_6 microcrystals show a group of sharp peaks between 600- 650 nm because of electronic transitions (^2E_g to $^4A_{2g}$) of Mn^{4+} ion, and whose PL maximum wavelength emission is centered at 630 nm. Moreover, several samples of Mn^{4+} doped K_2TiF_6 microcrystals exhibit a high PLQY near to 100 %. Optical (Photoluminescence spectroscopy), structural (X ray diffraction and FTIR spectroscopy) and morphological (TEM) characterization was conducted in order to analyze the properties of microwave synthesized red phosphors.

Keywords: Fluorolytic sol-gel synthesis, Fluoride based compound, Luminescent Materials
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Reference: Nicolas Goubard-Bretesch8, Erhard Kemnitz, and Nicola Pinna. Fluorolytic Sol–Gel Route and Electrochemical Properties of Polyanionic Transition-Metal Phosphate Fluorides. Chem. Eur. J. 2019, 25, 6189 – 6195 DOI: 10.1002/chem.201900186**.**
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[LPM-230] OPTICALLY STIMULATED LUMINESCENCE PROPERTIES OF THULIUM-DOPED MAGNESIUM PYROPHOSPHATE

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Continuous-Wave Optically Stimulated Luminescence (CW-OSL) is the emission of a material previously exposed to ionizing radiation and stimulated using light with a determined wavelength. The CW-OSL method is used in different applications such as: radiation protection (occupational and patient dosimetry, emergency response, area radiation monitoring), archeological and geological dating, food irradiation, accident dosimetry and material research. In this work the CW-OSL properties of dose-response, repeatability and fading of Thulium-doped Magnesium Pyrophosphate ($Mg_2P_2O_7:Tm^{3+}$) material were studied. $Mg_2P_2O_7:Tm^{3+}$ powders were synthesized using the solvent evaporation method. The photoluminescence (PL) emission and excitation spectra of the powders were analyzed. X-Ray diffraction patterns were measured to determine the crystalline structure of material. CW-OSL measurements were performed using an optical stimulation with blue light (458 nm) during 200 s. The stimulated emissions of powders were detected in the UV region through a set of filters Hoya U340 and Delta BP 365/50 EX. A blue emission (440-470 nm) of Tm^{3+} ions due to $^1D_2 \rightarrow {}^3F_4$ transition is observed in the PL emission spectrum and a UV band at 350 nm related to energy absorption from $^3H_6$ground level to $^1D_2$ excited level of Tm^{3+} ions is shown in the PL excitation spectrum. A monoclinic crystalline phase is determined by XRD in the of $Mg_2P_2O_2:Tm^{3+}$ material. The $Mg_2P_2O_7:Tm^{3+}$ powders were exposed to ^{90}Sr beta particles from 0.1 to 200 Gy. The powders show an intense CW-OSL curve with a fast decay within 5 s after stimulation. The CW-OSL intensity increases with the beta dose up to 200 Gy. A linear response from 0.1 to 65 Gy and a supra-linear range of 75-200 Gy are observed in the CW-OSL dose response test. After ten cycles of irradiation at 1 Gy and CW-OLS reading the $Mg_2P_2O_7:Tm^{3+}$ powders exhibit a well repeatability with a variation coefficient of 0.75%. The CW-OSL intensity of powders decreases with the storage time increase. The $Mg_2P_2O_7:Tm^{3+}$ phosphor shows well CW-OSL properties for its application in radiation dosimetry.

Keywords: Magnesium pyrophosphate, Thulium, CW-OSL, ^{90}Sr beta radiation.
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References: L. Yuan, Y. Jin, Y. Su, H. Wu, Y. Hu, S. Yang, Optically Stimulated Luminescence Phosphors: Principles, Applications, and Prospects, Laser Photonics Rev. 14 (2020) 2000123. https://doi.org/10.1002/lpor.202000123.
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[LPM-115] SYNTHESIS OF AL2(WO4)3:DY3+ PHOSPHORS USING EVAPORATION METHOD

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In this work, Dysprosium-doped Aluminum Tungstate $Al_2(WO_4)_3$ powders were synthesized via evaporation method using DI water as solvent, Aluminum Chloride ($AlCl_3$*AlCl3*) Dysprosium Chloride ($DyCl_3$*DyCl3*) and Sodium Tungstate (Na_2WO_4) as precursors; then it was submitted to heat treatment at 400°C for 2 hours. Evaporation is a procedure characterized by simple steps, high versatility and low cost. $Al_2(WO_4)_3$:Dy^{3+} optical properties were studied by photoluminescence (PL) spectrometry. Characteristic Dy^{3+} emission peaks at 481nm, 576nm, 669nm and 752nm were observed; $Al_2(WO_4)_3$*Al2(WO4)3* host presented photoluminescence emission peak at 391nm. Scanning Electron Microscopy and X-ray Difracction measurements will be discussed as well.

MICROELECTRONICS AND MEMS

CHAIRMEN

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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 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

[MEM-264] All Solution-Processed Hafnium Rich Hybrid Dielectrics Role in Hysteresis Free Metal-Oxide Thin-film Transistors

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Organic-inorganic (O-I) hybrid materials combine the great variability and interaction at molecular scale demonstrated to impact on properties, especially as gate dielectric thin films in thin-film transistors (TFTs). Benefits such as solution process, cost-effective and large-scale deposition, flexibility, and low-temperature process is critical for stimulating future flexible electronics device applications. Using the advantage of O-I hybrid materials, we present several $HfAlO_x$-PVP hybrid thin films in this study by incorporation of hafnium derivatives into pristine AlO_x-PVP hybrid solution. A facile dip-coating approach was used to deposit the hybrid thin films with a low processing temperature of 200 ^oC. We further studied the effect of Hf derivatives in hybrid thin films and their dielectric properties by varying the Hf/Al molar ratios. This study found that addition of Hf into hybrid thin films increased their dielectric characteristics more than AlO_x-PVP hybrid thin films. The dielectric properties performed on MIM capacitor structures showed low leakage current density of the order of $10^{-8}A/cm^2$. The frequency-dependent capacitance shows a high capacitance density up to 70 nF/cm^2 with low dielectric dispersion. These hybrid thin films further used as dielectric gate layers in solution-processed In_2O_3 TFTs to validate their electrical performance. The analysis of transfer curves of TFTs, revealing that the devices contain Hf rich hybrid dielectric films showed significant electrical performance with very low hysteresis, including saturation mobilities of 0.25 cm^2/Vs, a threshold voltage of 1.3V, a subthreshold swing of 0.37 V/dec and a high I_{on}/I_{off} current ratio of 10^6 respectively. Furthermore, we presented the feasibility of these hybrid dielectric layers in the fabrication of a-IGZO TFTs by RF magnetron sputtering other than In_2O_3 TFTs to examine the electrical characteristics such as electrical charge transport with other electrical parameters and demonstrated TFTs with mobilities of 3.39 cm^2/Vs, a threshold voltage of 2.2V, a subthreshold swing of 0.89 V/dec and a high I_{on}/I_{off} ratios of 10^6 respectively. In conclusion, the solution derived $HfAlO_x$-PVP hybrid dielectric thin films manifest potential dielectric aspirants for future low-cost and low temperature solution-based metal oxide TFT applications.

[MEM-170] COMPARISON OF THE OPTICAL PROPERTIES OF TITANIUM OXIDE NANOPARTICLES OBTAINED BY CHEMICAL AND GREEN SYNTHESIS BY MEANS OF THE SOL-GEL METHOD

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Abstract: In recent years, the green synthesis of nanomaterials has gained interest as an efficient and environmentally friendly method for obtaining metal oxide nanoparticles (NPs). In this work, the chemical and green synthesis of titanium dioxide (TiO2) nanoparticles by the sol-gel method is presented. Camellia sinensis extract (green tea) as reducing and stabilizing agent will be used. The morphological, structural and optical properties of the obtained nanostructures by the two methods were analyzed and compared. The morphology of the nanoparticles was analyzed by scanning electron microscopy (SEM). Micrographs showed quasi-spherical TiO2 nanoparticles. The structural properties of the TiO2 NPs were obtained by X-ray diffraction (XRD) and Raman spectroscopy. Crystalline phase formation of anatase was confirmed. Using UV-Vis spectroscopy, it was observed that the nanoparticles absorb in the UV range. The width of the forbidden band of the obtained NP's by green synthesis was greater than those synthesized chemically. The photoluminescence spectra shown bands located in the UV region, corresponding to the excitonic recombination of the electron-hole pair. The green method was viable, efficient, safe, simple, economical and ecological.

Keywords: titanium oxide, nanoparticles, green synthesis, sol-gel
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[MEM-53] ELECTROCHEMICAL SENSOR BASED ON COPPER-DECORATED SILICON NANOWALLS FOR THE DETECTION OF AMMONIA IN AQUEOUS SOLUTIONS

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Ammonia (NH_3) detection in aqueous systems is relevant because the presence of NH_3 is related to low quality of drinking water, hyperammonemia in COVID-19 patients, among others. In consequence, different types of sensors for aqueous ammonia solutions have been fabricated. Electrochemical sensors have arisen special attention due to their simple and affordable manufacturing processes, easy miniaturization, and good sensitivity. In the present project, we propose fabricating a new electrochemical sensor based on copper-decorated silicon nanowalls for the detection of NH_3 in aqueous solutions. Its detection mechanism is based on electrochemical reactions of copper (Cu) in NH_3 solutions **[1]**. Sensor's components are a) A working electrode made of copper nanoparticles that are deposited by an electroless wet chemical method. b) Silicon nanowalls prepared by Metal Assisted Chemical Etching (MacEtch), which serve as receptacles for the analyte. c) A counter electrode made of a noble metal film or wire.

We were able to synthesize Si nanowalls with a length of around 5μm, which assures that the sensed solution infiltrates to the bottom avoiding diffusion limitation. Using polyethylene glycol as a surfactant, Cu nanoparticles were evenly deposited by an electroless route on the surface of the silicon nanowalls. Solutions with different ammonia concentrations were analyzed by cyclic voltammetry using the sensor. Was identified a peak in the voltammogram whose intensity correlates with the concentration of ammonia in the solution. The voltammetric peak is associated with the oxidation of metallic Cu to Cu^{2+} due to the formation of cupric oxide and Cu-NH_3 complexes. Measuring solutions of different concentrations allowed to plot a calibration curve to determine the concentration of solutions with unknown ammonia concentrations. The present work represents a step forward towards the miniaturization of electrochemical sensors of liquid ammonia solutions. There is not such a device in the literature.

Reference: S. Yang, G. Zang, Q. Peng, J. Fan, Y. Liu, G. Zhang, Y. Zhao, H. Li, and Y. Zhang, In-situ growth of 3D rosette-like copper nanoparticles on carbon cloth for enhanced sensing of ammonia based on copper electrodissolution, Analytica Chimica Acta 1104 (2020) 60-68. https://doi.org/10.1016/j.aca.2020.01.010.
Keywords: microelectrochemical sensor, microstructured silicon, ammonia sensor
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[MEM-326] Flexible amorphous In-Ga-ZnO TFTs under simultaneous electrical and mechanical stress

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Flexible a-IGZO thin film transistors (TFTs) have been successfully demonstrated in applications such as displays, integrated circuits, sensors, and wearables. Some characterizations of flexible TFTs consist of measuring their electrical response under positive and negative gate bias stress (PBS and NBS) or under tensile bending at different bending radius. Nevertheless, in the literature there are few studies in which the flexible TFTs have been measured with a simultaneous mechanical and electrical stress. In this work, simultaneous mechanical and electrical stress were carried out under a tensile bending radius of 1, 2 and 4 mm, and a gate bias stress voltage of ±6 V during 3600 s. Bottom gate a-IGZO TFTs were fabricated on commercial 50 um thick Kapton HN polyimide by a complete photolithography process. All electrical characteristics under PBS and NBS presented an abnormal threshold voltage left shift which was mainly explained by the adsorption/desorption of water molecules at unpassivated the back channel. The Vth shift was modeled with the stretched exponential equation. Analyzed TFTs had a stable behavior under simultaneous stress until a 4 mm bending radius with electrical parameters Vth, SS, μ_{sat} and Ion/Ioff in the order of 0.7 V, 340 mV/dec, 6 cm^2/V-s and 5 x10^8, respectively.

Keywords: flexible electronics; IGZO; thin-film transistors
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[MEM-320] Nanowires of WO3 synthesized by HFCVD and CSVT techniques and their gas sensing properties

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Nanowires of tungsten oxide were obtained by two techniques, the first step consisted of depositing a porous layer via Hot Filament Chemical Vapor Deposition (HFCVD) and the second step was the growth of nanowires by Close Space Vapor Transport (CSVT). The material synthesized was annealed at 500 °C in air for 4 hours, the characterization shows nanowires of 5um in length, and the pattern of the material shows the phase transformation from $WO_{2.7}$ to WO_3 after annealing treatment. The gas sensing properties of the samples were studied through Au interdigitated electrodes fabricated over the silicon substrate but under the WO_3 nanostructures. The gas sensor properties were analyzed on a homemade test chamber using a synthetic airflow (flow, 0.1 l/min) and mixed with the testing gas 800 ppm for H_2, NO_2 and 700 ppm for acetone. The operating temperature was explored from 100 to 350 °C. The nanostructures show a gas sensing response of 27% to acetone (700 ppm) at 300 °C, the time response (t_{res}) and recovery (t_{rec}) were 162 s and 339 s, respectively. To hydrogen, the response was very low, 2% at 300 °C, t_{res} =90 s and t_{rec}=186 s. Finally, the response to NO_2 was 85% at an operating temperature of 200°C, and the t_{res} and t_{rec} were 123 s and 60 min, respectively. This report shows the growth of nanowires via CVD techniques, the material presents optimal properties for gas sensing mainly from NO_2. at 200,250 and 300°C. The material shows a low operating temperature compared to other similar works.

Keywords: chemical sensor, gas sensor, nanowires
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[MEM-347] Silicon microcavities for new surface science applications

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Silicon bulk micromachining is the primary technique for several well-known Microsystem applications. As a widely used academic tool, this technique is also the platform for scientific studies to develop novel 3D microstructures using silicon or other substrates. Some experimental microcavities, based on (0 0 1) silicon micromachining and aqueous potassium hydroxide (KOH) solutions, were analyzed in this work.
First, the precise alignment of squared-patterns parallel to the <1 1 0> axes of the oxidized substrates, lithography transferred over the photoresist, and finally, etching of squared cavities into the oxide film. After this selective etching step, the usually inverted pyramids develop by the anisotropy of the aqueous KOH solution into the (0 0 1) silicon. Then after stripping off the remaining oxide film, a second unmasked micromachining step is realized. This procedure reported by Kendall [XX] is under discussion because this unmasked anisotropic etching leads to developing aspheric cavities named micro-lenses.
The critical mechanism supporting this technique is the two-step etching following some fast-etching planes appearing around the surface squared cavity; after several hours, this procedure leads to rounded cavities taking advantage of the four-fold symmetry of the planar (0 0 1) surfaces.
About these rounded microstructures development, we identify the lack of thorough studies for these mechanisms leading to the controlled production of semi-circular structures, mainly when varied patterns are anisotropy evolving over these aspheric surfaces hosted into the low-index silicon.
In this contribution, new procedures for multi-step bulk micromachining based on (0 0 1) silicon substrates are presented, and additionally analyzes some mechanisms which produce varied aspheric cavities. Finally, some applications are part of the discussion for these novel micro-cavities.

Keywords: (0 0 1) Silicon, Bulk micromachining, KOH, Microlenses, High index planes
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[MEM-417] Synthesis of copper oxide thin films by the SILAR method as a semiconductor for potential sensor application.

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The search for materials based on metal oxides as thin films has increased in recent years due to the wide range of applications such as sensors, optical detectors, and photovoltaic devices. Copper oxide is a p-type semiconductor with a monoclinic crystal structure. This compound as the thin film is an excellent candidate for use in the production of microelectronic devices, due to its attractive microstructural, optical, and electrical properties. Copper oxide thin films were chemically synthesized on glass substrates using the successive ionic layers absorption and reaction (SILAR) method, which is an easy and inexpensive process. The chemical deposition consisted of 4 steps, using a solution of copper chloride complexed with ammonium hydroxide in deionized water as a cationic precursor, and deionized water at 90°C as an anionic precursor, an empty container as a drying stage, and finally a rinse bath in deionized water. The formation of thin films was identified thanks to deposition effects such as molar concentration of precursor materials, number of deposition cycles, pH of precursor solutions, immersion time and bath temperature, as well as final heat treatments. The resulting thin films were characterized and studied by X-ray diffraction (XRD), ultraviolet-visible spectroscopy (UV-Vis), scanning electron microscopy (SEM), and atomic force microscopy (AFM) characteristics. These analyses were performed to identify the structural, optical, and morphological properties of the metal oxide semiconductor material. Additionally, the electrical resistance was evaluated as a function of the finger gaps in interdigitated contacts, and the resistance response versus temperature for potential application in gas sensors.

Keywords: thin films, copper oxide, SILAR, semiconductor.
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[MEM-88] Zinc Oxide Mesoporous Electrospun Nanofibers

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Electrospinning is recognized as an efficient, powerful, and versatile method for generating mesoporous nanofibers based on different kind of materials like nanostructured oxide semiconductors. The main properties of the electrospun nanofibers, as the impact of solution parameters, such as molecular weight, viscosity and the polymer concentration as well as operating conditions have been extensively analyzed [1]. The present work reports the synthesis and structural, optical and morphological characterization of the zinc oxide (ZnO) nanofibers prepared by electrospinning technique. The synthesis process requires a starting solution of N,N-dimetilformamide, ethanol, and zinc nitrate as Zn precursor, under vigorous stirring for 2 hr. Then, poly(vinylpyrrolidone)(PVP) was added and continuously stirred to form a homogeneous viscous solution. Afterwards, electrospinning was performed at controlled operating conditions and looking for restricted environmental factors, such as relative humidity between 40-50 % and a temperature not higher than 22 °C. The above-mentioned polymer solutions were used subjected to 3 aging periods: 0, 7 and 13 days. Subsequently, the polymer fibers were calcined at 500 °C for 2 h in air. Structural characterization was executed through energy dispersive X-ray spectroscopy (EDS), whereas ultraviolet-visible (UV-Vis) and scanning electron microscopy (SEM) were utilized for the optical and morphological characterization, respectively. Finally, the main results obtained from these characterizations are presented.

Keywords: Electrospinning, Zinc Oxide, nanofibers, polymer solution, nanostructured oxide semiconductors

[MEM-410] Zinc oxide thin films by SILAR method as semiconductor material for sensor applications

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Zinc oxide thin films as n-type semiconductor material and hexagonal phase structure obtained by solution processes have great potential use in large area microelectronic devices as sensors, detectors diodes, transistors, solar cells, etc. The solution processes are considered substitutes for vacuum deposition methods of a huge cost reduction and enrichment of the structural, optical, and electrical characteristics. The zinc oxide was deposited on glass substrates by successive ionic layer adsorption and reaction (SILAR) method using a simple, economical, and easy process. The deposition method using 4 steps occurred from ammonium complexed zinc chloride in deionized water as a cationic precursor, hot deionized water at 90ºC as an anionic source, and two rinsing baths in-room deionized water after each precursor immersion. A post-annealing treatment in the air up to 400ºC for two hours was done to complete the zinc oxide phase formation. The ZnO thin film formation was obtained thanks to the parameter's deposition as immersion time, pH, the molar concentration of precursor materials as well as annealing. The structural, morphological, optical, and electrical characteristics of the resulting ZnO thin films were analyzed and discussed. Besides, the electrical resistance was evaluated versus temperature for potential application in gas sensors. On the other hand, it will be evaluated as photodetector material at wavelengths under 400 nm.

Keywords: zinc oxide, thin-film, SILAR, semiconductor.
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Sesión Oral

[MEM-357] ANALYSIS, DESIGN AND THEORETICAL EVALUATION FOR MICROFABRICATION OF SURFACE ACOUSTIC WAVE (SAW) SENSOR

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Surface Acoustic Wave (SAW) sensors have shown significant versatility in mechanical, biosensing, biochemical sensing, as well as compatibility with microfluidic systems; those sensors are based on transduction through a piezoelectric material like LiTaO3, LiNbO3, Quartz, Langasite, PVDF, etc. These materials use the electrical signal generated by the inverse piezoelectric effect; a signal created by the travel of acoustic waves on its surface. Different substrates or cuts can be chosen, such as 128°YX, 64°YX, 36°YX LiNbO3, YZ cut LiNbO3, ST-Quartz, so that certain types of waves are generated on its surface (e.g., Rayleigh, Leaky SAW, SH-SAW, Lamb wave, Love wave). This work contemplates the development of a microfabrication methodology and its specific application through the analysis of an SH-SAW sensor that was designed using a delay line configuration to implement a resonance frequency of 80MHz on a 64°YX cut LiNbO3 substrate. For the above, the most relevant design parameters (acoustic aperture, pitch design, bandwidth, number of fingers, etc.) are calculated and analyzed using transversal filters and circuit models employing mathematical modelling software Wolfram Mathematica® and COMSOL Multiphysics®. Microfabrication stages are experimentally demonstrated, morphological characterizations of the sensor are shown, and improvements are studied according to the analysis of manufacturing defects (short-circuited fingers, discontinuity) and their influence on sensor performance.

Keywords: Sensor, Surface acoustic waves, Delay line, Lithium Niobate.
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[MEM-223] FABRICATION AND CHARACTERIZATION OF P-N JUNCTIONS USING SnOx THIN FILMS FOR FLEXIBLE ELECTRONICS

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Tin oxide (SnO_x) has been widely used for the fabrication of transparent and flexible devices such as diodes and transistors because of its excellent optical and electronic properties. Also, it is well known that by varying the relative oxygen partial pressure (ppO_2) and the working pressure, the carrier type of the SnO_x thin films can change from p-type to n-type[1]. In this work, we obtained SnO_x thin films by DC magnetron sputtering varying the ppO_2 from 4.8 to 18.5%, the working pressure between 1.8 and 4.0 mTorr and using a power of 30 W. SnOx thin films were annealed at 180 °C for 30 min to ensure the complete formation of the SnO phase. The thin films were well-characterized by XRD, XPS, UV-vis, and Hall Effect. After the annealing at 180 °C, the films exhibited a tetragonal structure with Sn traces. P-type SnOx thin films were obtained in a ppO_2 range from 4.8% to 9.5%. XPS results demonstrated that the thin film deposited at ppO_2 of 8%, had Sn^{2+} content of 70%, and by further annealing it decreased to 34.3%. At ppO_2 of 18.5 % the Sn^{2+} content decreased from 42% to 39.8%, after annealing. SnOx film at ppO_2 of 18.5 % underwent less oxidation after annealing and showed n-type behavior. Using the conditions to obtain SnO_x thin films with n-type and p-type behavior, a p-n diode was fabricated using SnO_x thin film at a ppO_2 of 8.0 % and of 18.5 % on glass and polyimide substrates using lithography techniques. SnO_x junctions on polyimide exhibit I–V rectifying characteristics with a turn-on voltage of 2.24 V using Cr and ITO contacts. The diode fabricated on a flexible substrate retained its rectifying behavior even when it is bent, making it attractive for the transparent and flexible electronics.

Keywords: SnOx thin films, oxygen partial pressure, p-n junction, low temperature annealing, and flexible diode.
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Reference: J.A. Caraveo-Frescas, P.K. Nayak, H.A. Al-Jawhari, D.B. Granato, U. Schwingenschlögl, H.N. Alshareef, Record Mobility in Transparent p-Type Tin Monoxide Films and Devices by Phase Engineering, ACS Nano. 7 (2013) 5160–5167. https://doi.org/10.1021/nn400852r.
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[MEM-337] Parameter Extraction in Thin Film Transistors Using Supervised Learning

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Electronic simulation allows the design and testing of electronic devices or circuits prior to manufacturing, without the need to commit resources. Simulation software works by using mathematical models of the devices, which represent the behavior of the devices in the real world. The models are composed of parameters, which change from one device to another, but the value assigned to them, will define if the simulation will correspond to the behavior in the real world. For this reason it is of utmost importance to know the parameters of the devices, for which a process known as parameter extraction is performed. In the state of the art there are mainly analytical methods to perform this task, although methods based on genetic algorithms (GAs) have also been proposed as an alternative. Analytical methods require a lot of experience and knowledge in the operation of the device models, or defining the correct fitness function in the case of GAs to obtain good results. Therefore, an alternative to extract parameters based on supervised learning is proposed. Neural networks (NN)s, Random Forest (RF) and Support vector Regression (SVR) have been applied for parameter extraction in Thin Film Transistors (TFT). These methods are trained with sample I-V curves from which they must identify/predict the parameters that correspond to each sample. The proposed method has been shown to provide parameters that allow a modeling of experimental measurements of TFTs. Avoiding the need of having experience in parameter extraction and deep knowledge in the operation of the devices.

Keywords: Parameter extraction, Thin film transistors, Supervised learning, Machine learning, Electronic simulation.

[MEM-359] SIGNAL INTEGRITY FOR SURFACE ACOUSTIC WAVE DELAY LINE SENSOR USING MATCHING NETWORK

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The radiofrequency (RF) signal on a surface acoustic wave (SAW) sensor, in its configuration as a delay line, must have a special treatment at the input and output ports that will ensure an optimum performance of the sensor. A design of a complete SAW device must include external circuitry made of passive or active electronic elements that are connected to the input and output interdigital transducers (IDTs). The SAW sensor is considered as a 2-port network, and each port has a certain impedance level due to the design and fabrication of the IDTs. The consequence of an impedance mismatch is a poor transfer of the power signal to the SAW sensor. A part of the signal will be reflected from the input transducer to the source and on the other side, from the load to the output transducer. This work presents a methodology for the design of a matching network that ensures an optimum RF power transfer between the SAW sensor ports and circuits. First, a simulation of the frequency response of a SAW sensor with a resonance frequency of 112.96 MHz is shown, the simulation is programmed in *MATLAB* software. It is possible to calculate the admittance parameters of the sensor, and through them calculate the reflection coefficients S_{11} and S_{22}, the return loss and the voltage standing wave ratio (VSWR) of each SAW sensor port. Therefore, the design of the matching network topologies L and π are achieved through the resonance method and the Smith chart. This work shows that if a matching network is not used, 67% of the power signal could be reflected at the SAW sensor ports. Furthermore, we describe the advantages to the SAW sensor signal of having different quality factors Q from the two types of the matching network topologies.

Keywords: RF signal, SAW sensor, reflection coefficients, return loss, matching network.
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[MEM-91] Thin film phototransistors CdSe with TiSiOx-PVP hybrid gate dielectric, all-solution processed.

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Different molar concentration $TiSiO_x$-PVP dielectric, for a phototransistor application as a dielectric gate for a CdSe-based TFT are reported. Low temperature TiSiOx-PVP (200°C) solution process deposition with a molar precursors concentration 1:1:1, 1:2:1 and 1:2:2 of PVP:SiO_2:TiO_2, respectively, deposited by spin coating were performed. The samples were characterized morphologically and electrically, the dielectric properties were characterized by the fabrication of MIM and MIS devices. From 0 to 0.2MV/cm the leakage current density range was between 10^{-8}-10^{-5} A/cm^2 and the dielectric constant from 4 to 8 at 1MHz, with respect to the concentration. TFTs were fabricate with the selected hybrid dielectrics in ITO-coated glass substrate, the CdSe semiconductor was deposited by chemical bath deposition at 70°C. The TFT showed a very low hysteresis and operation voltage, subthreshold swing of 0.17 V/dec, threshold voltage of 1 V, on/off current ratio of 10^5 and mobility of 0.17 cm^2/Vs, finally, a wide light wavelength range photodetection capability was obtained.

Key words: solution process, hybrid dielectrics, CdSe TFTs.

[MEM-82] Thin film transistor and homojunction diode fabrication using room temperature deposited p-type ZnO:N

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Zinc oxide (ZnO) is one of the most extensively studied materials in recent decades. It is relatively easy to obtain n-type conductivity ZnO. On the other hand, the fabrication of p-type ZnO is not well established, and its reproducibility and long term stability are still under debate. Furthermore, according to most of the reports of p-type ZnO, temperature deposition and annealing processing above 400°C are required, which is incompatible with some applications such as device fabrication on flexible substrates. In this work, we present the low temperature (<200°C) microfabrication processing and electrical characterization of a p-channel thin film transistor (TFT) as well as a p-n homojunction diode. We employed reactive pulsed laser deposition (RPLD) at room temperature to deposit p-type nitrogen-doped zinc oxide (ZnO:N) thin films and n-type zinc oxide(ZnO) thin films. ZnO and ZnO:N had carrier concentration of -5.8×17cm^{-3} and +1×18cm^{-3}; mobility of 0.16 cm^2 V^{-1} s-^{1} and 0.5 cm^2 V^{-1} s-^{1}; resistivity of 10 ohm*cm and 5 ohm*cm, respectively. Both materials exhibited an Eg=3.29 eV, determined by cathodoluminescence. The homojunction diode had the following structure: bottom electrode, n-type ohmic contact, n-type ZnO, p-type ZnO:N, parylene-C as the insulating layer, and finally top electrodes. The diode exhibited rectification behavior and threshold voltage as low as 0.3 V. The thin film transistor had a staggered bottom gate architecture, with the following configuration: bottom gate, dielectric, p-type ZnO:N, semiconductor passivation/encapsulation layer, and source, drain and gate top electrodes. The TFT exhibited field effect modulation by positive gate voltage polarization, with I_{DS} current as high as -1×10^{-3} A. Both microdevices were fabricated employing photomask-assisted photolithography. The electrical nature of the devices allows us to conclude that we successfully achieved p-type behavior ZnO:N by room temperature RPLD.

MULTIFUNCTIONAL AND MAGNETICS MATERIALS

CHAIRMEN

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Materials capable of performing two or more primay functions, either simulteously 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 exaple) or single-phase materials that ma behave multifunctional under applied electric and/or magnetic fields. Besides, the technology around us has a fundaental 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 ceraics, which are used in electronic devices such as actuators, sensors, switches, capacitors, oscillators and ma also be used to mae 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 my phenomena that are in the frontier of knowledge such as “magnetoelectricity”, a property present in some multiferroic materials. For exaple, the fascinating magnetic spiral and helical structures that give place to an electrical polarization in some ceraics (maing 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 ma 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.

[MUL-11] 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 $Co_{0.25}Zn_{0.75}Fe_2O_4$ 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 $Co_{0.25}Zn_{0.75}Fe_2O_4$ 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 $Co_{0.25}Zn_{0.75}Fe_2O_4$ nanostructured material showed good mechanical stability, excellent magnetically 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.
Acknowledgments: This work was partially supported by Basic Science projects 2017 - 2018 A1-S-21323 and A1-S-21084, UABC-PTC-595 PRODEP-SEP, FORDECYT - CONACYT 272894, and DGAPA-UNAM, through research projects: PAPIIT IN103220, IG200320, IN110018, IN113219, and AG200320. Authors would like to thank the valuable technical support by Dr. Randy Dumas Quantum Design - Applications Department, Eloisa Aparicio, Eduardo Murillo, David Dominguez, Israel Gradilla, Francisco Ruíz, Jaime Mendoza, Michel F. Montañez, Maureen S. Cruz, Jessica I. Ortiz, and Luis A. Arce.

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[MUL-112] MAGNETIC PROPERTIES OF CaF2:Mn

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Mn-doped CaF_2 is a well-known material because of its thermoluminescent properties used in radiation dosimetry applications for the last four decades, however, due to the presence of manganese, it is possible to found some magnetic property in these compounds, what would them multifunctional materials. In this work, the magnetic properties of the Mn-doped CaF_2 powders synthesized by solid state reactions have been explored. The Mn content was varied in the range of 1 to 2.5 mol%. The phase identification and the solid solutions formation was confirmed by X-ray diffraction at room temperature. The solid solution limit was determined. The microstructure was observed by SEM and the magnetic properties were explored by measurements of magnetization as a function of the applied magnetic field. The obtained results are presented.

Keywords: CaF_2, magnetic properties, CaF_2:Mn, manganese doped compounds
Reference: N. Salah, N. D. Alharbi, S. S. Habib, and S. P. Lochab. Luminiscence properties of CaF_2 Nanostructure Activated by different Elements. Journal of Nanomaterials
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[MUL-407] MAGNETIC PROPERTIES OF NATURAL MATERIALS: THE CASE OF DESERT FLOWER

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The natural material's physical properties are a fascinating research subject because it is the basis of the comprehension of our world. In this case, the research on the physical properties of natural materials focused on the magnetic and related properties of "Desert Flower" because it is synthesized by nature in the presence of different kinds of minerals in the desert sands, where nanoparticles of iron oxides are very common. Thus, it could be interesting to know if these iron oxide nanoparticles are inside the "Desert Flowers" structure and if they have any effect on its physical properties. The research was carried out by first selecting the "Desert Flower" sample and then measuring the physical properties using X-ray Diffraction (DRX), Scanning Electron Microscopy (SEM), and Transmission Electron Microscopy (TEM), Vibrating Sample Magnetometry (VSM), and Electronic Properties Measurements (ETM). It was found that the sample was formed by gypsum and iron oxides in a fibrous microstructure. A magnetization close to 5 emu/g was found; its origin is from the iron oxide nanoparticles incrusted in the petal morphology. A magnetoresistance close to 1% was observed at an applied magnetic field of 1 T. Finally, the observed physical properties of this natural material give a piece of new knowledge to a better comprehension of our world.

Keywords: Natural materials; minerals; iron oxides; magnetic properties; magnetoresistance.
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[MUL-419] OPTICAL ABSOPRTION AND PHOTOVOLTAIC EFFECT OF LIQUID SUSPENSIONS OF IRON-DOPED LITHIUM NIOBATE POWDERS

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Abstract: lithium niobate (LN, chemical formula LiNbO3) is a ferroelectric material extendedly used in technological applications. Recent studies highlight its use as a photo-catalyzer to reduce carbon dioxide (CO2) and water treatment, having formic acid and formaldehydes as products. In the present work, the photovoltaic efficiency of liquid suspensions of LN doped with several iron (Fe) concentrations was assessed by means of cyclic voltammetrymeasurements. Six LN:Fe powders with variable doping concentration in the range 0.8-6.0 wt. % Fe2O3 have been prepared. They are derived from the synthesis of a common base material (the pristine structure), pure ferroelectric LN powders with the congruent chemical composition (LNCG, congruent point described by the ratio Li:Nb = 48.5:51.5). The pristine and LN:Fe samples were then subjected to thermal treatments in both reducing and oxidizing atmospheres, so that in total 21 samples were available for analysis –accounting also for samples without post-thermal treatment. All samples were characterized by X-Ray Diffraction and confocal Raman Spectroscopy. Mostly, pure ferroelectric solid solutions of LN:Fe were obtained, except for the two highest doping concentrations of 4.5 and 6.0 wt. % Fe2O3. Structural refinement procedures by the Rietveld method reveal that the percentage value of the secondary phase (Fe based) is marginal for the 4.5 doping concentration, regardless of the oxidation state of the samples. The photovoltaic studies show the viability of LN:Fe as a photo-assisted catalyzer (high doping concentrations). On the other hand, the (optical) absorbance of the pristine samples presents the expected linear behavior (Beer-Lambert law) in the ranges of 10-4 and 10-5 M(acetone), whereas the determined band gap (Tauc plot method) shows a reverse tendency (*Eg* lowers significantly as the concentration ratio is increased in the suspension) which is highly sensitive to the scattering properties of the suspended LN particles.

Keywords: lithium niobate, iron—doped, photo-assisted catalysis, optical absorption, liquid suspensions

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[MUL-180] Phase transition temperature study of VO2 to obtain metallic nanowires.

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ABSTRACT: The present work aims to study vanadium dioxide as a conductor controlled by the phase transition temperature. Variation of the electrical and optical properties occurs due to it changes from a monoclinic phase that it behaves as a semiconductor material to tetragonal rutile where it is presented as a metallic character. Metallic nanowires were obtained by using electrospinning technique. Vanadyl Acetylacetonate was used as an insertion in a PMMA matrix. Initial nanowires were calcinated to 600 °C. After thermal annealing, structural characterization and morphology were employed by using X-ray diffraction and scanning electron microscopy techniques, respectively, as well as UV-Vis spectroscopy range to determine the optical properties. XPS was used to obtain chemical environment information on VO2. While the electrical tests will be obtained using the two-point method, seeking to determine the electrical properties of the vanadium dioxide controlled by temperature at 68 °C.

Keywords: Electrospinning, VO2, Vanadyl Acetylacetonate, PMMA, metallic nanowires.
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One reference: S. Gnanasekar, P. Kollu, S.K.Jeong, A.N. Grace, Pt-free, low-cost and efficient counter electrode with carbon wrapped VO2 (M) nanofiber for dye-sensitized solar cells. 1-12 (2019)

[MUL-411] Synthesis of low and medium entropy alloys with cubic structure based on Fe, Co, Ni and Mn

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Abstract: Alloys based on transition metals with magnetocaloric effect have the potential to replace alloys used in magnetic refrigeration based on rare-earth elements. Among them, the low-entropy alloy of equal proportion between Fe, Co and Ni has a Curie temperature close to 1000 K, this alloy can have technological applications at room temperature if the Curie temperature is lowered. The main objective is to modify the proportion between the alloyed elements to lower the Curie temperature. 7 new alloys were synthesized using an electric arc melting furnace with the following atomic ratios between Fe:Co:Ni = 25:25:50, 20:20:60, 15:15:70, 10:10:80 and Fe:Co:Ni:Mn = 9.5:9.5:76:5, 8.5:8.5:68:15, 7.5:7.5:60:25. It was determined that the low and medium entropy alloys present an FCC structure without impurities, the lattice parameters obtained by X-ray diffraction patterns indicate a correlation between the changes of these parameters with the degree of substitution, there was a decrease in the FeCoNi alloys; instead, the FeCoNiMn alloys there was an increase. In addition, a reduction of the Curie temperature from 1000 K to 855 K was determined by modifying the degree of magnetic interaction between the three ferromagnetic elements in the low-entropy alloy. It is possible to adjust the Curie temperature in alloys based on Fe, Co, and Ni by modifying the proportion of these elements, however, to lower this temperature further, incorporating and increasing the concentration of Mn in the alloy will cause a dilution effect since this is a non-magnetic element.

Keywords: Low entropy alloy; Magnetic properties; Curie Temperature; X-ray diffraction, Crystal structure.
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This work was supported by: Consejo Nacional de Ciencia y Tecnología, national traditional doctorate scholarship program, scholarship number: 817062

[MUL-113] THE EFFECT OF THE Co CONTENT ON MAGNETIC PROPERTIES OF CaF2

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Recently, calcium fluoride, CaF_2, has aroused great interest on account of its diverse properties. It has been developed as a good thermoluminescent when it is doped with manganese. It has excellent UV transmittance, surpassing that of fused silica and it has been observed magnetic order at room-temperature in powders containing small amounts of impurities of CeO_2 even though in pure form it is a diamagnetic material.
In this work, the effect of the concentration of Co on magnetic properties of the Co-doped CaF_2 solid solutions have been explored. Solid solutions were synthesized by solid state reactions. The Co content was varied in the range of 1 to 2.5 mol%. The phase identification and the solid solutions formation was confirmed by X-ray diffraction at room temperature. The solid solution limit was determined. The microstructure was observed by SEM and the magnetic properties were explored by measurements of magnetization as a function of the applied magnetic field. The obtained results are presented.

Keywords: CaF_2, magnetic properties, CaF_2:Co, CaF_2 solid solutions
Reference: R.M. Rakhmatullin, V.V. Semashko, A.V. Lovchev, A.A. Rodionov, I.F. Gilmutdinov, A.G. Kiiamov. Magnetic properties of doped CaF2 powders,
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Sesión Oral

[MUL-19] ANALYSIS OF A POLYMORPHIC PHASE TRANSITION IN KNNLiTaLa0.01 USING TEMPERATURE-VARYING RAMAN SPECROSCOPY

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KNNLiTaLa0.01 is a promising lead-free piezoelectric material therefore its characterization is important for future technological applications. Using Raman spectroscopy, a study of a polymorphic phase transition in the KNNLiTaLa0.01 compound was performed. An analysis of the behavior with temperature, wavenumber and half width at full maximum of the individual bands corresponding to the vibration modes of the $(Nb/Ta)O_6$ octahedra of the compound's structure, was realized. Through this analysis it was concluded that the polymorphic phase transition of the KNNLiTaLa0.01 compound occurs not at a precise temperature but within the 90 to 105°C temperature interval. Additionally, using the Hard Mode Spectroscopy method, the value of the critical exponent of the order parameter was determined to be $\beta \approx ½$, indicative of a second order transition.

[MUL-126] EFFECT OF SILICON OXIDE SHELL THICKNESS ON MAGNETITE CORE: MAGNETIC, MORPHOLOGICAL AND ELECTRICAL CHARACTERIZATION

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Magnetite and silicon oxide (SiOx) nanoparticles (NPs) stand out from other materials because of their ferrimagnetic characteristics, uniform size distribution, functional surface, and versatility in terms of synthesis. Magnetite NPs were synthesized by the coprecipitation method. Using ferrous and ferric chloride salts (molar ratio of 2:1) and aqueous NH4OH solution. Over the magnetite core, it was grown a SiOx shell by the Stöber method. First, the previously synthetized magnetite (as core), was redispersed in tetraethyl orthosilicate (TEOS) (precursor for SiOx shell), and those volumes were calculated for theoretical shell thicknesses of 5, 10, 15 and 20 nm. Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM) images of magnetite NPs revealed that most of the particles are spherical with a regular average size (16.67 nm) and agglomerated. SEM images of the core-shell revealed irregular shell surfaces around the magnetite NPs. SAED (Selected Area Electron Diffraction) analysis for the core-shell NPs characterized crystallographic planes of oxidized magnetite species such as maghemite and hematite as well as the presence of SiOx. In the electronic paramagnetic resonance (EPR) spectra of 5 nm core magnetite and bare magnetite, a broad signal representing hysteresis is shown. The wave amplitude of the EPR resonance signal is due to the random orientation of the ferromagnetic particles, which scatter in the directions of the anisotropic field produced in the 10 to 20 nm thick samples by the coalescence between magnetite and silicon oxide originating an interface signal. A thin film transistor (TFT) was used to obtain the electrical properties of the core-shell NPs through output curves. Reflecting a semiconductor behaviour in the theoretical core-shell of 10, 15 and 20 nm obtaining the value of charge carrier mobilities and evaluating the saturation current for each sample.

Keywords: Magnetite, ferrimagnetic, core-shell, nanoparticles, silicon oxide.
Reference: de Mendonça, E. S. D. T., de Faria, A. C. B., Dias, S. C. L., Aragón, F. F. H., Mantilla, J. C., Coaquira, J. A. H., & Dias, J. A., Effects of silica coating on the magnetic properties of magnetite nanoparticles, Surfaces and Interfaces 14 (2019) 34-43. https://doi.org/10.1016/j.surfin.2018.11.005
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[MUL-92] Great magnetocaloric properties of polyurethane foam matrix composite with embedded lanthanum manganite particles

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This work deals with the effect that a porous structure causes on the magnetocaloric properties of substituted lanthanum manganite with the formula $La_{0.67}Ca_{0.28}Sr_{0.05}MnO_3$. A composite with a foam structure was fabricated using a polyurethane matrix and embedded manganite particles at three different amounts. The magnetocaloric effect was determined indirectly by mathematical adjustment of the experimental magnetization curves as a function of temperature, according to the phenomenological model proposed by Hamad. Based on the phenomenological parameters, the magnetic entropy change, ΔS_m (H, T), was calculated at 1.5 T and 3.0 T. Also, the Curie temperature, the relative cooling power, RCP, the heat capacity, ΔCp, and the order of the ferromagnetic-paramagnetic transition of all the samples were determined. Results show a highlighting increase of the relative cooling power when the manganite particles are dispersed in the polymeric matrix. In addition, the magnetocaloric properties turned out to be a function of the amount of manganite embedded in the matrix. Better results were obtained at a lower manganite content. In all the studied cases, the magnetocaloric properties of the foam composite are better than that of the powder. This behavior is attributable to a change in the interaction state of the manganite particles due to the confinement that they undergo in the polymeric matrix

[MUL-418] PROBE OF THE OPTICAL SECOND HARMONIC RESPONSE FROM MULTIFERROIC IRON-DOPED LITHIUM NIOBATE POWDERS

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Abstract: emphasis is put in this contribution to (optical) Second Harmonic Generation (SHG) as a characterization tool of random granular media. Recently, it has been reported that earthquakelike dynamics can be quantitatively described in detail at the laboratory scale, by performing shear experiments in granular media. In principle, remote, non-invasive SHG could be proposed as a probe to describe and predict seismic phenomena. Thus, a search follows immediately for novel seismic sensors (or gravisensors), which could operate under similar principles used by plants to maintain their vertical posture as they grow. Six LN:Fe powders with variable doping concentration in the range 0.8-6.0 wt. % Fe2O3 have been prepared. They are derived from the synthesis of a common base material (the pristine structure), pure ferroelectric LN powders with the congruent chemical composition (LNCG, congruent point described by the ratio Li:Nb = 48.5:51.5). The pristine and LN:Fe samples were then subjected to thermal treatments in both reducing and oxidizing atmospheres, so that in total 21 samples were available for analysis – accounting also for samples without post-thermal treatment. All samples were characterized by X-Ray Diffraction and confocal Raman Spectroscopy. Representative sets of samples also have been studied in detail regarding SHG, both in presence and absence of an external constant magnetic field, with emphasis on the reduced LN:Fe samples. Detailed SHG measurements convey the obtention of intensity depth profiles plus rotation of the linear polarization of the fundamental wave at selected depths, as previously reported in a contribution achieved by close collaboration between our researching groups. On this instance, however, we have focused the polarization analysis on a single depth, that at which the SHG intensities are maximal; distortions in the polarization-resolved plots can be traced because the SHG contribution from ballistic photons dominates that of multiply scattered photons which is naturally unpolarized.

Keywords: lithium niobate, second harmonic generation, ferroelectricity, ferromagnetism, granular media

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[MUL-446] Quantifying dipolar interactions in nanowire arrays using asymmetries in magnetization and demagnetization curves

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Arrays or assemblies of magnetic particles are of great interest since they show an extensive palette of properties that combine individual as well as collective magnetic effects, that lead to novel fundamental effects while also having a great potential for novel applications. Interaction effects in magnetic particle arrays play a very important role since they modify the energy landscape of the individual particles in the array. A direct consequence of the interaction field is that the properties measured on the entire array differ from those of the individual constituents, resulting in two fundamentally important problems: (1) understanding how the the properties of the array can be controlled o tailored using the intrinsic properties of the individual particles and the interaction between them, and (2) elucidate the intrinsic properties of the individual particles by interpreting the measurements obtained from the array which contain the additional contributions of the interaction field. Both problems require knowledge of the interaction field. In this sense, we propose and validate a method to quantify the interaction field based on the assumption that the interaction field can be related to asymmetries between magnetization and demagnetization curves. To this end, arrays of magnetic nanowires have been used and interaction effects have been studied using minor loops as well as complementary remanence curves. The results show that the method allows quantifying the interaction field as an average value or as a set of measurements that provide an interaction field distribution. We discuss the validity, limitations as well as possible improvements of the method to provide an accurate value of the average interaction field as well as for the interaction field distribution.

[MUL-339] VOLTAGE-CONTROLLED RESISTANCE SWITCHING IN THERMALLY BIASED VO2 PLANAR MICRO-DEVICE

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Complex metal oxides are now being under extensive research as they are a feasible alternative to extend the functionality of oxide electronics for information processing and storage beyond CMOS scalability in the nanotechnology industry. Researchers expect that this alternative could cope with the physical limits and their quantum effects. It is important to look for novel devices with enhanced storage density and long retention time. Novel devices could be based on recently discovered properties, such as the Structural Phase Transition and the Metal-Insulator Transition. They may be compatible with the integration processes of CMOS devices and capable of supplying the next generation of universal memories and processors. However, a scalability limit on the size of such devices is not clear and it is necessary to make a robust device. Vanadium dioxide (VO2) undergoes both mentioned transitions at a critical temperature of 68°. Below this Tc it exhibits a semiconductor behavior (monoclinic structure) while for temperatures higher than Tc it exhibits a metallic behavior (tetragonal structure.) In this work, VO2 370 nm films were grown (DC sputtering) on Al_2O_3 (0001) substrates. With these films microdevices were fabricated using contact UV photolithography. We found that it was feasible to control the threshold voltage of the transition by an external voltage in a thermally biased two-terminal 60, 36, 33 and 20 volts, respectively. I vs. V curves show a pronounced hysteresis and an abrupt jump in electrical conductivity indicating a clear transition. Some advantages of our device are: robustness, simple architecture and integration, and excellent performance in noisy surroundings. However, its high frequency response has not been yet evaluated and the power required may be high. Our oxide film is thicker than most devices reported by others.

Keywords: vanadium dioxide, Metal to Insulator Transition, Structural Phase Transition, resistance switching, photolithography.
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Reference: [1] A. Pergament, G. Stefanovich, and A. Velichko, Oxide Electronics and Vanadium Dioxide Perspective: A Review, J. Sel. Top. Nano Electron. Comput. (2014) vol. 1, no. 1, pp. 24–43.
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NANOSTRUCTURES

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Dear Friends and Colleagues,

We take pleasure to invite you to participate in the Nanostructures symposium of the XV international conference on surfaces, materials and vacuum. Participants interested in presenting an oral or poster contribution are invited to submit an abstract to the following link until June 30th:

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.

We look forward to welcoming you.

[NSN-436] A simple process to obtain Bi2Te3 hexagonal nanoplates

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In this report, we introduce the results of the synthesis and study of the physicochemical properties of hexagonal Bi_2Te_3 nanoplates obtained at atmospheric pressure and low temperature. The most attractive approach of this work was the obtaining of Bi_2Te_3 hexagonal nanoplates without employing expensive equipment, but by using a simple technique at atmospheric pressure in a simple convection oven at low temperature. The Bi_2Te_3 was processed into powder and drop-casted deposited on commercial glass substrates for its chemical, structural and optical analysis. Results of electron microscopy analysis indicate that our simplified method allowed the crystallization of Bi_2Te_3 in highly crystalline hexagonal nanoplates, grown along the basal plane corresponding to the rhombohedral crystalline phase of Bi_2Te_3, which resulted oriented in the (101) direction. The hexagonal crystals exhibited an extension of up to several hundred nanometers, with thicknesses minor than the Bohr radius of the exciton for Bi_2Te_3, within the interval of 20 to 40 nm, and with an interplanar spacing of 0.37 nm, which confirms the growth of the nanostructure along the basal plane of the rhombohedral crystalline phase of Bi_2Te_3. Likewise, Raman spectroscopy exhibited a vibrational mode around 120 cm^{-1}, corresponding to the mode, which appears due to the breaking of the symmetry of the crystal in the C axis of the rhombohedral structure of Bi_2Te_3, so that the thickness of the crystal is an order magnitude less than its extension. Finally, chemical characterization by XPS showed that despite the strong reactivity of the Te^{2-} ion precursor with the ambient oxygen does not inhibit the Bi_2Te_3 crystallization in hexagonal nanoplates under atmospheric pressure conditions at a lower temperature than that reported in other works.

Keywords: Thermoelectric, bismuth telluride, chalcogenides, atmospheric pressure, nanoplates.
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[NSN-179] AB INITIO BOND ELASTIC CONSTANTS IN SILIPHENE

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Carbon-substituted in silicene (siliphene), is a modified phase of silicene whose interest in recent years has increased due to its possible applications based on its mechanical and electronic properties. The semiconductor character of the material has been suggested in the literature, as well as a semimetal behavior. Elastic bond constants are useful in finite element-based predictive models for nanostructures. In this work we calculate the mechanical properties, in particular the bond constants K_r and K_f that are obtained from isotropic and axial strains, respectively. Calculations and comparisons of the electronic and phonon dispersion behavior for the material are presented. We perform calculations using density functional theory (DFT), using the GGA correlation exchange potential without spin polarization, 400 eV cutoff energy, and a 10x10x10 k-point grid for all calculations.

Keywords: Graphene, silicene, constantes elásticas de enlace.
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Reference: Khosravi, M., Badehian, H.A. & Habibinejad, M. A Comparison of the Structural, Electronic, Mechanical and Phonon Properties of Silicene and Carbon-Substituted Silicene from First Principles. J. Korean Phys. Soc. 77, 1183–1187 (2020). https://doi.org/10.3938/jkps.77.1183.
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[NSN-208] AB INITIO ELECTRONIC AND VIBRATIONAL PROPERTIES OF B12N12 FULLERENE

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Boron-nitrogen fullerenes have been investigated for several years, due to their interesting structures and physical, chemical and thermal properties. Currently, they are still being studied due to their possible application in fields such as molecular electronics and medicine. In this work we calculate the electronic and vibrational properties of fullerene B12N12 in order to compare the calculations made with the exchange and correlation functionals GGA and HSE06. The density functional theory implemented in the VASP code is used, which employs plane waves and pseudopotentials. A cutoff energy of 520eV and a 1x1x1 k-point grid is used.

Keywords: Nitrides, fullerene, electronic properties.
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Reference: Li, J & He, Tao & Yang, G. (2012). An all-purpose building block: B12N12 fullerene. Nanoscale. 4. 1665-70. 10.1039/c2nr11808d. DOI: 10.1039/c2nr11808d
This work was supported by: Universidad Autónoma de Yucatán.

[NSN-184] Ab Initio Study of the Single-Atom Promoted MoS2 Nanotriangular Models: Adsorption, Diffusion, and Incorporation of Noble Metals

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Transition metal dichalcogenides (TMDs) are a vast class of two-dimensional materials with the general formula MX_2, where M is a transition metal (TM), and X is a chalcogen element. The interest in TMDs has brought their application as ideal catalytic models in the fuel enhancement process for the removal of Nitrogen, Sulfur, metallic atoms, and enhancement of hydrocarbons. The higher catalytic activity of TMDs has been correlated with the incorporation of noble metals on MoS_2. Moreover, in light of the experimentally observed triangular morphologies in which the MoS_2 system stabilizes under sulfiding conditions, the edge termination has been taken into account as a further descriptor of the distinctive catalytic activity exhibited by these structures. Several inquiries about the precise location of the promoter adatoms, edge termination role, or the existence of a size-dependent catalytic effect remain an open debate. In this work, employing density functional theory, we describe the adsorption, diffusion, and incorporation mechanisms of single atom TM: Ru, Rh, and Pd to form promoted MoS_2 triangular structures. The models are consistent with the experimentally observed terminations -Mo(10-10) and S(-1010)-. Our results show that in both systems, the adatoms adsorb on a hollow site over the basal plane; however, a lateral four-fold configuration with the S atoms over the edge is the lowest energy configuration. Two diffusion trajectories -starting from the basal plane toward the lateral site- are presented for each termination. We have employed the surface formation energy (SFE) formalism to analyze the stability of incorporations considering exchanges between adatoms and one Mo atom at the center, lateral edge, and tip against the lateral adsorption. Upon varying the chemical potential limits, the analysis unveils that for Mo poor conditions, the incorporation is favored only in the lateral site but depends on the adatom's size.

Keywords: Transition-metal dichalcogenides, edge-termination, stability, promoter, diffusion, DFT.
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J.I. Paez-Ornelas, R. Ponce-Pérez, H.N. Fernández-Escamilla et al. The effect of shape and size in the stability of triangular Janus MoSSe quantum dots. Sci Rep 11, 21061 (2021). https://doi.org/10.1038/s41598-021-00287-6
This work was supported by DGAPA-UNAM projects IA100822, IN110820, and IG200320. Calculations were performed in the DGCTIC-UNAM Supercomputing Center, projects LANCAD-UNAM-DGTIC-368 and LANCADUNAM-DGTIC-150. J.G.S. acknowledges LNS-BUAP and THUBAT KAAL IPICYT supercomputing center, projects 202201042N and TKII-JGSA001, for computational resources. We thank E. Murillo and Aldo Rodriguez-Guerrero for their technical support.

[NSN-142] An ecological approach for the synthesis of multi-shape silver nanocrystals

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Abstract: Eco-friendly methods have been a highly efficient alternative in nanomaterial synthesis methods. The advantage of using low cost and low toxicity materials represents a great possibility to apply nanoparticles in unexplored areas of medicine and industry. In addition to other nanotechnological applications such as catalysis, electrocatalysis, optoelectronics, sensors, coatings and photothermal therapies. A novel bottom-up synthesis method for obtaining multi-form silver nanoparticles at room temperature in suspension with high stability 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 with different geometrical shapes (nanoprisms, nanorods, nanorings, among others). The EDS spectrum gave evidence of the chemical composition of the synthesized nanoparticles. Optical absorption measurements showed an absorption band characteristic of the surface plasmon resonance (SPR) of the silver nanoparticles. It has been found in several studies that the SPR can be more intense in non-spherical nanoparticles. Therefore, a multi-form nanoparticle solution could represent an advantage. The obtained nanoparticles were incorporated in coatings, with the purpose of taking advantage of the antimicrobial properties of AgNPs.

Keywords: Nanomaterial synthesis; Silver nanoparticles; Characterization of nanomaterials; bottom-up synthesis method; Surface plasmon resonance (SPR)
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Reference: Restrepo, C. V., & Villa, C. C. (2021). Synthesis of silver nanoparticles, influence of capping agents, and dependence on size and shape: A review. Environmental Nanotechnology, Monitoring & Management, 15, 100428. https://doi.org/10.1016/j.enmm.2021.100428

[NSN-293] APPLICATIONS OF GRAPHENE IN BREAST CANCER TREATMENT

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Breast cancer is considered as a health problem worldwide and is the second most frequent cancer with 1.7 million diagnosed cases worldwide. The strategies to reduce and control breast cancer have focused on its prevention, early detection, and treatment. However, the current treatments are neither capable to stop its propagation and/or recurrence on healthy cells. Furthermore, breast cancer treatments are not specific and harm healthy tissues and cells. It is well known, that the activity of anticancer drugs is greatly attenuated by the time drug reaches its target, which causes the ineffectiveness of the treatment and increase off-target effects. To achieve the effectiveness of breast cancer treatment it is necessary that the drug be administered in the proper dosage and shows its maximum activity in cancer cells. Recently, there has been an increasing number of scientific evidence that offer new alternatives for the design and development of novel anti-breast cancer drugs using desirable nanomaterials that have the capability of increasing local concentration of drugs in and around cancer cells, thereby reducing the potential toxicity toward healthy cells. Carbon-based nanomaterials are an emerging technology with promising applications in medicine, particularly for detecting, diagnosing, and treating breast cancer. Among the wide variety of carbon-based nanomaterials, graphene is of particular interest to scientific community due to their ultra-high surface area, versatile chemical functionalization, biocompatibility, as well as its unique physical, chemical, and mechanical properties. Scientific evidence shows that graphene-based materials could induce apoptosis in cancer cells while showing low toxicity due to their carbon structure. Therefore, these materials can be used as nanodrugs, or biological carriers (nanocarriers) to introduce small molecules such as nucleic acids or drugs into human cells to achieve treatment goals. This generates new possibilities for the development of innovative systems to the treatment of breast cancer and can be used to detect this disease at much earlier stages. Thus, in this conference we present the current status and future potential applications of graphene in the treatment of breast cancer.

Keywords: breast cancer; graphene; treatment; carbon nanomaterial
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[NSN-135] BiOI-BASED NANOCOMPOUNDS APPLIED AS ADSORBENTS AND PHOTOCATALYSTS OF ORGANIC CONTAMINANTS IN AQUEOUS SOLUTIONS

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ABSTRACT: According to the United Nations (UN), more than 40% of the population is affected by access to water. In addition, there is global concern about the contamination of this vital liquid. Different techniques have been applied to treat contaminated water, among which adsorption and photocatalysis stand out, which together provide greater overall efficiency to the elimination of dyes and pharmaceuticals. In this work, BiOI-based nanocomposites (NCs) decorated with graphene (G) and silver (Ag) were synthesized by solvothermal route: BiOI, G/BiOI, Ag/BiOI, Ag/G/BiOI. The NCs were characterized by several analytical techniques: XRD, zeta potential, N2 physisorption, photoluminescence, SEM, Raman, and UV-Vis DRS. The NCs exhibited micro flower-like morphology constituted by BiOI nanosheets and specific areas (SBET) between 55 and 63 m2/g. Adsorption and photodegradation of rhodamine B (RhB) and tetracycline (TC) were studied. The as-synthesized NCs exhibited adsorption capacities of RhB and TC varied from 36 to 39 and from 83 to 86 mg/g, respectively. The adsorption capacities of TC on the NCs were higher than reported in the literature [1], and the G/BiOI NC presented the highest sorption capacity. The degradation percentages of RhB using NCs resulted in the interval of 86 - 100 % in 480 min, using 19 W white LEDs (SMD, 5050) as an illumination source. On the other hand, TC degradation varied from 70 to 81 % within 45 min of applying 100 W blue LEDs (COB) to irradiate the suspension. The Ag/BiOI NC exhibited the highest performance to degrade RhB and TC.

Keywords: BiOI, photocatalysis, adsorption, rhodamine B, tetracycline.
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Reference: [1] R. Hao, X. Xiao, X. Zuo, J. Nan, W. Zhang, Efficient adsorption and visible-light photocatalytic degradation of tetracycline hydrochloride using mesoporous BiOI microspheres, Journal of Hazardous Materials. 209–210 (2012) 137–145. https://doi.org/10.1016/j.jhazmat.2012.01.006.
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[NSN-233] BISMUTH VANADATE-BASED NANOSTRUCTURES WITH ENHANCED PHOTOCATALYTIC PERFORMANCE FOR DEGRADING ORGANIC POLLUTANTS AND INACTIVATING MICROORGANISMS

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ABSTRACT: World Health Organization (WHO) defines contaminated water as water that cannot be used for essential activities and is considered an unhealthy resource by containing bacteria and organic pollutants. The presence of these pollutants in water represents a health risk and is estimated to produce more than 500,000 deaths worldwide [1]. From the view of sustainable development, the application of polluted water treatment technologies of low cost and high efficiency is vital. Heterogeneous photocatalysis, a semiconductor-based technology, is viable and considered green [2]. In the present work, bismuth vanadate nanostructures ($BiVO_4$-NEs) were synthesized and decorated with Graphene (G) and Silver (Ag): $BiVO_4$, G/$BiVO_4$, Ag/$BiVO_4$ y G/Ag/$BiVO_4$ with the aim of photodegrade dyes and photoinactivate bacteria. Physicochemical characterization of NEs was performed by different analytical techniques: XRD, TEM, Zeta Potential, N_2 physisorption, photoluminescence, Raman, and UV-Vis DRS. The photodegradation of Violet Crystal (VC) and the inactivation of *E. coli* were also studied. The NEs exhibited branched morphology and presented a rougher surface due to the deposited silver particles. XRD analysis showed the $BiVO_4$ monoclinic crystalline phase and crystallite sizes around 43 nm. The degradation percentage of VC achieved by NEs varied from 73 to 100 % within 180 min, using blue LEDs as the illumination source (19 W). The photoinactivation of E. *coli* (100%) was attained at 60 min of irradiation with Ag/$BiVO_4$ and by using G/Ag/$BiVO_4$ at 180 min. The NE that exhibited the highest performance in VC photodegradation and *E. coli* inactivation was G/Ag/$BiVO_4$. Trapping experiments and reuse cycles were performed to determine oxidative species that cause the VC photodegradation and *E. coli* inactivation and evaluate the possibility of NEs reuse.

Keywords: $BiVO_4$; synthesis; photocatalysis; violet crystal; *E. coli* photoinactivation.
References: [1] M. Pal, Y. Ayele, A. Hadush, S. Panigrahi, and V. J. Jadhav, "Public Health Hazards Due to Unsafe Drinking Water," *Air Water Borne Dis.*, vol. 7, no. June, pp. 1–6, 2018, doi: 10.4172/2167-7719.1000138. [2] C. Regmi, D. Dhakal, and S. W. Lee, "Visible-light-induced Ag/BiVO4 semiconductor with enhanced photocatalytic and antibacterial performance," *Nanotechnology*, vol. 29, no. 6, 2018, doi: 10.1088/1361-6528/aaa052.
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[NSN-312] BRAGG MIRROR OF SIO2 AND TIO2 FOR LIGHT COUPLING BASED ON PEROVSKITES

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Alternate layers of SiO2 and TiO2 were deposited by AACVD/pyrolysis at different thicknesses in order to obtain resonant structures at a given wavelength (Bragg-mirror). During the growth of the films, the difference in refractive index and thickness were analyzed by following parameters: deposition flow, substrate temperature, molar concentration, distances and deposition times. Also, a layer of different perovskites were deposited on the multilayers obtained to improve the intensity of light emitted. The resulting films were characterized by XRD, ellipsometry, SEM, UV-Vis and fotoluminiscente analysis.

[NSN-251] CDSE NANOPARTICLES PROCESSED BY LASER FRAGMENTATION IN LIQUIDS

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Laser Fragmentation in Liquids (LFL) is a physical technique to produce metallic and semiconductor nanoparticles (NPs). The synthesized NPs are pure and ligand free. Among the advantages of this technique we found: the experiment is simple, low cost and safe. For medical and biological applications, the NPs could be recovered with other semiconductor materials like silicon oxide or zinc sulfide. To process cadmiun selenide (CdSe) nanoparticles, CdSe powder at different concentrations was used in a constant volume of acetone (40 ml), in order to get a colloidal solution. A Nd:YAG pulsed laser was used to irradiate the colloidal solutions during 30 minutes, a lens was used to concentrate the energy in a focal spot. The laser was tuned in the 3rd harmonic to get 355 nm wavelength, with 30 Hz of frequency. After samples irradiation, a change in color was observed, the solution got homogeneous yellow tone that was increased with the output power and the concentration of the CdSe powder. The transmittance specter was taken with the Spectrometer Perkin Elmer Lambda 35 and the band gap shift was observed. For the Raman and Photoluminescence characterizations, 2 ml of the solutions were evaporated on glass and silicon substrates.

Keywords: Nanoparticles, CdSe, fragmentation, quantum dots
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[NSN-428] CHEMICAL AND OPTICAL PROPERTIES OF CUBIC InxGa1-xN/GaN QUANTUM WELLS

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The $In_xGa_{1-x}N$ compound represents a potential and viable alternative for solid-state lighting applications among the nitride family, such as LEDs [1]. We report the growth of $In_xGa_{1-x}N$/GaN quantum wells (QWs) in metastable-cubic phase (c-$In_xGa_{1-x}N$/GaN) by conventional Molecular Beam Epitaxy (conventional MBE) on GaAs (001) substrate. 10 nm-thick QWs with 30 nm-thick GaN barriers were grown. A chemical abruptness of the interfaces in these applications and a homogeneous atomic distribution in the wells must be achieved. We used secondary ion mass spectroscopy (SIMS) to analyze these features in QWs grown. The In-depth profile of three c-$n_xGa_{1-x}N$ QWs grown by conventional MBE was observed. Moreover, our studies provide information on the stable atomic arrangement of c-$In_xGa_{1-x}N$ QWs by X-ray photoelectron spectrometry (XPS). With optical techniques, we studied the excitonic transitions in the visible spectrum range from 495 to 570 nm; these emissions were obtained in the green wavelengths for QWs. These emissions are in good agreement with the theoretical calculations performed, where the excitonic binding energy was calculated according to the matricial model. Our work can facilitate the design of the active region for LEDs.

Keywords: c-$In_xGa_{1-x}N$ quantum wells, cubic-metastable phase.
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[NSN-47] CONFINEMENT STATES IN QUANTUM DOTS OF INAS EMBEDDED IN ALGAAS ASYMMETRIC MATRIXES.

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A low-dimensional system (LDS) is one where the degrees-of-freedom electrons, phonons, or photons is restricted from full three dimensions of our world. Motivated by a constant stream of striking discoveries and also by the potential for, and realization of, new state-of-the-art electronic device architectures the LDS encouraged lots of investigations during the past thirty years. The semiconductor quantum dots (QDs) are a particular LDS where the motion of electrons is restricted to zero dimensions and likewise, novel physical properties are expected. High quality QDs can be self-assembled by employing deposition techniques like molecular beam epitaxy, and in order to develop QD-based devices further mechanism to successfully attack them must be investigated. To achieve this, it is necessary to have great control over the growth parameters, which is quite a challenging since diffusion, segregation, alloy intermixing, or strain effects are wholly involved. For this work, we use finite element methods feedbacked with experimental observations to study the InAs QDs embedded in (Al)GaAs matrixes. Experimentally is observed that AlGaAs capping affects less the morphology of the pyramidal islands, the QDs density is shortened and the WL thickness is thinner for the growth on GaAs surfaces, as compared with Al containing surfaces. Considering the aforementioned results, 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 behavior presented in heavy hole (HH) and light hole (LH) depending on whether we are under constant strain or there are changes in the structure between the simulated heterostructures. Also, we can see some changes in the electronic transitions of the electrons and holes depending on the geometry presented in the QD. Resulting in changes such as the confinement capacity depending on the geometry of the QD.
Keywords: InAs-quantum dots, multi-stacked, strain distribution, diffusion parameters, critical thickness, band structure.
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[NSN-390] CONTROLED SYNTHESIS, CHARACTERIZATION AND PHOTOCATALYTIC APPLICATIONS OF ELECTROSPUN TIO2 NANOFIBERS OBTAINED FROM DIFFERENT CHEMICAL PRECURSORS

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The obtaining of TiO_2 nanofibers synthesized from two different chemical precursors titanium tetrabutoxide (TNBT) and titanium isopropoxide (TTIP) by the electrospinning technique with controlled morphology and crystal structure is reported. The crystalline phase of the TiO_2 nanofibers was controlled by heat treatment at 450 °C for 3 h. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) confirmed the formation of nanofibers with a well-defined shape, without the presence of defects. By Raman scattering it was found that the TiO_2 nanofibers presented anatase CP, which was corroborated by X-ray diffraction. The functional groups were obtained by FTIR infrared spectroscopy and by energy dispersive spectroscopy (EDS) the chemical structure of the TiO_2 nanofibers. In addition, the photocatalytic properties of TiO_2 nanofibers in the decolorization of Remazol Black B azo dye were evaluated. The Ti precursors used in the synthesis of TiO_2 nanofibers had an effect on the physicochemical properties. the fibers prepared with the TTIP precursor showed a smaller crystal size, a larger surface area, while the samples prepared with TNBT showed a smaller bandgap energy. The photocatalyst prepared with titanium isopropoxide as precursor showed the most remarkable efficacy in the decolorization rate of Remazol Black B azo dye, this is the result of smaller diameter and smaller specific surface area.

Keywords: Titanium dioxide nanofibers, Electrospinning, Titanium tetrabutoxide, Titanium isopropoxide.
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[NSN-40] CONTROLLED SELF-ASSEMBLY OF METALLIC AND BIMETALLIC NANOPARTICLES ON DEEP EUTECTIC SOLVENT USING VACUUM THERMAL EVAPORATION FOR EFFICIENT SERS SUBSTRATES

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Controlled assembly of noble metallic nanoparticles (NPs) has become most attractive approach to fabricate highly efficient surface enhanced Raman spectroscopy (SERS) substrate for sensitive detection of biomolecules at a single molecular level. However, controlled assembly and regulating the gap between plasmonic metal NPs to achieve abundant ¨hot spots¨ at the target area still remains a great challenge. In this work, we report a simple and versatile method for controlled assembly of Ag, Au and Ag/Au NPs networks onto surface of deep eutectic solvents (DESs) using vacuum thermal evaporation technique. By varying the deposition parameters such as applied current and pressure inside the chamber, enables to modulation of Ag NPs size, shape, and density of Ag NPs assembly. The results demonstrate that the depsotion of Ag, Au and Au-Ag at high pressure ($2x10^{-4}$ mbars), highly porous metallic and bimetallic NPs networks were formed with controlled gaps. Moreover, the thickness of the films was also modulated by simply varying the amont of Ag and Au metal wires used for deposition onto DESs. The resultant Ag NPs assemblies exhibits abundant of SERS hot spots for highly sensitive detection of biomolecules such as Rhodamine (R6G) and Crystal violet (CV). These simple, and low-cost approach adapted in this work pave the way for scalable fabrication of an active SERS substrate for ultra-sensitive SERS detection of various biomolecules.

Keywords: Metallic NPs, bimetallic NPs, self-assembly, deep eutectic solvents, surface enhanced Raman spectroscopy.
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Referece: V. S. Raghuwanshi, M. Ochmann, F. Polzer, A. Hoell and K. Rademann, Self-assembly of gold nanoparticles on deep eutectic solvent (DES) surfaces, *Chem. Commun*., **2014**, 50 (2014) 8693–8696. https://doi.org/10.1039/C4CC02588A
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[NSN-241] EFFECT OF REDUCING AGENT CONCENTRATION ON THE SYNTHESIS OF GOLD NANOPARTICLES FUNCTIONALIZED WITH AMOXICILLIN.

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Antibiotics are less effective, although resistance to antibiotics occurs naturally, its appearance and spread have been increasing rapidly due to the inappropriate use of antibiotics in recent decades and, the transfer of genes encoding antibiotic resistance. Bacteria constantly mutate; therefore, their defense mechanisms mutate, as well. This leads to high mortality in patients with infections and a high cost for the recovery of health. The projections for the future are not very encouraging, which has led to consider antimicrobial resistance as a global health problem and to be the object of study by researchers. Nanotechnology plays a key role in antimicrobial resistance due to materials being modified at the nanometer scale, allowing large numbers of molecules to assemble to have a dynamic interface. These nanomaterials act as carriers, and their design is mainly focused on introducing the temporal and spatial release of the payload of antibiotics. By using nanoparticles as vehicles for the administration of antibiotics, either by encapsulating the antibiotic or by attaching it to the surface of the nanoparticle, the antimicrobial can be protected from enzymes, molecules, or other agents that can degrade and deactivate its effect. As an alternative to the problem, the synthesis of gold nanoparticles functionalized with amoxicillin (AuNPs@amox) has been developed, using the chemical reduction of Au^{+3} to Au^{0} generated by the amino groups of the antibiotic. That occurs by varying the concentrations of the precursor agent ($HAuCl_4$) and the reducing agent (Amoxicillin, $C_{16}H_{19}N_3O_5S$), as well as the reaction time in the synthesis. In the characterization of AuNPs@amox, UV-Vis spectroscopy and transmission electron microscopy were used to determine their morphology, size, and elemental composition. Quasi-spherical gold nanoparticles with a bimodal behavior were obtained, with a size distribution between 15-20 nm for the large ones and 1-2 nm for the small ones.

Keywords: *AuNPs, antibiotic, antimicrobial resistance, functionalization, nanotechnology.*
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[NSN-72] EFFECT OF STRAIN ON SURFACE PLASMON OF GRAPHENE EMBEDDED IN ONE-DIMENSIONAL PHOTONIC CRYSTAL.

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Graphene supports surface plasmons in the terahertz range, and compared with noble-metal plasmons, they show an extreme level of field confinement and relatively long propagations distance, with the advantage of being highly tunable via electrostatic field. In this work, charge density excitations in uniform strained graphene are carried out for one and double-graphene layer structures. Because strain induces anisotropy in the graphene optical conductivity, the strength and strain orientation plays and important role to manipulate the variation of graphene plasmon energy, propagation length and penetration depth of the surface plasmon in the homogeneous environment, which may be useful to tune graphene properties in plasmonic devices to enhance light-matter interactions.

Keywords: graphene, strain, propagation, penetration.
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G. Khalandi, A. Namda, S. Roshan Entezar, Tension induced surface plasmon-polaritons at graphene-based structure. Superlattices and Microstructures (2017). https://doi.org/10.1016/j.spmi.2016.11.070.
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[NSN-393] ENHANCED PHOTOLUMINESCENCE OF InP@ZnS NANOCRYSTALS In(MA)x/P(TMS)3 RATIO OF -DEPENDENT PHOTOLUMINESCENCE

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In this work presents the results obtained on the synthesis and characterization of InP@ZnS quantum dots (QDs) grown by a one-step chemical synthesis method without injection of hot precursors, varying the ratio of $In(MA)_x/P(TMS)_3$ (0.2,0.3,0.4). The effect of the indium myristate precursor concentration on the optical, structural properties InP@ZnS QDs was studied. By X-ray diffraction (XRD) were shown the presence of zincblende crystalline phases of the InP and ZnS and was estimated the InP@ZnS QDs size with Scherrer-Debye equation, which was ranging from 3.75 to 9.72 nm as confirmed by high resolution transmission electron microscopy (HR-TEM). It was found a color variation of the InP@ZnS QDs in solution due to the quantum confinement effects when the nanoparticle sizes are smaller than the exciton Bohr radius. The bandgap energy of the QD was determined from the absorption spectra, finding that it depends on the myristate concentration, which was ranged from 2.90-3.21 eV. In addition, an enhanced PL emission was obtained due to a passivation effect on the ZnS-covered InP QDs. In the photoluminescence (PL) spectra at room temperature, emission peaks were observed in the range of 2.19 to 2.91 eV. Additionally, photoluminescence was studied as a function of temperature in the range of 20 to 300 K, finding that the main luminescent band does not obey the Varshni equation.

[NSN-323] EVALUATION OF THE HARDNESS ON THE SURFACE OF MEDIUM AND LOW CARBON STEEL DUE TO THE USE AND EFFECT OF TIO2 AND MNO NANOPARTICLES

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Several cuts of a low carbon steel plate (ASTM A36) and medium carbon steel (ASTM 1045) were made to prepare different samples of size 10.16x5.08x1.27 cm, which were polished on the upper face to eliminate the polluting residues and oxidizing material. Each sample was covered with different nanoparticles on the surface. Two different types of nanoparticles with different sizes were used. We have two oxides: TiO_2 (21 nm) and MnO (50 nm). Each sample was placed in a steel hearth box with a lid, each box, in turn, was introduced into a muffle to carry out heat treatment at 950°C for 24 hours. After this time and without low the muffle temperature, each of the boxes with every sample was removed the muffle to implement a cooling process by not severe thermal shock at room temperature. A surface layer of iron oxide, and nanoparticles, was formed on each plate; these layers were ground in a ceramic mortar to obtain powders, which were characterized using the X-ray diffraction technique to find the phases present in these layers. Semiquantitative phase analysis was obtained using HighScore Plus software. As a result, the reaction between nanoparticles and the steel surface at 950°C gave us different percentages of iron oxides such as FeO, Fe_2O_3, and Fe_3O_4. We obtained non-stoichiometric Fe compounds and others with different crystallography and composition according to the different nanoparticles used in the process. We observed the penetration depth level of the nanoparticles in each sample according to the width of the surface layer removed each steel plate.

Keywords: low carbon steel, medium carbon steel, iron oxide, temperature, nanoparticles
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Reference: Jiménez-Jiménez, A., Paniagua-Mercado, A. M., García-Bórquez, A., López-Hirata, V. M., De Ita-De la Torre, A. S., Mejía-García, C., ... & Miguel-Díaz, E. (2020). Modification of mechanical properties of submerged arc welds by adding Mn2O3–or TiO2–NPs directly to the beveled surface of low-carbon steels. *Materials Research Express*, *6*(12), 1265j8.
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[NSN-304] EXPERIMENTAL DIFFUSION RESEARCH ON Ni80Cr20 AND Cu70Ni30 BINARY ALLOYS

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Abstract: The interdiffusion behavior in metallic alloys controls many technological processes, such as nitriding, carburizing, and carbonitriding. The understanding of these processes will allow us to design effective thermal treatments. In this work, we study experimentally the interdiffusion zone behavior at 800°C by means of a diffusion couple of Ni80Cr20 and Cu70Ni30 binary alloys. The Cu-Ni binary alloy is an ideal isomorphic system, however, the addition of a third alloying element such as Cr introduces an immiscibility gap that makes these alloys susceptible to heat treatment. Diffusion-couples were solution treated at 1000°C for 100 h and then water-quenched subsequently aged at 800°C for 0.5 h. Interdiffusion zone was analyzed by HRTEM, SEM and nanohardness measurements. Linear EDS-SEM permitted to obtain the concentration profile showing the difference in chromium composition in the CuNi region. HRTEM showed the change in size and volume of the nanoparticles in the interdiffusion zone during aging. Nanohardness values indicated hardening during isothermal aging due to the presence of chromium-rich manometric precipitates in the interdiffusion zone.

Keywords: Diffusion-couples, isothermal aging, precipitates and concentration profile.
This work was supported by SIP project 20221932 and CNMN-IPN

[NSN-254] FABRICATION OF ENCAPSULATED ZEOLITE POLYETHYLENE TEREPHTHALATE NANOFIBERS

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There are different techniques for the generation of nanostructures and microstructures of fibers where specifically the electrospinning technique has been targeted in recent years as an accessible method for the manufacture of different organic and synthetic materials and widely used by the scientific community because due to its efficiencies, relative simplicity, and low cost. In the electrospinning technique, the encapsulation of materials has been widely used such as zeolites, which are both natural and artificial crystalline aluminosilicates and due to their high cation exchange capacity, surface area, porosity, and water retention capacity are principally used in the agricultural industry, water treatment, air purification, and photocatalysis. In this work, the characteristics of the nanofibers will be evaluated by the electrospinning method from plastic waste bottles (PET) at 30% and with the encapsulation of zeolite at percentages of 0.1, 1 and 1.5% respectively. The control parameters for the electrospinning technique are the voltage of 10-25 kV, with a feed rate of 1-0.5 mL/h and a rotating collector speed of 1500 rpm. Morphological characterization and analysis of the nanofibers were carried out using SEM, FTIR, and RX techniques, mainly to observe the incorporation of zeolite into the nanofibers and its possible applications.

Keywords: PET, nanofibers, electrospinning, plastic waste, zeolites encapsulation
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[NSN-32] GREEN SYNTHESES OF SILVER NANOPARTICLES USING GARAMBULLO (MYRTILLOCACTUS GEOMETRIZANS) CHARACTERIZATION AND APPLICATION IN ORTHOPEDIC CASTS.

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Green synthesis consists of minimizing or, if it is possible, to eliminate polluting products by carrying out a chemical process to avoid further damage to the environment or to health. San Luis Potosí has á wide diversity of regional flora and fauna, the characteristics of berries and fruits have been studied, but little application of them is known and little or nothing oriented to nanotechnology. The objective of this work is to use the fruit from the Myrtillocactus geometrizans (garambullo) plant, in its dehydrated, fresh, ripe and green state, and its stem for the synthesis of silver nanoparticles, performing Vis-NIR spectroscopy to observe the formation of plasmons, DLS for size and PZ and TEM to characterize them. A total of 72 syntheses were carried out with their respective replicas and it was verified that, depending on their concentrations, pH variation and type of extract, the sizes obtained were from 1.5 to 400 nm, in addition bacteriological tests, using microdilution method, were carried out against the most common microorganisms from skin and exposed wounds, Staphylococcus aureus and Escherichia coli. The application that was given to the obtained nanoparticles was to reduce the probable infection in unfavorable conditions for its optimization or in poor care of the splint with plaster. The plasters were immersed in the synthesis carried out, allowed to dry for 72 h and their mechanical properties were measured using the 3-point bending tests guided by the ASTMDA standards for ceramic materials. Approximate sizes were obtained with the same method in its replica as well as PZ, its bactericidal and inhibitory capacity against bacteria worked in pure solution and with the plaster itself was demonstrated, the last one using Kirby Bauer method.

Key words: green synthesis, garambullo, silver nanoparticles, orthopedic cast.
Author for correspondence: edgar0292@outlook.com
Reference: Salinas Estevané, Juan Pablo y Sánchez Cervantes, (2012) La química verde en la síntesis de nanoestructuras. Ingenierías. 15 (54) 7-16 http://eprints.uanl.mx/10484/1/54_la_quimica.pdf
This work was supported by: Facultad de Ciencias, Universidad Autónoma de San Luis Potosí

[NSN-37] GREEN SYNTHESIS OF SELENIUM NANOPARTICLES USING PLUCHEA SERICEA (CACHANILLA) AQUEUS EXTRACT, AS AN ANTIBACTERIAL AGENT FOR THE FOOD PACKAGING INDUSTRY.

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The use of natural extracts for the synthesis of nanoparticles is attracting much interest due to their compatibility to the environment and low cost compared to conventional methods. In this study Selenium nanoparticles were synthesized by green method using ascorbic acid and *Pluchea Sericea* (Cachanilla) aqueous extract (a native plant of Baja California, Mexico) as reducing and stabilizing agents, respectively. For shape, size, particle distribution, and Z potential were characterized by Dynamic Light Scattering (DLS), UV-VIS, and Scanning Electron Microscope (SEM). UV-Visible spectroscopic analysis showed the absorbance peak at 261.36 nm, which indicates the presence of Selenium, Dynamic Light Scatering (DLS) results showed Z potential of 46.1 Mv, and the diameter of the Selenium Nanoparticles is 35.14-77.04 nm indicated by SEM. Finally, Selenium Nanoparticles were tested on strains of *E. coli* and *S. aureus* (bacteria recurrent in contaminated food in supermarkets), and showed good antibacterial activity. The results suggest that Selenium Nanoparticles significantly reduce the growth effect of the bacteria evaluated, opening the way for the use in the food packaging industry as antibacterial agent.

Keywords: Nanoparticles, Selenium, green synthesis, pluchea sericea.
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Reference: Alghuthaymi, M. A., Diab, A. M., Elzahy, A. F., Mazrou, K. E., Tayel, A. A. y Moussa, S. H. (2021). Green Biosynthesized Selenium Nanoparticles by Cinnamon Extract and Their Antimicrobial Activity and Application as Edible Coatings with Nano-Chitosan. Journal of Food Quality, 2021, 1–10. https://doi.org/10.1155/2021/6670709
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[NSN-424] Growth of InGaN and InAlN nanostructures on Si(111) substrates

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The bandgap energy of III-N compounds can be varied over a wide energy range (0.7-6.2 eV) by introducing indium atoms to form semiconductor alloys. Furthermore, in the form of nanostructures, III-N alloys emit light very efficiently [1]. However, the mechanism of incorporation of indium atoms in III-N compounds is still poorly understood. For this reason, in this work we studied the indium incorporation in InxGa1-xN and InxAl1-xN nanostructures embedded in Ga(Al)N barriers grown by molecular beam epitaxy (MBE) on Si(111) substrates. The Si substrates were cleaned by the Ishizaka-Shiraki method [2] and then introduced into de MBE system. In order to obtain high-quality III-N epilayers on Si substrate, an AlN buffer layer was used to reduce the lattice and thermal mismatch with Si, this AlN buffer also prevents the formation of an amorphous SiN layer at the interface. We studied the effect of varying the growth temperature on the concentration of indium in the InGaN and InAlN nanostructures. The In concentration in the samples was obtained by secondary ion mass spectrometry (SIMS). The structural properties were studied by x-ray diffraction (XRD), secondary electron microscopy (SEM) and atomic force microscopy (AFM). The optical properties of the nanostructures were evaluated by photoreflectance and photoluminescence spectroscopy.

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[2] A. Ishizaka and Y. Shiraki J. Electrochem. Soc. 133 (1986) 666

[NSN-48] Hexagonal MoO3 nanotubes synthesis: Removal of methylene blue by a photocatalytic process

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One of the main problems that can be attacked using the photocatalytic processes is the wastewater treatment. For instance, in the textile industry, 200 liters per kilogram of wastewater are produced using dyes. The present work describes the methodology to synthesize hexagonal nanotubes of molybdenum trioxide (NT-h:MoO_3) and their characterization. It was found an enhanced methylene blue (MB) degradation under light irradiation as a function of the NT´s amount. In particular, we used 10 and 20 mg of NT-h:MoO_3. Moreover, for 20 mg of NT´s although the MB degradation is favored even at 20 min of irradiation, we could observe in the UV-Vis absorption spectra evidence of the generation of sub-products during the photocatalytic process. The morphology of the NT-h:MoO_3 was analyzed by scanning electron microscopy (SEM), the crystallinity was studied by X-ray diffraction (XRD), chemical bonding by Raman, and Infrared (FTIR) spectroscopies, while the MB degradation was investigated using UV-Vis spectroscopy.

Keywords: Molybdenum trioxide, photocatalytic activity, chemical synthesis, SEM.
References: [1] M. Morales-Luna, S.A. Tomás, M.A. Arvizu, M. Pérez-González, E. Campos-Gonzalez, The evolution of the Mo^{5+} oxidation state in the thermochromic effect of MoO_3 thin films deposited by rf magnetron sputtering, J. Alloys Compd. 722 (2017) 938-945. https://doi.org/10.1016/j.jallcom.2017.06.149
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[NSN-387] IMPACT OF PVP AGING ON THE SYNTHESIS OF SILVER NANOPARTICLES.

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The interest of study of silver nanoparticles (Ag NP´s) is due to the applications in electronics, clothes, paints, cosmetics, bactericides, biofungicides, biomedical, pharmaceutical and food industry [1]. A lot of methods for production of Ag NP´s are based on the reduction of silver nitrate ($AgNO_3$) and the use of polyvinylpyrrolidone (PVP) to prevent agglomerates. The effect of PVP solution aging in the sintesis of Ag NP´s has not been investigated. For this reason, in this work a follow-up of the effect of PVP aging; for which PVP was dissolved in water and the NP's were prepared with aged solution for 0, 2, 4 and 8 days. Absorption spectra were obtained by UV-vis spectroscopy in the range of 300-800 nm. In all the samples the presence of the plasmon centered around 400-450 nm with an approximate FWHM of 220 nm. The absortion spectra show that the signal corresponding to the plasmon is asymmetric, which could be associated whith the presence of spherical Ag NP´s with different sizes. It was observed that the intensity of peak of Plamon absorption increases as the PVP solution ages. By Scanning electron microscopy (SEM) show an Ag NP's distribution of different sizes between 40-100 nm, which is consistent with that observed by UV-vis spectroscopy.

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[NSN-102] IMPROVED SYNTHESIS AND PHOTO-THERMAL PROPERTIES OF SILICA-GOLD NANOSTRUCTURES

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Silica-gold nanostructures (SGNs) have been used for the ablation of cancerous tumors and for the localized delivery of drugs due to their ability to transform near-infrared (NIR) irradiation into heat [1]. Once SGNs are located in the desired area, they elevate their temperature while irradiated with NIR laser. The scattering and dispersion coefficients of human skin, subcutaneous and mucous tissues are reduced when the wavelength of the irradiation is between 600-1300nm, which allows for the laser to access the location of the SGNs without affecting any tissue. NIR irradiation will then turn into heat which could be used for hyperthermia and/or the localized release of drugs. Because of the wide range of possible applications for the SGNs, this work presents the optimization of their synthesis method. The silica cores were synthesized using the Stöber method, and the gold nanoparticles were deposited over the cores by modifying the method presented by Kah. These modifications reduced the synthesis time by 83%, and even though the gold nanoparticles only cover the core partially, the photo-thermal properties were kept. The silica core and gold semi-shell dimensions were evaluated by scanning and transmission electron microscopy, respectively. The cores have a diameter of 62±5nm with a gold semi-shell of ≈3nm. To compare the photo-thermal efficiency of a semi-shell with a full-shell, SGNs were also synthesized with a core of 62±5nm and a full gold shell of ≈5nm. Both nanostructures were irradiated with laser of 852 nm 3.2mW, and the temperature changes were recorded with a thermal imager. The nanostructures increased their temperature by 36 C and 37 C for the semi-shell and the full-shell, respectively. This increment in temperature is sufficient to induce necrosis on cancerous cells, as well as to induce localized drug release, which would significantly reduce the side effects of conventional treatments.

Keywords: Silica-gold nanostructures, photo-thermal ablation, NIR
Author for correspondence: rosa.ruvalcaba@cimav.edu.mx
Reference: [1] A. R. Rastinehad, H. Anastos, E. Wajswol, J. S. Winoker, J. P. Sfakianos, S. K. Doppalapudi, M. R. Carrick, C. J. Knauer, B. Taouli, S. C. Lewis, et al., Proceedings of the National Academy of Sciences, **116**(37), 18590–18596, (2019). https://doi.org/10.1073/pnas.1906929116.
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[NSN-416] IN-SITU STUDY OF INAS QUANTUM DOTS ENCAPSULATED IN ASYMMETRIC (AL)GAAS CONFINEMENT BARRIERS.

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Their exciting physical properties and the potential applications in the development of optoelectronic devices have stimulated plenty of research on semiconductor quantum dots (QDs) in the past two decades, or so. There still great interest to conduct basic research on QDs advantageous properties, which include the mechanisms of high quantum yield, high photostability, high molar extinction coefficients, collective electron spin manipulation, among others. Additionally, their unique quantum properties like increased density of states and energy level discretization conduces to significant advantages when applied to electronic and optoelectronic devices. Self-assembling via strain relaxation is the main mechanism of synthesis to be considered for such applications and to obtain effective experimental QDs devices is necessary to grow a successful vertical stacked QDs in the active region of the devices. Nevertheless, structural parameters get more challenging as each layer of QDs is added since the strain itself boost no-desired processes of surface diffusion, segregation between layers and alloy intermixing. In this work, the strain distribution during the multistacking of QDs layers is studied. We have tailored the InAs adatoms mobility by changing the layer over which they are self-assembled, i.e. either GaAs or AlGaAs. The reduced mobility of In adatoms conduced to larger QDs density relieving the interface strain. On the other hand, by changing the capping material, an important interfaces diffusion takes place, presumably related with strain redistribution. When are covered by AlGaAs the QDs are less affected in comparison with the GaAs capping, preserving the morphology and avoiding materials alloying. Lastly, asymmetric high-resolution x-ray scans were performed to evaluate the residual strain in the whole stacked heterostructure.

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[NSN-33] INCORPORATION OF SILVER NANOPARTICLES INTO SiO2 FILMS

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Our concern to conserve and preserve our environment has led us to increase research focused on the development of biodegradable containers and/or containers incorporating the use of starch on our films; without forgetting to improve its physical and chemical properties, thus forming organic-inorganic films with various areas of application, as they are especially in the textile, industrial, scientific, medical and food area.

The use of antibacterial materials and coatings for the creation of films for the specific use of food packaging and other uses in the food industry. For higher and better results, antibacterial sensitivity tests were performed for inhibition halos to determine the susceptibility of a microorganism to silver nanoparticle films, from exposure of a standardized concentration of two bacteria used: Escherichia coli (E. coli) and Staphylococcus aureus (S. Aureus). In addition, the films were characterized by VIS-NIR spectroscopy, DLS analysis, Transmission Electron Microscopy (TEM), Fourier Transform Infrared Spectroscopy (FTIR) and Atomic Force Microscopy (AFM).

Homogeneous, fracture-free and translucent films were obtained using the sol-gel method by means of simultaneous polycondensation and gelation of what were the different precursors of starch, glycerol and TEOS. **[1]** The best result was obtained in the films of 3% glycerol and 3% TEOS. The addition and proportional increase of TEOS significantly influences its gelling and resistance, in addition to its biodegradation process.

The incorporation of AgNPs does not modify in any way the described properties, that is, it is possible to incorporate Ag or some other material in order to improve and develop our films for food use or any other. In addition to incorporating silver, it is possible to clearly observe how it inhibits the halo to microorganisms sown at the beginning of the tests.

Keywords: Nanoparticles, silver, synthesis, films, sol-gel.

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Reference: [1] Horst, C., Pagno, C., & Flores, S. &. (2020). Hybrid starch/silica films with improved mechanical properties. *Science and Technology*, 52-65.

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[NSN-207] INTERACTION OF POSSIBLE RESONANT CAVITIES WITH SURFACE PLASMONS

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Superfluidity and superconductivity have their origin in Bose-Einstein condensation while polariton condensates introduce novel concepts for non-equilibrium condensation. The aim is to have a coherent laser output that exhibits temporal and spatial coherence. Given the existence of possible resonant cavities on SERS substrates, shown as a kind of pores within a layer of gold nanoparticles, one beam photons interacting with existing plasmons in the NP Au layer, these exhibit plasmon excitations of surface localized through an indirect interaction of the plasmons with the resonant cavities. For the study of these interactions where the system consists of polaritonic modes that are coupled to dye molecules. We assume that each molecule is a two-level system coupled to a harmonic oscillator that describes the rotational degrees of freedom of the molecule [1]. The Hamiltonian used is described in the supplementary reference information [3]. The interaction of photons and plasmons is expected to show condensation effects. For this purpose, ultrafast spectroscopy studies are carried out in order to analyze the absorption and emission behavior of SERS substrates.

Keywords: Plasmons, resonant cavities, polariton, condensation
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Reference: [1] Hakala, T. K., Moilanen, A. J., Vakevainen, A. I., Guo, R., Martikainen, J.-P., Daskalakis, K. S., . . . T¨orm¨a, P. (2018). Bose–Einstein condensation in a plasmonic lattice and Supplementary information . Nature Physics, 14(7), 739–744. doi:10.1038/s41567-018-0109-9
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[NSN-43] KINETIC STUDY OF THE SIZE GROWTH OF QUANTUM DOTS SYNTHESIZED BY THE SONOCHEMICAL PROCESS

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In this work, the growth kinetics of silver sulfide quantum dots obtained by the sonochemical process is presented. Nowadays the use of quantum dots is significant in the application fields of electronics, energy, and biomedical, due to its excellent potential properties in optics and electrics. But some of the issues faced in the use of this material is the production because the residues are toxic and the time to synthesize it is too long. For these reasons the new generation of quantum dots, it is focusing on the environmental impact and the facility of synthesis through novel methods such as sonochemical methods, in the presented work the structures obtained had a size range between 2-10 nm, and its morphology is regularly semicircular with excellent dispersion and stability in solution. The scattered light analysis presented spectra with only one peak suggesting a homogeneous size of the particle and the TEM images exhibit a regular size distribution and great dispersion without cumulus of particles. Finally, the crucial step in the process according to the kinetic study occurs between 10 to 16 minutes, in this stage, the size growth is exponential, and the diameter increased from 2 nm to 10 nm.

Keywords: growth kinetics, quantum dots, sonochemical process
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[NSN-278] LaMnO3-TYPE PEROVSKITE SYNTHESIS BY COMBUSTION AND MOLTEN SALT METHODS ASSISTED BY MICROWAVE

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Perovskite-type oxides have flexible physicochemical properties closely related to their crystalline structure, which have been highlighted in recent materials science research. Their characteristics make them good candidates for use in applications ranging from solar cell, storage devices and fuel cell. However, there is still no low-cost and energy-saving route to obtain perovskite-type materials. Fast chemistry has emerged as an alternative for obtaining high-purity and industrially scalable materials. Here, some methods such as combustion and molten salts can be assisted by microwaves, obtaining excelent electrochemical properties. In this work, the chemical synthesis of lanthanum manganite ($LaMnO_3$) by the combustion and molten salts methods assisted by microwaves is presented. The perovskites obtained were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). X-ray diffraction allowed us to identify the cubic-type crystal structure (PDF 75-0440) and orthorhombic-type crystal structure (PDF 89-0682) for the perovskites sintethized by combustions and molten salts, respectively. Crystallite sizes were ~15nm for the cubic phase and ~24 nm for the orthorhombic phase. Results showed that the microwave-assisted chemical synthesis of the $LaMnO_3$ perovskite offered energy and time savings compared with the traditional chemical methods. The electrochemical properties for oxygen reduction (ORR) and oxygen evolution (OER) reactions were assessed.

Keywords: Perovskite, $LaMnO_3$,combustion, molten salts, microwaves.
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[NSN-196] MICROWAVE ASSISTED SYNTHESIS OF CARBON QUANTUM DOTS AND ITS ABSORPTION/EMISSION CHARACTERIZATION

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From the second half of the last century up to date, carbon-based nanomaterials have raised great expectation. Nanostructures like nanotubes, fullerene, graphene and nanodiamonds have been found to possess extraordinary physico-chemical properties. On the other hand, Carbon Quantum Dots (CQD) stand out by their optical and biochemical properties that make them optimal candidates for applications like bioimaging and biosensors. Still far from optimized applications, the CQD synthesis and characterization is an area of intensive research; great diversity of methods and precursors are being tested and a wide variation of properties is being discovered. In this work, a green method was employed to synthesize CQD. Dextrose/water solution (11.1 w %) was used as precursor, energy was dosed as microwaves to the reactor, and the reaction time was between 2 and 10 min. UV-vis spectroscopy was used as a first approach to characterize the products. Transmision electron microscopy (TEM) was used to determine their dimension, Fourier transform infrared spectroscopy (FTIR) was used to confirm the functional groups -C=C-, -CO, –OH, -COOH, that are expected to conform the synthesized nanostructures. Thermal lens (TL) and photoluminescence (PLS) spectroscopy will be used to determine the quantum efficiency and yield. As the synthesis was performed in aqueous media, with a biocompatible precursor that generates no other chemical groups than the listed before, this research is expected to generate highly biocompatible CQD, to be confirmed.

Keywords: Quantum Dots, Green synthesis, Biocompatibility.
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[NSN-415] MOLECULAR BEAM EPITAXIAL GROWTH OF GANAS MULTI-QUANTUM WELL HETEROSTRUCTURES.

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Research for efficiently convert solar light energy into electricity using photovoltaic (PV) technologies or solar cells (SCs) was started a long time ago, novel materials and new designs of solar cells (SC_s) have been proposed. Up to now, the highest conversion efficiencies have been achieved with tandem or multi-junction SCs, technologies that comprise the simultaneous absorption of photons of different wavelengths. This strategy allows for capturing a broader region of the solar spectra, as compared to conventional solar cells based on single pn junctions. An alternative approach to achieve the multi-wavelength photon absorption is throughout highly mismatched alloys (HMA) like GaNAs. For this material the decoupling in electronegativity and size of the atomic radii of the N with Ga, generates a splitting conduction band (CB) letting unaltered the balance band (VB). The low and high energy CBs after splitting have been called as minus (-) and plus (+) bands, respectively. Thus, in a single layer three different transitions are allowed: VB→CB–, VB→CB+ and CB–→CB+. In this work, a novel quantum well heterostructure is proposed to further increase the quantity of electronic transitions. The GaNAs HMA alloy was sandwiched between AlGaAs barriers with mole fraction x_{Al} from 0 to1 to selectively achieve the confinement of CB+ and/or CB–. 3d finite element model was employed to determine the confinement quantum states. Simulations indicated that some eigenfunctions of both bands are overlapped depending on the AlGaAs barriers. Conversely, in spite that the activation of bands was corroborated by photoreflectance spectroscopy, there was not clear evidence of quantum confined states related with CB+, suggesting that CB- is the sole energy band that contributes to the electron confinement. The experimental-theoretical controversy is explained in terms of the deallocation of the impurity levels of N in the host matrix.

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[NSN-21] N 1S CORE-LEVEL BINDING ENERGIES IN NITROGEN-DOPED CARBON NANOTUBES: A COMBINED EXPERIMENTAL AND THEORICAL STUDY.

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ABSTRACT: We present a combined experimental and theoretical study dedicated to analyzing N 1s core-level binding energies (CLBE) in N-doped carbon nanotubes (N-CNTs). N-CNTs were synthesized using the CVD technique, and then subjected to acid treatments (nitric and sulfuric acid) yielding multiwalled carbon nanotubes with functional groups, which were characterized by scanning and transmission electron microscopy of the which we obtained appreciable images of carbon nanotubes with diameters around 70-90 nm and lengths of 200 μm, were also characterized by RAMAN, SEM, TEM and XPS microscopy. Extensive density functional theory (DFT) calculations are performed on various single and double-walled N-CNT models where the CLBEs of N 1 are determined using Koopman's theorem. However, peak deconvolution is characterized by five broad Gaussian curves that overlap considerably with each other, with different widths and heights, implying a more complex distribution of N atoms within CNTs. DFT calculations reveal a strong dependence of CLBE values on the local atomic environment. The above distributions of theoretical CLBEs also overlap strongly, implying that some peaks in the XPS spectra must be understood as composite signals where the coexistence of different N defects is present. We found, in agreement with the experimental data, that the independent molecular nitrogen and the encapsulated (weakly interacting) N2 within the hollow core of model CNTs have very similar CLBEs. In addition, we predict that the chemisorbed N2 in the defect regions of the nanotube walls, as well as the intercalated (highly confined) nitrogen molecules between the carbon layers, have N1s binding energy values that are considerably higher compared to N1s. with the N2 encapsulated, which makes its identification possible.

KEYWORDS: Carbon nanotubes, XPs and Koopman's theorem.
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REFERENCE: Mihai V. Putz*. Koopmans' Analysis of Chemical Hardness with Spectral-Like Resolution. Hindawi Publishing Corporation, The ScientificWorld Journal, Volume 2013 |Article ID 348415 | https://doi.org/10.1155/2013/348415
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[NSN-296] N-DOPED CARBON NANOTUBES FROM PINE TURPENTINE AND ITS PERFORMANCE IN THE BASIC METHYLENE BLUE (AB9) ADSORPTION

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The discovery of a purple compound on the Industrial Revolution by oxidation of the aniline set the beginning of the synthetic dye era. In the present there are about 10,000 different kinds of pigments and dyes which are most used by the Textile Industry but they are so dangerous to rivers, lakes and sea. It has been shown carbon nanostructures like CNT's and graphene oxides are good synthetic dye adsorbents but their synthesis involves polluting carbon sources for this reason the use of pine turpentine as renewable carbon source extracted from Michoacan pines. The synthesis of CNT's was made using Spray Pyrolysis technique with pine turpentine and ferrocene as catalyst at 800°C and 5 LPM of argon as carrier. Doped carbon nanotubes (DCN) were synthetized using Pyridine and Imidazole as nitrogen sources at different concentrations. The synthetized nanostructures were analyzed by Raman Spectroscopy, X-Ray Diffraction (XRD) and Transmission electronic Microscopy (TEM). Raman Spectroscopy shows D, G and G' peaks corresponding to sp^2 nanostructured carbon with highly crystallinity and good wall arrangement. XRD shows 26°, 44° and 54° peaks corresponding to graphitic planes and tiny peaks corresponding to the incorporation of nitrogen in carbon nanotube structure. Using TEM let us know that nitrogen doping was successfully due the presence of bamboo-like structures in the CNT's. Adsorption studies were made using UV-Vis Spectroscopy in different temperature and pH ranges obtaining 97% remotion at 180 min whit imidazole doped carbon nanotubes.

Keywords: Nitrogen, Pine, Turpentine, Remotion, DCN
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[NSN-227] NiOx THIN FILMS GROWN FROM COLLOIDAL NANOCRYSTALS FOR APPLICATION IN FLEXIBLE OPTOELECTRONIC DEVICES

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Non-stoichiometric nickel oxide (NiO_x) is a transparent conductive oxide (TCO) with interesting properties for many optoelectronic applications, among them light sensors. It has a band gap of ~3.8 eV, a transmittance of almost 90%, a resistivity of less than 10^3 Ω·cm, and an excellent chemical stability. Moreover, in contrast to the most TCOs used in optoelectronic and electronic devices, it is a p-type semiconductor. NiO_x thin films have been deposited using various techniques, including Atomic Layer Deposition, Chemical Vapor Deposition, Sputtering, Pulsed Laser Deposition and e-beam evaporation. However, these techniques require high vacuum and expensive equipment. In this work, we present a simple, low-temperature, and low-cost method for synthesis and deposition of NiO_x thin films from a colloidal dispersion of NiO_x nanocrystals. As an example for application of these films in optoelectronic devices we study flexible photosensors based of NiO_x layers deposited by spin-coating technique using various ligands.

Keywords: NiO_x thin films, colloidal nanocrystals, flexible optical sensors, low temperature process

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[NSN-87] NOVEL AND GREEN SYNTHESIS OF BI2WO6/BIVO4 HETEROJUNCTIONS WITH PHOTOCATALYTIC ACTIVITY UNDER LEDs ILLUMINATION

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Abstract: $Bi_2WO_6/BiVO_4$ (BiW/BiV) heterojunctions with different loads of BiW were successfully prepared by a metathesis-assisted molten salts route, a green and high-yield synthesis. The photocatalytic activity is affected by BiW content in heterojunctions. Besides, silver nanoparticles (Ag-NPs) and graphene (G) were loaded to 1BiW/1BiV heterojunction. The Ag/1BiW/BiV heterojunction is constituted by plate and spherical-like particles of BiV and BiW, respectively. TEM studies confirmed the junction zone between BiV, BiW, and Ag-NPs in Ag/BiW/1BiV. The P25 (TiO_2) exhibited lower photocatalytic activity than Ag/1BiW/1BiV. The rhodamine B (RhB) degradation ($\%X_{RhB}$) over Ag/1BiW/BiV reached 100% within 210 min under blue LEDs irradiation. Besides, the RhB degradation is dependent on the initial dye concentration and catalyst dosage. The scavenger tests revealed that the main oxidative species inducing the RhB degradation were h^+ and $\bullet O_2^-$, and the carrier transfer mechanism in Ag/1BiW/1BiV was postulated. After four reuse cycles, the Ag/1BiW/1BiV heterojunction exhibited high chemical stability.

Keywords: $Bi_2WO_6/BiVO_4$, green-synthesis, nanoparticles, heterojunctions, photocatalysis
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[1] M. Humayun, F. Raziq, A. Khan, W. Luo, Modification strategies of TiO_2 for potential applications in photocatalysis: A critical review, Green Chem Lett Rev. 11 (2018) 86–102. https://doi.org/10.1080/17518253.2018.1440324.
This work was supported by The National Council of Science and Technology (CONACYT, Mexico) through CB-2016-285350 and INFRA-2018-294130 projects. Dirección de Apoyo a la Investigación y Posgrado de la Universidad de Guanajuato (DAIP).

[NSN-270] OBTAINING SILVER NANOPARTICLES BY GREEN SYNTHESIS USING NOPAL MUCILAGE

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Silver nanoparticles have been studied for their wide use as bactericides, fungicides, infection control, coatings of textile materials, as well as being used in the treatment of wounds and burns. Therefore, the objective of this study was to synthesize and characterize silver nanoparticles (NpAg) using the so-called green synthesis, which is effective, simple and low cost, with the advantage that it has a friendly environmental impact. This green synthesis was made from nopal mucilage (Opuntia ficus-indica), which was extracted and filtered, and used as a precursor for the nanoparticles. For the synthesis, 0.2 g of cactus extract were used, which were dissolved in 80 ml of deionized water and a 5mM $AgNO_3$ solution. The Ag/Mucilage solution was mixed using a temperature of 60 ºC for 30 min. The solution turned from clear to brown, which was indicative of NpAg formation. Subsequently, the solution was dried at 100°C and then exposed to 500°C. The NpAg were characterized both in aqueous solution and in powder form, through UV-Vis spectroscopy techniques. The results showed that a plasmon resonance was present around 430 nm, attributed to the Ag particles. The structural characterization was carried out by X-ray diffraction, Infrared spectroscopy and particle size analysis. By the previous techniques, the presence of NPAg with a particle size of around 20nm was corroborated. In this study, the Opuntia ficus-indica extract provided a reducing medium for the production of NPAg through a simple and efficient process, obtaining desirable particle sizes with a wide potential for use.

keywords: nanoparticles, greensynthesis, nopal mucilage
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[NSN-301] ONE-STEP CONFINEMENT OF BIMETALLIC Au-M NANOPARTICLES (WHERE M: Ag OR Cu) IN MESOPOROUS OXIDES AS AN EFFECTIVE CATALYST IN THE REDUCTION OF NITROPHENOL ISOMERS

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Recently, the catalysts based on bimetallic nanoparticles confined in metal oxides have become attractive in applications such as photodegradation of organic dyes, hydrogen production and catalytic reduction of nitroaromatic compounds. However, the synthesis of these catalysts is arduous and commonly involves more than three stages [1]. In this work, we present the microwave-assisted one-pot synthesis of catalysts based on mono and bimetallic nanoparticles (Au, AuAg and AuCu) confined into the oxides: Fe_2O_3, TiO_2 and CeO_2. The physicochemical properties of obtained samples were studied using STEM, XRD, UV-Vis spectroscopy, DLS and Z potential techniques. Results confirmed the effective formation of oxides matrix capping metallic nanoparticles, characterized by quasispherical shape and sizes between 200 to 400 nm. In addition, catalytic activity and stability were evaluated using the reduction of nitrophenol isomers in situ monitored by in-situ UV-Vis spectroscopy. The catalytic activity depends on the composition of the catalyst as well as the reagent molecule (2-, 3- and 4-nitrophenol). The Au-M@TiO_2 and Au-M@Fe_2O_3 catalysts were stable up to 5 catalytic cycles in reducing 4-nitrophenol to 4-aminophenol. These results highlight the development of a one-pot methodology for nanomaterials synthesis with catalytic performance comparable to their reference supported catalysts, commonly presented in the literature.

Keywords: Bimetallic-nanoparticles, Nanoreactor, nitroaromatic-reduction brenda.acosta@uaslp.mx

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[NSN-83] PERFORMANCE EVALUATION OF A SINGLE-CHAMBER SOLID OXIDE FUEL CELLS USING SDC AND DSC ELECTROLYTES AS THIN FILMS.

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Single-chamber solid oxide fuel cells (SC-SOFC) are interesting devices since they present technological advantages over conventional double-chamber cells; this visualizes them as the novel energy systems for application in portable systems. Two types of substrates are used in this research YSZ 3% mol and YSZ 8% mol. GDC/SDC and SDC/GDC thin films were grown on these substrates by cathodic-erosion utilizing a radio frequency source for one hour. The charge transport was measured in four different fuel cells. For all the cells, the anode used was NiO (60%) – $Ce_{0.9}Gd_{0.1}O_2$ and for the cathode $La_{0.8}Sr_{0.2}MnO_3$ (50%) – $Ce_{0.9}Gd_{0.1}O_2$. Sol-gel Synthesis was employed to obtain manometric powders of these compositions. The cells were formed using a co-linear geometry, i.e, the anode and cathode deposited by screen-printing parallel to each other and separated by ≈1 mm of electrolyte. The cells were fed with methane gas and air. The electrolytes grown on YSZ 3% mol substrates reached a thickness of 100 nm, while those grown on YSZ 8% mol increased in thickness by 50% (150 nm). Power density results indicate that cells grown on 8% mol YSZ substrates achieve higher current density.

Keywords: SC-SOFC, Impedance, GDC, SDC, YSZ
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Reference: Palacios, D. O., Rojas, A. R., Holguín, J. R., Moller, J. D., & Esparza-Ponce, H. E. (2015). EVALUATION OF STABILITY OF TARGET HOMEMADE BY EFFECT OF TEMPERATURE, POWER AND FLOW IN THE DEPOSITION OF ZIRCONIA STABILIZED 8% Y^ sub 2^ O^ sub 3^ THIN FILMS WITH RF SPUTTERING. *International Journal of Materials Engineering and Technology*, *13*(1), 23.
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[NSN-321] PHOTOCATALYTIC ACTIVITY OF HETEROUNIONS ZnO@BiOX (X=Cl. Br, I), A STRUCTURAL AND ELECTRONIC INTERACTION STUDY.

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In this work we show the effect of varying the chemical composition of the halogen (X=Cl, Br, I), as well as its chemical nature on the photocatalytic activity of heterojunctions, 1:1, type ZnO@BiOX (where X= Cl, Br, I) in the photo-degradation of the dye rhodamine-B at high concentrations. It was observed that the photocatalytic activity of the heterojunction activated with visible light (λ > 420nm), is better in the samples that contain the BiOBr/BiOCl combination, obtaining the activity peak when using the molar ratio of the halogen BiOCl with respect to the BiOBr of 25 % (0.25:0.75 respectively), obtaining a degradation constant k = 0.143 s^{-1}. This can be explained by the interaction between the n-type (ZnO) and p-type (BiOX) semiconductors that favor an effective separation of the photogenerated exciton ( ) and the effective transfer of charge between the BiOCl and BiOBr, this results in a significant increase in the lifetime of the photogenerated species. The synthesis of the materials was carried out by solvothermal method using as base material the ZnO previously synthesized by co-precipitation method. The different samples were characterized by means of X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), ultraviolet-visible-near-infrared spectroscopy (Uv-vis-NIR) and Raman spectroscopy.

Keywords: ZnO, BiOX, photocatalysis, rhodamine-B, visible light, solvothermal.
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Reference: L.Lin,etal.,Fabrication of a three-dimensional BiOBr/BiOI photocatalyst with enhance dvisible light photocatalytic performance, Ceramics International(2014), http://dx.doi.org/10.1016/j.ceramint.2014.03.039
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[NSN-289] PRODUCTION OF NANOTOROIDAL CARBON STRUCTURES FROM BIOGAS WITH COBALT AND MOLYBDEN CATALYST SUPPORTED ON SBA-15

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Carbon nanostructures synthesis was dominated by the use of no renewable carbon sources like benzene, toluene and its use are so pollutant and risky for health for that reason new carbon sources like biogas a bio renewable gas are investigated. Carbon science became a solid science with the discoveries of carbon nanotubes (CNT) by Ijima and Donald Bethune. These materials are attractive for his amazing properties like his resistance enhancement by adhering metals in his surface and his highly synthetic dye adsorptive capacity. There are so many techniques for the develop of these nanomaterials like Arc Discharge, Spray Pyrolysis and Chemical Vapor Deposition (CVD). CVD technique has been used for his high yields and the easy control of the synthesis variables. In this project biogas has been used as the carbon source obtained from a restaurant organic waste using a modified UASB reactor. Carbon nanostructures were synthetized using CVD technique at 750 °C and 7 LPM of biogas. Mesoporous silica was synthetized using Sol-Gel method. Catalyst was prepared supporting Co and Mo as a catalytic metal on SBA-15. Synthetized materials were analyzed using Raman Spectroscopy, X-Ray Diffraction (XRD) and Transmission Electronic Microscopy (TEM). The synthetized nanostructures were a huge amount of toroidal structures with a range of 5-15 walls obtained using TEM. Raman Spectroscopy showed D and G peaks that represent sp^2 nanostructured carbon. X-ray Diffraction showed peaks in 26°, 44° and 54° corresponding to graphite planes. Biogas is an attractive carbon source for his low cost and its relatively easy obtaining.

Keywords: CNT, Biogas, toroidal, SBA-15, CVD
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[NSN-363] PSEUDOBOEHMITE AS AN ADSORBENT MATERIAL OF POLLUTING ORGANIC MOLECULES IN WASTEWATER

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According to ONU nowadays water pollution is a problem that has not been solved and the main issue is due to the absence of correct management and treatment of human, industrial and agricultural waste. In this work, we find a way to remove pollutants from water, taking into account the surface affinity of pseudoboehmite. Considering this affinity with polluting molecules, of an organic type, such as sodium citrate, the synthesis of pseudoboehmite and gold nanoparticles coated with sodium citrate was carried out. The synthesis of pseudoboehmite was from a solution of aluminum sulfate ($Al_2(SO_4)$) and ammonia gas (NH_3), while nanoparticles were synthesized from a concentration of chlorine auric acid ($HAuCl_4$), deionized water, and sodium citrate. After that, pseudoboehmite was mixed at different concentrations with gold nanoparticles coated with sodium citrate for its characterization using X-ray diffraction technique and UV-Vis spectrometry. It was concluded that pseudoboehmite adsorbs the sodium citrate removing successfully this contaminant from water, being an easy and not expensive option to produce with the same result with other types of pollutant organic molecules.

Key Words: Pseudoboehmite, organic molecules, wastewater, gold nanoparticles, pollution, sodium citrate
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References: Auxilio, A.R. *et al.* (2008) 'Functionalised pseudo-boehmite nanoparticles as an excellent adsorbent material for anionic dyes', *J. Mater. Chem.*, 18(21), pp. 2466–2474. doi:10.1039/B715545J.
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[NSN-414] RAMAN CHARACTERIZATION OF HEMT HETEROSTRUCTURES GROWN ON (631) HIGH INDEX SUBSTRATES.

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Throughout the years and since its discovery the Raman scattering studies have provided valuable information about chemical structures and physical forms of the substances. The versatility of this technique to stablish optical configurations to align the electric field of the electromagnetic wave of excitation and detection adds the capability of gathering information of the symmetry and order/disorder of the molecular structure of the samples. In particular, when applied to study semiconductor nanostructures assembled on high index crystallographic planes, the Raman spectra comprises information related to the near surface anisotropy due to the unidimensional (1D) arrangement, strain and lattice disorder. In this work we studied the structural properties of AlGaAs/GaAs (631) high electronic mobility transistors (HEMTS) grown by molecular beam epitaxy. The intrinsic anisotropic and kinetic properties of the (631) plane allow the self-assembling of 1D quantum wires (QWs) whose geometry essentially depends on the growth temperature and III/V molecular beam fluxes ratio. However, the n-type doping necessary for devices like HEMTs takes place at substrate temperatures where the 1D order is not allowed. Therefore, we explore tin impurification of the AlGaAs barrier of the device to overcome this issue. In order to determine the crystal properties due to the Sn incorporation the parallel and perpendicular directions to the corrugations was evaluated, which correspond to the Z(XX)-Z and Z(YY)-Z RS configurations, where X=[-113] and Y=[-8 19 -9]. The RS analysis shows a clear dependence of the L- intensity located at 256 cm^{-1} with the Sn doping, while the lattice disorder occasioned by the impurity changes the GaAs-like LO/TO intensity ratio, getting further from the ideal ratio depicted by the Raman selection rules. Finally, an original stereographic projection analysis of the RS is presented for even higher index directions.

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[NSN-84] REAL-TIME THERMO-OPTICAL PHOTODEGRADATION MONITORING OF TOXIC DYE WATERS BY PHOTOCATALYTIC ACTION OF SEMICONDUCTOR NANOPARTICLES USING THE PHOTOTHERMAL TECHNIQUE

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Environmental pollution problems, especially in wastewater associated with the textile industry, are due to the fact that these contain chemical components such as: organic dyes, surfactants and additives, which have a significant impact on aquatic ecosystems that affect the health of both aquatic and aquatic species as well as human health, resulting in serious consequences in the rest of the ecosystems, being many of the organic dyes present in wastewater toxic or carcinogenic compounds. In this research project, $AgTiO_2$ and Ag_2CrO_4 nanoparticles were synthesized, to evaluate their photocatalytic activity when irradiated by sunlight (at different exposure times) to cause the degradation of organic dyes such as methyl blue, methyl orange, rhodamine 6G and gentian violet. Photothermal and optical techniques such as Thermal Lens Spectroscopy (TLS), Thermal Wave Resonant Cavity (TWRC) and UV-Vis spectroscopy were used to assess the degradation of organic dyes. Auxiliary techniques were used for its complementary characterization such as: Transmission Electron Microscopy (TEM) to measure the size and distribution of $AgTiO_2$ and Ag_2CrO_4 nanoparticles. To measure its structure, morphology and functional groups, X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR) and X-ray Photon Spectroscopy (XPS) were used.

Keywords: photodegradation, photothermal techniques, nanoparticles, water remediation
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[NSN-100] Removal of total As from aqueous solutions using nZVI@GO heterostructures

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Industrial development has caused changes that affect the environment globally. The contamination of aquifers by heavy metals is a problem of great relevance in Mexico and other countries. Therefore, ensuring the availability of good quality water is a priority. For this reason, new technologies must be generated to treat influents, effluents, and water recovery systems. The use of zero-valence iron (nZVI) nanoparticles and the synergy of their properties with those of graphene oxide (GO) have recently been reported in water treatment processes due to their ability to easily modify the structural properties and physicochemical properties of toxic metals. This work presents the development of heterostructures based on nZVI nanoparticles and GO. The nZVI@GO synthesis was carried out in a reactor using reducing agents such as sodium borohydride. The resulting material was characterized by transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), and X-ray diffraction techniques. Finally, the heterostructures were evaluated in the adsorption of As (III), one of the emerging contaminants present in waters at the national level. The results show an increase in the dispersion of nZVI using GO as a substrate and a more significant elimination of the contaminant with less material compared to previous works where nZVI alone was evaluated.

Keywords: Graphene oxide, heterostructures, nZVI, arsenic, water pollutants

[NSN-73] ROLE OF PLASMON MODES ON THE OPTICAL REFLECTIVITY OF GRAPHENE UNDER UNIFORM STRAIN

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In recent years, the tunable plasmon modes on the terahertz region, has attracted significant interest motivated by grapheneí,'s unique high carrier mobility, electrically or chemically tunable carrier density, long-lived and strong plasmon excitation confinement. In the context of optoelectronics and nanophotonics, graphene is considered as promising plasmonic material working in the mid-infrared and terahertz spectral windows. Assuming that graphene is a strictly 2D material, generalized Fresnel coefficients are derived as a function of the incident angles and the anisotropic in-plane optical conductivity of graphene. As an application, our general findings are particularized for uniform strained graphene. Effectsa uniaxial strain on plasmon modes and the reflectance are performed as a function of the magnitude and direction of the strain.

Keywords: Reflectivity, Graphene, Strain

A. G. Ardakani, Z. Ghasemi, M. M. Golshan. A new transfer matrix for invesigation of surface plasmon modes in multilayer structures containing anisotropic graphene layers, Eur. Phys. J. Plus, (2017)132: 206 DOI 10.1140/epjp/i2017-11468-x

[NSN-116] SIMPLE SYNTHESIS METHOD AND CHARACTERIZATION OF PEROVSKITE-TYPE NdFeO3 NANOPARTICLES FOR GAS SENSING APPLICATIONS

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Perovskite structures with general formula ABO_3 are of great interest in different technological applications, e.g. catalysts, gas sensors, magnetic devices, electrodes for solid oxide fuel cells (SOFC), among others. This work presents the synthesis of $NdFeO_3$ with perovskite-type structure by a simple, economic and reproducible method. The crystal structure, surface morphology, composition, and particle size were analyzed by X-ray diffraction, scanning electron microscopy, and transmission electron microscopy. Microwave radiation was applied for solvent evaporation. The thermal decomposition of the precursors leads to the formation of $NdFeO_3$. The oxide was synthesized at 800 °C and crystallized in an orthorhombic structure with cell parameters a = 5.58, b = 7.76 and c = 5.45 Å, space group Pnma (62). The perovskite´s surface shows a fibrous appearance due to a continuous connectivity between particles, generating cavities among them. La composición elemental de la superficie fue analizada por EDS. The TEM analyses confirmed the formation of $NdFeO_3$ nanoparticles. Starting with the $NdFeO_3$ synthesized powders, pellets were made and tested as gas sensors in propane and carbon monoxide gases. The nanoparticles were clearly sensitive to the studied gases at concentrations of 0–300 ppm, and temperatures of 25, 100, 200, and 300 °C. The response of the material increased with both the increase in temperature and gas concentration.

Keywords: Perovskites, Sol-gel synthesis, Nanoparticles, Gas sensors.
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J. W. Fergus, Perovskite oxides for semiconductor-based gas sensors, Sens Actuators B 123 (2007) 1169–1179. https://doi.org/10.1016/j.snb.2006.10.051

This investigation was carried out following the line of research “Nanostructured Semiconductor Oxides” of the academic group UDGCA-895 “Nano- structured Semiconductors” of CUCEI, University of Guadalajara.

[NSN-237] STRUCTURAL AND OPTICAL STUDIES OF MIXED Ti-Ce COMPOUNDS SYNTHETIZED BY HYDROTHERMAL METHOD

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Mixed compounds based on TiO_2 and CeO_2 structures were synthetized via hydrothermal process, varying the different concentrations between the titanium and the cerium. Samples where prepared by hydrothermal method using titanium and cerium precursors under a highly concentrated sodium hydroxide solution at 130 °C during 60 hours. Obtained compounds were characterized by DRX, Raman Spectroscopy, UV-Vis-NIR, TEM and HR-TEM. DRX diffractograms were analyzed by Rietveld's method to identify compounds present in each sample, this analysis showed the presence of a solid solution phase $Na_{0.5}Ce_{0.5}TiO_3$. UV-Vis-NIR diffuse reflectance spectrum were treated by Kubelka-Munk's method to find the optical gap associated to each sample. The Raman spectrum of the samples showed structural differences between the pure samples and the mixed compounds.

Keywords: Hydrothermal, Solid-Solutions, Mixed Compounds, Cerium, Titanium
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Reference: Hernández-Arteaga, J. G. R., Ojeda-Galván, H. J., Alanis, J., Rodríguez-Aranda, M. C., Villabona-Leal, E. G., Mendoza-Mendoza, E., Ulloa-Castillo, N. A., Quintana, M., Navarro-Contreras, H. R., & Rodríguez, A. G., Thermal tuning of the morphology of hydrothermally synthesized CeO2 nanotubes for photocatalytic applications. In Ceramics International (2022) Vol. 48, Issue 12, pp. 17802–17815). Elsevier BV. https://doi.org/10.1016/j.ceramint.2022.03.051
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[NSN-136] STRUCTURAL CHARACTERIZATION OF GAAS NANOCORRUGATED AND NON-CORRUGATED LAYERS INSIDE ALGAAS BARRIERS WITH A SYMMETRICAL SILICON-DELTA-DOPING GROWN BY MBE

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The way that the dopants are incorporated in semiconductor nanostructures is critical for the fabrication of highly functional electronic devices. For example, in the fabrication of AlGaAs/GaAs heterostructures which are widely used in the fabrication of bipolar transistors or MOSFETs; the doping is usually incorporated as modulated doping. However, this modulated doping of the active layers could introduce crystal defects that negatively affect the performance of the electronic devices. On the other hand, the use of low-dimensional systems such as wires or quantum wells has shown to be of great interest to further improve the performance of different devices. In this work, a study was carried out on the crystalline quality of samples grown as a function of the growth temperature, from 640 to 720 °C of the GaAs active layer. The samples were fabricated by Molecular Beam Epitaxy using GaAs (631) and (100) substrates to induce the formation of corrugated (with different uniformity) and non-corrugated interfaces in GaAs wells inside AlGaAs barriers. The structural characterization was carried out by HRDRX, AFM, and Raman spectroscopy. The samples (100), in which abrupt interfaces are expected, to change very little, which is consistent with what has already been reported. On the other hand, the literature tells us that the surface morphology of the (631) samples varies strongly with temperature [1], our sample with a temperature of 690 °C presents surface corrugation indicative of 1D systems (Quantum Wires) which is important for applications and the study of unique effects in this type of system. The results indicate a similar or even better crystalline quality for both, the GaAs and AlGaAs films, as compared with others reports using a modulated doping.

Keywords: Quantum Wire, GaAs, HRDRX, Raman.
Author for correspondence: elihuhazels@yahoo.com.mx
[1] E. Cruz-Hernández, S. Shimomura, and V. H. Méndez-García, Highly ordered self-assembled nanoscale periodic faceting in GaAs(631) homoepitaxial growth, Appl. Phys. Lett. 101 (2012) 073112. https://doi.org/10.1063/1.4746423
This work was supported by the Consejo Nacional de Ciencia y Tecnología (CONACyT, México) through Grants CB-2015-01-257434.

[NSN-242] STUDY OF NANOMATERIALS BASED ON METAL OXIDES SUBJECTED TO HIGH PRESSURE AND TEMPERATURE CHARACTERIZED BY RAMAN SPECTROSCOPY IN SITU.

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Abstract: Nanotechnology has attracted considerable attention to a broad range of advanced potential technological applications because at the nanometric scale the properties change. Metal oxide nanoparticles represent a field of materials chemistry which attracts considerable interest due to the applications of these compounds. The implications of these materials on fields such as medicine, information technology, catalysis, energy storage and sensing has driven much research in developing synthetic pathways to such nanostructures. In addition, changes in temperature and pressure can lead to the improvement or deterioration of certain properties in nanomaterials. In this review, we will consider three different oxides: zinc oxide ZnO, cerium oxide CeO_2 and zinc vanadate $Zn_3(VO_4)_2$ synthesized by hydrothermal. The structural properties due to high pressure and high temperature will be studied via in situ Raman spectroscopy in order to determine the bulk module, the Grüneisen parameter and compare the results of photocatalytic applications.

Keywords: metal oxide, ZnO, CeO_2, $Zn_3(VO_4)_2$, Hydrothermal, Raman.
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Reference: Rubén Mendoza-Cruz, et al, Orthorhombic distortion in Au nanoparticles induced by high pressure, CrystEngComm, 21(2019) 3451-3459. https://doi.org/10.1039/C9CE00104B

[NSN-188] Study of the effect of the morphology of silver nanoparticles in the catalytic reduction of organic dyes

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The field of study of silver nanoparticles has grown recently, due to their chemical and physical properties, which vary with their size and shape. The study of these nanoparticles is based mainly on the properties of the localized surface plasmon, which can be used in different applications: Surface-enhanced Raman Scattering, sensors, electronic devices, environmental applications, catalysis and photocatalysis, antibacterial agents or anticancer therapies.
Dyes are organic compounds widely used in the textile industry. The waste produced by this industry is discarded without pretreatment, affecting the quality of the water.
The study of this research was focused on the synthesis of silver nanoparticles with different morphologies, to be used as catalysts in the reduction of organic dyes.
Anisotropic nanoparticles were synthesized from spherical particles using high-power LEDs that emit at different wavelengths. Silver nanoparticles were characterized by UV-Vis spectroscopy and scanning electron microscopy to determine their morphology and size. Subsequently, the reduction studies of the methylene blue dye were carried out.

Key Words: Silver nanoparticles, LED, Dyes, Catalysts.
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[NSN-93] STUDY OF ZNS AND AU NANOHETEROSTRUCTURES CORESHELL TYPE FABRICATED BY LASER ABLATION AND EMBEDDED IN A CERAMIC MATRIX

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ABSTRACT: ZnS and Au nanoheterostructures were fabricated by physical methods. The nanoheterostructures obtained consist in a ZnS@Au and Au@ZnS coreshell type mixture. The fabrication of these samples was implemented by an innovative laser ablation in liquid media strategy. This technique offers a mechanism for manufacturing nanoheterostructures through a fast and clean process. The samples obtained were embedded in a ceramic matrix manufactured by sol-gel for its implementation in potential photocatalytic applications. Its potential for implementation in fuel cells is evidenced, as well as in organic dyes degradation. Using first principles, the material structure was modeled, as well its catalytic properties.

Keywords: coreshell nanoparticles, laser ablation, nanoheterostructures, porous silica, photocatalitic applications
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Reference: M. Madkour and F. A. Sagheer, Au/ZnS and Ag/ZnS nanoheterostructures as regenerated nanophotocatalysts for photocatalytic degradation of organic dyes, Optical Materials Express.7(2017) 158-169. https://opg.optica.org/ome/fulltext.cfm?uri=ome-7-1-158&id=355963
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[NSN-139] SYNTHESIS AND CHARACTERIZATION OF IRON OXIDE NANOPARTICLES AND CARBON NANOSTRUCTURES FROM BIOMASS USING GREEN CHEMISTRY

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Nowadays different materials such as carbon nanostructures (graphene, carbon nanotubes), conductor polymers (polyaniline, polypyrrole), metal oxides (manganese oxide, copper oxide), nitrides (vanadium nitride, nickel nitride), sulfides (molybdenum sulfide, iron sulfide) obtained by different methods are used to develop supercapacitors,[1] where some of them are made through synthesis techniques that use hazardous chemicals and sophisticated equipment. One viable solution to reduce the contamination impact is the use of green chemistry to obtain some of these materials because it is ecological, easy and cheap. We reported the preliminary results of the synthesis and characterization of iron oxide nanoparticles using natural extracts as reducing agents, for example, sarcodon clavatus. Also, it is reported amorphous, biochar, porous and activated carbon structures are obtained from biomass, which comes from orange, lemon, bamboo, peanut, eucalyptus, potato, papaya, pineapple, green tea, mate herb, horsetail, corn leaf with thermal treatment at 250°C. We will present the results of the characterization of SEM, DRX, EDS, elemental mapping, DLS of the samples obtained in our research work. The aim of this research is to obtain a composite material of iron oxide nanoparticles and carbon structure to be used in the future as supercapacitor source material.

Keywords: green chemistry, nanoparticles, carbon structure, iron oxide, biomass
References: [1] S. Rajagopal, R. P. Vallikkattil, M. M. Ibrahim, and D. G. Velev, Electrode Materials for Supercapacitors in Hybrid Electric Vehicles: Challenges and Current Progress, Condens. Matter 7 (2022) 6. https://doi.org/10.3390/condmat7010006.

[NSN-34] SYNTHESIS AND CHARACTERIZATION OF MESOPOROUS SILICA NANOPARTICLES

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Mesoporous nanoparticles (MSNs) are investigated due to their physical, chemical, biological properties, their surface functionalization, ability to contain, transport and release active biological substances against a stimulus, so they have received attention in areas, such as catalysis, adsorption, separation, chromatography, chemical sensors, bioscience therapies, oncology, biomedicine and biotechnology, the size can range from 25 to 200 nm, which can be varied by synthesis parameters and by adding additive agents such as: alcohols, amines, inorganic bases and inorganic salts.
The aim of this work is to synthesize mesoporous SiO2 nanoparticles, using a simple method with sizes of 90 - 185 nm and spherical morphology, in order to selectively charge and release, which was amoxicillin.
To prepare MSN, it was made by the Stöber Process, where in a beaker was added ethanol, H2O (water) and NH4OH (ammonium hydroxide), stirred on a plate, added TEOS with a peristaltic pump, obtaining a white mixture, centrifuged to obtain a white powder. Finally, the powder is washed with deionized water, to remove the precursor TEOS.
In total 9 MSN synthesis were performed, to determine the synthesis with the necessary specifications such as reagent concentration, zeta potential lower than -30 mV and size of the MSN, achieving specifications, loaded and released the MSN with amoxicillin, performing antibacterial tests, where it was observed that it has bactericidal characteristics, which was what was sought.
The objective was reached to prepare MSN of the required size, becoming a promising material of the future in medicine, for its characteristics for the release of drugs or substances biologically, avoiding damage to organs or cells in good condition. Without forgetting that synthesis is a process that controls pore size, structure, biocompatibility and low toxicity.

Keywords: MSN, load, release, synthesize, size.
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Reference: Naiara I. Vazquez, Z. G. (7 de ABRIL de 2017). Synthesis of mesoporous silica nanoparticles by sol–gel as nanocontainer for future drug delivery applications. *ELSEVIER*, doi:https://doi.org/10.1016/j.bsecv.2017.03.002
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[NSN-36] SYNTHESIS AND CHARACTERIZATION OF MNFE2O4 NANOPARTICLES: INFLUENCE OF BETA-CYCLODEXTRIN ON THEIR MICROSTRUCTURE

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Manganese ferrite has a wide interest in the photocatalytic degradation of organic contaminants in water, due to its high stability and strong magnetic property, in addition to being friendly due to its low toxicity. The investigations are being studied with the aim of improving its physical chemical properties and thus improve the catalytic performance.
In this work we report a simple way to synthesize manganese ferrite ($MnFe_2O_4$) nanostructures by the coprecipitation method, using Fe chloride and Mn sulfate as metal precursors, and β-cyclodextrin (β-CD) acting as coating agent. Synthesis was accompanied by the hydrothermal method at different temperatures 120 and 140 °C for 24 h. These samples were named as β-CD-$MnFe_2O_4$. For comparison, pure $MnFe_2O_4$ was also prepared by a similar procedure, without the addition of β-CD.
X-ray diffraction (XRD) analysis of the β-CD-$MnFe_2O_4$ sample prepared without a reactor and the sample at 120°C indicated little crystallinity of the material, while the sample at 140°C indicated the presence of a single phase. crystal corresponding to $MnFe_2O_4$. The crystallite size of these samples increased with temperature from 2.7 nm to 4.7 nm. On the other hand, the sample obtained at 140°C is mesoporous with a high value of specific surface area 240 m_2g^{-1}. The XRD of the samples without cyclodextrin showed good crystallinity at all synthesized temperatures, however, the size of the crystallite was 23 nm, much larger than the samples obtained with cyclodextrin.
In the degradation of methylene blue, the samples obtained with cyclodextrin presented a better catalytic performance than pure $MnFe_2O_4$ in terms of activation of hydrogen peroxide (H_2O_2) to degrade methylene blue (AM) at neutral pH. The results indicate that β-CD-$MnFe_2O_4$ is promising for the degradation of organic species in aqueous systems, overcoming the disadvantages of pure $MnFe_2O_4$.

Keywords: Nanoparticles, methylene blue, manganese ferrite, cyclodextrin
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Reference: Zhou X, Kong L, Jing Z, et al. The art of writing a scientific article,Journal of Hazardous Materials (2020). https://doi.org/10.1016/j.jhazmat.2020.122528
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[NSN-273] SYNTHESIS AND CHARACTERIZATION OF PHOTOCATALYSTS OF TiO2 - Ag

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Heterogeneous photocatalysis has proven to be effective in removing a wide range of contaminants. Using titanium dioxide (TiO_2) which improves its performance when doped with nanostructures that are mostly metals. In this work, TiO_2 photocatalysts with different contents of silver nanoparticles (Ag) were synthesized by means of the sol-gel method assisted by a microwave reactor and subsequently subjected to thermal treatments between 400°C - 700ºC. The materials were analyzed by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Scanning Electron Microscopy (SEM) and Diffuse Reflectance Spectroscopy to study the influence of silver and heat treatments on the properties. structural and optics of TiO_2.

Keyword: photocatalysis, TiO_2, silver nanoparticles.
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[NSN-333] Synthesis and Characterization of silver nanoparticles with the use of commercial teas as reducing agents.

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Nowadays, the development of synthesis methods of silver nanoparticles (Ag NPs) that involve the use of non-aggressive agents with the environment has taken great relevance. The easiest method is the one known as green synthesis, which usually is made of plant extract, taking advantage of the reducing properties we find in their phenolic groups. This research proposes the use of commercial teas, that can be found in any convenience store, and their extracts are obtained and then used to synthesize the silver nanoparticles. In this research was used a hot plate stirrer to obtain the Ag NPs with silver nitrate (AgNO3) and teas, such as chamomile, lemongrass, and ginger-lemon; the nanoparticles obtained were characterized by ultraviolet-visible spectroscopy (UV-vis), scanning electron microscope (SEM) and dynamic light scattering (DLS).

Keywords: Silver nanoparticles, green synthesis, commercial teas.

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[NSN-265] SYNTHESIS AND CHARACTERIZATION OF TiO2 POWDERS DOPED WITH Ni AND Ag BY SOL GEL METHOD

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Impurifying a material through the use of elements or compounds (copper, gold, nickel hydroxide, tungsten, carbon nanotubes (CNT), etc.) is a common practice that is carried out to improve or attenuate some property; In the case of multifunctional materials such as ilmenites or titanium oxide, doping can alter more than one property and limit their possible applications. In the present work, the synthesis of TiO_2 doped with Ni and Ag (10% w) was carried out by the sol gel method to modify the electronic properties of TiO_2. The sample was dried at 100°C and heat treated at 500°C. It was structurally and morphologically characterized by: X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). The dried sample presents crystallization towards the anatase phase of TiO_2, metallic silver and a tendency to crystallize $NiTiO_3$, while at 500 ºC, the anatase phase shows a crystallinity of more than 80%, $NiTiO_3$ is crystalline and silver remains as metallic silver. However, the main anatase peak is slightly displaced, possibly due to the insertion of silver atoms in the interstitial space of the anatase structure.FTIR spectroscopy shows the characteristic Ti-O bonds typical of Titania, as well as at 1624 cm^{-1} of the Ni-O-Ti bond. The SEM images show that the particles tend to agglomerate.

keywords: sol gel, ilmenites.
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[NSN-362] SYNTHESIS AND CHARACTERIZATION OF ZnO NANOPARTICLES BY LASER ABLATION OF SOLIDS IN LIQUIDS

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Laser ablation is a process in which the laser removes or vaporizes material from the surface of a solid object by striking it, a laser with an optical system is concentrated on the surface to be ablated.
For this experiment we used a metal our target is Zn.
We made several samples where the laser ablation technique used, changing some variables such as its energy, time and liquid such as alcohols, biodistilled water and glycerin, in all the experiments carried out so far only our Zn nanoparticles have been oxidized.
"Zinc oxide is chemically and thermally stable, it has a gap of 3.37eV and it excitation junction energy is 60eV. The benefits of using this compound are that it is low cost, has excellent electrical and optical properties, and is applied in microelectronic devices, solar cells, biological sensors, photocatalytic agents."(Barrón Dannareli,2018, p.10).
On this specific occasion, tests will be carried out to see its possible application as a bactericide in some products such as talcum powder.
Due to the fact that the size of the synthesized material can be controlled by changing some synthesis parameters, such as wavelength, fluence, and duration of the laser pulse, as well as changes in pH or temperature in the liquid medium, the technique of UV-VIS spectroscopy in which the samples will be measured every day to see their oxidation evolution.

Keywords: Nanoparticles, laser ablation, sprectroscopy, experiments, bactericide.
Reference: [1] Barrón Dannareli, "Capítulo 2-Fundamentos teóricos", Síntesis y caracterización de nanopartículas de óxido de Zinc por las técnica de ablación láser de sólidos en líquidos, Universidad autónoma de Baja California, p.10-18, 2018

[NSN-160] SYNTHESIS OF CARBON NANOSPHERES BY PYROLYSIS OF POLYCARBONATE

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Nanotechnology has developed with the creation of new materials, and particularly, with the discovery of new carbon nanostructures due to their properties and important applications in different fields. The objective for this work was to synthesize carbon nanospheres by pyrolysis from polycarbonate. Polycarbonate is a plastic which is used in many fields and now the different recycling methods of it are looked. The samples obtained during the synthesis process were characterized through Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), Raman spectroscopy, Fourier Transform Infrared spectroscopy (FTIR), and X-ray diffraction (XRD). The reactor consists of a quartz tube inside an electric furnace connected to a flowmeter. High purity argon gas was used as an inert medium to prevent combustion and as carrier gas with two flows: 20 ml/min and 60 ml/min. Polycarbonate was used as carbon precursor. The synthesis temperatures were 650, 700, 750 and 800 degrees centigrade. The morphology and size of nanostructures were determined with SEM. The micrographs showed that the synthesized nanostructures have a spherical morphology and show some coalescence, the diameters of the carbon spheres obtained are from 50 to 400 nm. EDS demonstrated high carbon (greater than 93 wt%) and low oxygen contents. The D and G bands, characteristics of carbon nanomaterials, were identified by Raman spectroscopy. FTIR analysis demonstrated the typical bands of carbon nanomaterials functional groups as -OH, CH_x, CO, C=C. X-Ray Diffraction, used to see the crystallinity of the obtained products, performed in a range of 5 to 80 degrees 2θ, showed a broad band at 26 degrees. These obtained carbon spheres can be used in the different fields, like electronics, energy storage, drug delivery etc.

Keywords: carbon spheres, pyrolysis, polycarbonate, nanomaterial
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[NSN-381] SYNTHESIS OF SILICON CARBIDE NANOPARTICLES BY LASER ABLATION OF SOLIDS IN LIQUIDS TECHNIQUE

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In this work we report the synthesis of silicon carbide nanoparticles by laser ablation of solids in liquids (LASL) method using different types of liquids for the synthesis. The purpose of this work is for the study of the optical properties and behavior of the colloidal silicon carbide nanoparticles in different solutions and looking at the behavior of a photosensitive resin when silicon carbide NPs are added, analyzing the original resin with the one with NPs comparing their optical and mechanical properties.
Using the laser equipment of CUCEI labs, the laser configuration was changed so it can be able to shoot at a delay of 7 microseconds for a higher energy emission. The laser was able to hit the silicon carbide target inside of a beaker fully covered with the solutions that we are working on (distilled water, methanol, ethanol, isopropanol, and a resin) thanks to an optical lens arrangement on the other room. When the laser was fired the sample could be observed through a camera to verify the ablation is correctly happening, for each experiment the time of ablation was kept constant in all the solutions. Colloids were optically characterized by UV-Vis spectroscopy and the hardened resin was tested for tensile stress behavior.

[NSN-346] SYNTHESIS OF SILVER NANOPARTICLES AND ITS APPLICATION AS A CONDUCTIVE INK FOR FLEXIBLE AND PRINTING ELECTRONICS.

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The use of materials with conductive properties, such as metallic nanoparticles, is currently a component of great interest since it favors the production of electrical circuits and devices using flexible substrates. Through printing electronics, an easy application and manipulation of these conductive materials can be carried out for their development in flexible electronics. In this work, the synthesis of silver nanoparticles was carried out for their potential application as a conductive ink in flexible electronics. Nanoparticles were obtained using sodium borohydride ($NaBH_4$) and sodium citrate ($C_6H_5Na_3O_7$) as reductive agent. It was observed that with the use of these reagents at an optimal concentration, silver nanoparticles are obtained, using silver nitrate ($AgNO_3$). as precursor agent. The conductivity of the obtained product was tested by placing it on strips of paper connected to an LED. The characterization of the ink was carried out through I-V measurements, as well as flexibility of the formed prototype. Finally, the formation of a conductive ink was carried out by integrating the formed nanoparticles, which was adapted to a conventional printer.

Keywords: Silver nanoparticles, printing electronics, flexible electronics.
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[NSN-322] SYNTHESIS OF SILVER NANOPARTICLES BY ELECTROCHEMICAL METHOD

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In this work, silver nanoparticles (AgNP) were synthesized by electrochemical method, using a metallic silver cathode and anode in deionized water. The polarity was inverted every 60 seconds generating a voltage variation in order to obtain three different concentrations: 16 ppm, 24 ppm and 34 ppm. The synthesized nanoparticles were structurally, optically and morphologically characterized by XRD, UV-Vis and Transmission Electron Microscopy (TEM), respectively. XRD patterns showed the peaks at 38.11 and 64.42 from Ag. The surface plasmon resonance peak in absorption spectra on silver colloidal solution showed absorption from 422 nm to 429 nm. TEM measurement provided an average particle size for the concentrations of 16 ppm, 24 ppm and 34 ppm of 4.23 nm, 3.95 nm and 3.27 nm, respectively.

Keywords: silver nanoparticles, electrochemical method, XRD, UV-Vis, TEM.
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[NSN-366] SYNTHESIS OF SILVER NANOPARTICLES BY LASER ABLATION OF SOLIDS IN LIQUIDS AND THEIR POTENTIAL APPLICATION IN SURFACE ENHANCED RAMAN SPECTROSCOPY (SERS)

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This project was carried out by laser ablation of solids in liquids, which in this case our target was silver. As liquid media we used different alcohols and doubly distilled water, in this way, silver nanoparticles were obtained which were suspended in the liquid to be used.
Multiple samples were fabricated at different conditions such as laser energy, ablation time and the liquid where our target was immersed, the samples changed in the optical and physical characteristics depending on the synthesis condition, the most noticeable feature would be the color of the suspensions.
The multiple samples were analyzed by UV-VIS spectroscopy in order to see the absorption by surface plasmon resonance. To investigate if nanoparticles produce SERS effect, a pellet of TiO2 was measured by Raman spectroscopy, afterwards, drops of suspensions were added to the surface and it was measured again.

Keywords: Laser Ablation Silver Nanoparticles SERS.
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[NSN-110] SYNTHESIS, CHARACTERIZATION, AND GAS SENSOR APPLICATION OF NANOSTRUCTURED COBALT MANGANITE

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Abstract: Cobalt manganite ($CoMn_2O_4$) is a semiconductor material that has been used as an anode in lithium-ion batteries, supercapacitors, and electrocatalysts due to its high stability, low toxicity, and excellent electrochemical behavior [1]. To date, $CoMn_2O_4$ has been little studied in the field of gas sensor. Therefore, in this work we synthesized, characterized, and investigated the detection properties of nanostructured cobalt manganite. $CoMn_2O_4$ was synthesized by a simple microwave-assisted colloidal method. The samples obtained were characterized by X-ray diffraction, Raman spectroscopy, scanning electron microscopy and ultraviolet-visible spectroscopy. The crystalline phase of $CoMn_2O_4$ was obtained at a calcination temperature of 400 °C, while the main Raman vibration bands confirmed the spinel structure of cobalt manganite. The surface morphology of $CoMn_2O_4$ revealed a porous microstructure with irregularly shaped pores, and a particle size distribution ranging from 30 to 100 nm was estimated. In addition, three characteristic absorption bands of $CoMn_2O_4$ were located at 314, 631, and 680 nm. Detection measurements showed that $CoMn_2O_4$ is sensitive to ethanol in the range of 10 to 50 ppm at an operating temperature of 185 °C with a stable, reproducible, and repeatable response. The decrease in resistance of $CoMn_2O_4$ in the presence of ethanol indicated n-type semiconductor behavior. Due to the good detection performance of the nanostructured $CoMn_2O_4$, it could be used as a sensor to detect ethanol.

Keywords: Cobalt manganite, nanoparticles, gas sensor, ethanol
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Reference: [1] H. Jiu, N. Ren, L. Jiang, Q. Zhang, Y. Gao, Y. Meng, and L. Zhang, Hierarchical porous $CoMn_2O_4$ microspheres with sub-nanoparticles as advanced anode for high-performance lithium-ion batteries, J. Solid State Electrochem. 22 (2018) 2747–2755. https://doi.org/10.1007/s10008-018-3987-y.
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[NSN-235] THERMAL EVOLUTION OF THE STRUCTURAL, OPTICAL AND VISIBLE LIGHT PHOTOCATALYTIC PROPERTIES OF Zn-V-O SYSTEMS

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Several compounds of the Zn-V-O system were prepared via a precipitation process, some samples were subjected to a subsequent hydrothermal process. The resulting materials consisted of a single vanadium compound $Zn_3(OH)_2V_2O_7{\cdot}2H_2O$, hydrated zinc hydroxy-vanadate. Calcination at 300, 500, 700 and 850 ^oC, resulted in the formation of five other Zn-V-O compounds, which evolved from the hydrated zinc hydroxy-vanadate compound. The relevant compound in photocatalysis, zinc vanadate $Zn_3V_2O_8$, was synthetized at 500 ^oC and higher temperatures. The samples obtained at different calcination temperatures were characterized in their structural, optical and photocatalytic response. It was observed that the best photocatalytical response under visible illumination was obtained with the material calcined at 500 ^oC, which presents a heterojunction between the $Zn_3V_2O_8$ and the ZnO binary compound.

Keywords: Zn-V-O family, Calcination, Photocatalysis, visible light, dyes; MB
Author for correspondence: a259046@alumnos.uaslp.mx
References: Villabona-Leal, E. G., Escobar-Villanueva, A. G., Ovando-Medina, V. M., Pérez-Pérez, E. B., Díaz-Flores, P. E., Romero-Galarza, A., & Marquez-Herrera, A. Semiconducting polypyrrole@TiO2 pure anatase nanoparticles for photodegradation of reactive red 120 azo dye. In Journal of Materials Science: Materials in Electronics (2020) (Vol. 31, Issue 15, pp. 12178–12190). Springer Science and Business Media LLC. https://doi.org/10.1007/s10854-020-03764-2
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[NSN-85] THERMAL STUDY OF MAGNETIC NANOPARTICLES IN WATER-BASED NANOFLUIDS FOR APPLICATIONS IN BIOMEDICINE

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Superparamagnetic magnetite (Fe_3O_4) nanoparticles (NPs) are a promising option in the field of biomedicine, as well as in hyperthermia therapies, drug delivery and imaging, among others. Fe_3O_4 NPs of less than 20 nm in size are able to organize themselves when a nearby magnetic field is encountered and lose magnetization when this field is removed. A simple methodology has been developed to synthesize these nanoferrous particles, using the precipitation method for Fe_3O_4 NPs. They were characterized by Fourier Transform Infrared Spectroscopy (FTIR), UV-vis spectroscopy and X-ray diffraction (XRD). A laser was used to heat and recorded using a thermal camera to know their behavior. For such applications, an important parameter is thermal conductivity as a function of nanoferrous concentration and nanoparticle size, using the thermal wave resonant cavity characterization (TWRC) technique. The experimental data were fitted to various classical models such as the Maxwell model and the neural network model to describe the thermal conductivity of nanoferrous metals. These investigations have immediate applications in drug transport and imaging (1).

Keywords: magnetic nanoparticles, nanofluids, biomedicine, characterization
Author for correspondence: jimenezp@fis.cinvestav.mx
Reference: Ghazanfari MR, Kashefi M, Shams SF, Jaafari MR., Biochem Res Int. 2016, (2016). https://doi.org/10.1155/2016/7840161
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[NSN-202] THERMO-OPTICAL CHARACTERIZATION OF CARBONIZED POLYACRYLONITRILE (PAN) NANOFIBERS AND EXFOLIATION OF FIBERS FOR DETERMINATION OF QUANTUM EFFICIENCY

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Polyacrylonitrile (PAN) fibers were obtained by the electrospinning technique which were calcined in a nitrogen atmosphere, these were put in isopropyl alcohol to be exfoliated and subsequently centrifuged. For the scanning electron microscopy (SEM) micrographs carbonized fibers with a diameter of 211±0.74 nm were observed. From energy dispersive X-ray spectroscopy (EDS) percentage elements obtained values were 98.5% carbon, 1.5% oxygen and 0% nitrogen. X-ray diffraction pattern showed two diffraction peaks (002) and (101) associated with graphite oxide. Raman spectroscopy demonstrates two main bands D and G associated with sp2 and sp3 hybridizations, as well as defects. The X-ray photoelectron spectroscopy (XPS) corroborated the bonds of these energies for the hybridizations after exfoliation of carbonized fibers. From transmission electron microscopy (TEM) particles of approximately 10 nm were seen and high resolution-TEM (HRTEM) showed an interplanar distance of 0.19 nm with direction (002) associated with graphene oxide. Fluorescence showed 2 energy bands one in 2.52 eV and 2.84 eV as well as photoluminescence 2.69 and 2.98 eV associated with structural defects. Besides the information about nonradiative efficiency, absolute values of fluorescence quantum efficiency and *ds/dT* were determined through the wavelength TL method by using a discrete excitation wavelength 514.

Keywords: photoluminescence, thermal lens, polyacrylonitrile fibers, quantum efficiency
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This work has been supported by: SIP project, COFAA and CONACYT

[NSN-217] TUNING THE LOCAL DENSITY OF STATES WITH APPLIED PRESSURE IN DEFECTIVE ONE-DIMENSIONAL PHOTONIC CRYSTALS

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ABSTRACT: In this work, we calculate the local density of states using dyadic Green's functions for a defective one-dimensional photonic crystal of finite size composed of alternating air and semiconductor layers. Photonic crystals are heterostructures built from periodic arrangements of materials with different refractive indexes. We consider that the refractive index of semiconductor materials, such as GaAs, Si, and SiO_2, changes with the amount of the applied pressure. Herein, spatial periodicity is broken as one of the semiconductor layers increases its layers. We determined the existence of a confined mode within the cavity with a maximum value of the local density of states. Currently, in the photonic crystal field, designing sensors of ultra-compact size and fast response is preferred. One of the sensors used in the one-dimensional photonic crystal is the pressure sensor. The results show that, as pressure increases, the local density of states decreases within the confined mode. However, for the GaAs cavity, the results reveal that increased pressure favors the appearance of a more significant number of confined modes at frequencies within the second photonic band gaps.

Keywords: Photonic crystal, local density of states, dyadic Green's functions, pressure, photonic band gaps.
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Reference: F. Segovia-Chaves, H. Vinck, and E.P. Navarro, Local density of states in a one-dimensional photonic crystal with a semiconducting cavity, Results in Physics 33 (2022) 105129. https://doi.org/10.1016/j.rinp.2021.105129.
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[NSN-154] TUNNELING EFFECT BETWEEN MULTIPLE-QUANTUM WELL AND OPTICAL TRANSITIONS OF GALLIUM ARSENIDE QUANTUM WIRES AND WELL: THEORETICAL AND EXPERIMENTAL STUDY.

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The synthesis of one-dimensional(1D) arrays, such as III–V semiconductor quantum wires (QWRs) is an important topic of study due to the unique quantum effects predicted for 1D systems and by the numerous potential applications of these nanostructures in electronic and optoelectronic, in addition to the possibility of improving existing applications. Similarly, the tunnel effect is one of the physical phenomena that has generated interest for possible applications [1]. In this work, the theoretical study of the quantum tunneling effect in GaAs/AlGaAs systems was carried out for different configurations of the finite periodic type, ranging from 2 to 5 quantum wells for different well and barrier sizes. The Schrödinger equation was solved using the transfer matrix method with the Kroning-Penney model as reference. It was found that the transmission coefficient presents a resonant behavior and reaches the maximum value of 1 at resonant energies. On the other hand, from the results of the photoreflectance spectroscopy technique (PR), the experimental transition energies corresponding to the quantum wires and the quantum well of GaAs were obtained, and these energies were compared with the theoretically calculated optical transitions, which showed good agreement. Also, the transitions identified in the type of confinement and the type of heavy hole or light hole transition were studied.

Keywords: Tunneling, Quantum Wire, GaAs, photoreflectance.
Author for correspondence: elihuhazels@yahoo.com.mx
Reference: [1] R. Méndez Camacho and E. Cruz Hernández, Tunneling between parallel one-dimensional Wigner crystals, Sci Rep. 12 (2022) 4470. https://doi.org/10.1038/s41598-022-08367-x
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Sesión Oral

[NSN-187] ATOMIC-SCALE UNDERSTANDING OF THE Na AND Cl TRAPPING ON THE Mo1.33C(OH)2-MXene

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Drinking water scarcity in arid and semi-arid regions is a reality that may turn into a global healthcare problem in the next few years. The scientific community is always looking for new materials to achieve effective sea and brackish water desalination to reduce water scarcity. Commonly, theoretical, and experimental methods make a synergy to better understand and explain the chemical and physical processes in water desalination electrodes. In this way, experimental evidence pointed Mo1.33CTx MXene as an efficient ion intercalation material, in which both Ná and Cl are removed. However, the atomic-scale understanding of the physicochemical processes due to the Na and Cl interaction with the MXene is still unknown. We report the Ná and Cl interaction with an OH functionalized Mo1.33C monolayer through a comprehensive first-principles density functional theory assessment. Results demonstrate that Na atoms attach to Oxygen, whereas Cl atoms bond through hydrogen bonds to the functional groups in the MXene, these bonds have two energy contributions: electrostatic and charge transfer, which increases its adsorption energy. Electrostatic potential isosurfaces, Bader charge analysis, and non-covalent interactions index help clarify the way Ná and Cl attach to the MXene layer. Oxygen atoms have an affinity for the electropositive Ná atoms, which after interaction oxidize to Ná, whereas hydrogen atoms—of the hydroxyl groups—interact with the electronegative Cl atoms, which upon adsorption reduce to Cl. Our findings explain why OH-functionalized Mo1.33C can efficiently remove both Na and Cl atoms based on their affinities with the functional groups present in the MXene layer.

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[NSN-412] AUXETIC MATERIALS BASED ON GRAPHENE DERIVATIVES AND NANOCOMPOSITES

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The development in design and technology in the field of engineering requires the use of smart and high-performance materials to meet the highest specifications. General requirements of such materials include specific combination of properties and low production costs. Among smart materials, auxetic materials represent a great potential for many industries, as a response to the emerging field of negative Poisson's ratio materials. To improve the inherent properties of an auxetic material or add properties of interest to the material, certain conditions are required. Thus, the design of nanocomposites stands out as an important alternative for the development of auxetic materials with improved characteristics, such as its impact and indentation resistance, fracture toughness, stiffness, energy absorption, among others. The effective preparation and development of auxetic material is the key issue for its use in future applications. The scope of the present work goes from the understanding of the structure and properties relation of both matrix and reinforcement to achieve a permanent auxetic response in the nanocomposite. Furthermore, taking advantage of the excellent properties of chemically derived graphene materials. A successful auxetic material will be the one which can be produced on a commercial-scale with the desired properties.

Keywords: Graphene Derivatives, Auxetic Properties, Nanocomposites.
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[NSN-246] BIMETALLIC SILVER-GOLD (AG/AU) NANOPARTICLES BY PULSED LASER ABLATION IN LIQUID (PLAL) AND THEIR COATINGS DEVELOPED BY ELECTROPHORETIC DEPOSITION (EPD)

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Abstract: Nanoparticles have interesting properties and being new bimetallic ones, draw much more attention from researchers for their optical, electronic, magnetic, chemical, and biological application. Pulsed laser ablation in Liquid (PLAL) is an efficient synthesis method for developing metallic, semiconducting, and ceramic nanoparticles. In this work, nanocolloids of bimetallic silver/gold (Ag/Au) nanoparticles were obtained by ablation using a Nd: YAG laser of 532 nm wavelength, with an energy of 90 mJ, with a pulse switch of 10 nanoseconds, frequency 100 Hz. The optical properties of Ag/Au nanocolloids were analyzed by UV-visible-NIR spectroscopy. Transmission Electron Microscopy (TEM) analysis was used for the morphology, structure, and sizes of these bimetallic nanoparticles. Electrophoretic deposition was then used to develop coatings from these bimetallic nanocolloids. The coating is obtained on different substrates under various electrophoretic deposition parameters, such as voltage, current and time. Elemental composition and analysis of chemical states of nanoparticles as well as coatings are done by X-ray photoelectron spectroscopy (XPS), morphological analysis of bimetallic coatings is performed by scanning electron microscopy (SEM). The reflectance spectra for the developed coating are also obtained using UVvisible-NIR. The results of this study show that electrophoretic deposition is effective for the development of bimetallic nanoparticle coatings from their laser-synthesized nanocolloids.

Keywords: Bimetallic nanoparticles, Pulsed laser ablation in liquid, Electrophoretic deposition, Coatings, Material characterization
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One reference : G. Ortiz-Arana, M. Talavera-Rojas, V. Velázquez-Ordoñez, and J. Acosta-Dibarrat, “Aplicaciones de las nanopartículas metálicas en las ciencias veterinarias,” Rev. MVZ Cordoba, vol. 26, no. 3, pp. 1–12, 2021, doi: 10.21897/RMVZ.2123.
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[NSN-420] CARBON NANOSTRUCTURES IN WATER REMEDIATION: ROLE OF DIMENSION AND FUNCTIONALIZATION IN ADSORPTION AND PHOTOCATALYSIS

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Carbon nanostructures such as multi-walled nanotubes, single-walled nanotubes, graphene or graphenic materials, and graphene quantum dots have been extensively researched in the last 20 years, and due to their outstanding properties have been proposed for diverse possible applications. Although these materials are based on the same graphitic sp2 hybridization, the differences in their structures have allowed diversifying their properties; thus, there are significant variants that play an important role in the performance of these nanostructures depending on the field in which could be employed. Due to their outstanding mechanical, thermal, electrical, and optical properties these materials have been proposed to be used in composite materials, catalysis support, electronic devices, and biomedical applications among others. However, in addition to the mentioned properties, other important features in carbon nanostructures are surface area, point of zero charge, and band gap, these surface and structure characteristics depend on graphitization degree, surface functionalization, and dimension. Therefore, the whole of the mentioned features and properties have made carbon nanostructures an important option in water remediation, removing diverse pollutants by adsorption or photocatalysis. This invited talk presents a summary of the results found in the Advanced Materials and Nanotechnology group, related to the adsorption capacities for removal of dyes and hexavalent chromium from aqueous solution achieved by different carbon nanostructures. The role that plays dimension, functionalization, and graphitization degree in this process depending on rate-controlling mechanisms and equilibrium data are analyzed. Also, the performance of carbon nanomaterials as photocatalysts depending on oxidation degree and dimension is revealed, in the degradation of phenolic organic pollutants. Finally, some results found in current research of graphene quantum dots functionalized by biomolecules as photocatalysts in the degradation of methylene blue in water are shown and discussed. Concluding remarks will also be presented in full context.

Keywords: Carbon nanostructures, water remediation, adsorption, photocatalysis, dimension.
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[NSN-408] DESIGNING PLASMONIC NANOSTRUCTURES FOR MOLECULAR SENSING AND PHOTOCHROMIC SMART WINDOWS

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Plasmonics is the study of light at the nanometer scale. Plasmonic research has received a tremendous boost recently due to the vast possibility of utilizing plasmonic nanostructures in diverse technological fields which include ambiental remediation, therapeutics, biomedicine, energy harvesting, and many others. However, for each of these technological applications, we need plasmonic nanostructures of specific characteristics and functionality, which can be induced only by manipulating their design. For example, pure metallic nanostructures of different sizes and shapes exhibit surface plasmon resonance at different energies. On aggregation, the electric field around them gets modified. On the other hand, when anchored with or embedded in some semiconductor or dielectric material, electron transfer occurs at their interfaces, generating new functionality of the composite. In this talk, I will present some examples and research results to demonstrate how we can design and fabricate plasmonic nanostructures of specific functionalities for applying them in molecular sensing and for fabricating efficient photochromatic windows.

Keywords: *Plasmonics, Metal nanoparticle, Core@shell nanoparticles, SERS-based sensing, Photochromatic window.*
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[NSN-31] GRAPHENE OXIDE AND MAGNETITE NANOPARTICLES NANOCOMPOSITES FROM AGRO-INDUSTRIAL WASTES FOR CATALYST APPLICATIONS

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Graphene oxide (GO) is a carbon nanomaterial, which is useful and promising for applications in electronics, optics, chemistry, energy storage and biology. Due to the presence of hydroxyl, carboxyl and epoxy functional groups on the basal and edge plane of GO, this material is easily dispersed in aqueous solvents, making its processing and usage more convenient. In addition, the strong hydrophilicity of GO guarantees that it is a good candidate for many applications, including drug delivery, harmful cell treatment and water purification. GO is usually obtained using the Hummers'method by oxidizing graphite, where a considerable volume of strong acid wastes are generated. Nowadays, the use of green chemistry in the research of nanomaterials has the purpose of decrease and eliminate the presence of toxic and contaminating compounds during the synthesis of GO. In the present work, we produce GO through pyrolysis of different agro-industrial wastes, which are: peanut shell (PSP), post-use commercial ground (PMCB) and artisanal (PXCB) coffee and were compared with GO produced by the Hummers' method. The different properties of the products obtained from the green synthesis and the Hummers' method were compared using FTIR for the detection of functional groups and Raman spectroscopy for the detection of D (disorder) and G (graphitization) bands that are characteristic of GO. Afterwards, the GO of different materials were functionalized with magnetite by chemical co-precipitation for use as catalysts. The functional groups present in the nanomaterial obtained are used as nucleation centers for the formation of metal oxides. Therefore, a major number of functional groups present in the surface will cause the formation of metal oxide nuclei, obtaining metal oxide nanoparticles with good dispersion on GO sheets for energy and environmental applications such as generation of biofuels, adsorptive removal of dyes in water and antimicrobial activity in wastewater treatment plants.

Keywords: Graphene oxide; agro-industrial wastes; nanoparticle; magnetite; nanocomposites
One reference: Somanathan, T., Prasad, K., Ostrikov, K. K., Saravanan, A., & Krishna, V. M. (2015). Graphene oxide synthesis from agro waste. Nanomaterials, 5(2), 826–834. https://doi.org/10.3390/nano5020826
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[NSN-30] HETEROSTRUCTURES OF GRAPHENE OXIDE AND FEW LAYERS GRAPHENE FOR MEMEBRANES.

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Van der Waals Heterostructures are defined as an arrangement of bidimensional (2D) crystals layer by layer that can be designed in a chosen sequence. These heterostructures of 2D materials are a new exciting field for new properties, like hydrophilic and hydrophobic nature of heterostructures of few layers graphene (FLG) and graphene oxide (GO). Among the applications proposed, membranes present lot of opportunities for heterostructures in mechanical stabilization of the materials to exposure of water or organic solvents, and for control of pores for effective molecular separations. One example is GO exposure to water was already found unsuitable for long term stability. But heterostructures adding FLG or partially reduced graphene oxide (PrGO) to the GO are useful. In this work we address the use of GO as main component for desalination application due to water easy slip through pores. The methodology includes synthesis of GO by modified Hummer's method, synthesis of few layers graphene (FLG) by ultrasound method, characterization of these materials by Raman spectroscopy, UV-Visible spectroscopy employment for the characterization of the mixtures of FLG and GO, and permeability of the membranes for water and for a sodium chloride solution. We use weight percentage of GO and FLG in the assembly for the membranes, which is related to the weight of a GO sheet and FLG sheets. That is why, we expect that the number of sheets of each material for a same mass weight in the membrane will be different, and then we address calculations for idealized sheets that propose a coverage phenomenon in the conformation of the heterostructure GO-FLG.

Keywords: Graphene Oxide, Few Layers Graphene, Heterostructure, Membrane, 2D Materials.
Reference: A. K. Geim, I. V. Grigorieva, (2013), Van der Waals heterostructures, Nature Perspective Research, Vol 499, (419-425), doi: 10.1038/nature12385
This work was supported by: CONACYT Ciencia Básica CB-A1S-8817 “Diseño Molecular de Materiales 2D para la construcción de Membranas Artificiales Inteligentes” CONACYT Scholarship no. 744836

[NSN-308] Hybrid structures of zinc oxide-macroporous silicon as a posible alternative in gas detection

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Nowadays, the effort to obtain nanostructures/hybrids from semiconducting materials has attracted a considerable interest in the scientific community due to the possible superior functional properties that they could be present compared to the individual components assembling composites. Among the related experimental works, zinc oxide (ZnO) stands out due to its morphological and physical properties. ZnO is a semiconductor material with a direct bandgap of 3.37 eV and a high excitation binding energy of 60 meV. On the other hand, ZnO has been recognized as promising material for some electronic and optoelectronic applications, such as solar cells, transparent conductors, surface acoustic wave devices, gas sensors, etc. ZnO deposited on porous samples as porous silicon nanostructures can present divers morphologies such as nanorods, nanobelts, nanowires, etc. The advantages of using such morphologies derive from the large surface-to-volume ratio, high specific area, and roughness surface that they can present. The open structure and large surface area of PS make it a good candidate for templates and gas sensing applications[0]. In the effort to propose a new functional material for possible sensing gas applications, we have deposited ZnO films on mPS using sol-gel spin coating and ultrasonic spray pyrolysis (USP) techniques. The changes in the growth of ZnO films on mPS were studied using an UV-visible spectrometer, X-ray diffractometer (XRD), scanning electron microscopy (SEM) and atomic force microscopy (AFM). XRD analysis revealed a beneficial influence of mPS on the structural properties of ZnO films. SEM micrographs showed the growth and coverage of ZnO granular and flake-like crystals inside the pore of the substrate. The root mean square roughness (RMS) measured by AFM in the ZnO grown on the mPS substrate was higher up to one order of magnitude compared than reference samples. The results prove that the methods used in this work are effective to cover porous and obtain nano-morphologies of ZnO. These morphologies could be useful for making highly sensitive gas sensors.

Keywords: Zinc oxide, macroporous silicon, ultrasonic spray pyrolysis, spin coating, sol-gel.
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[NSN-171] LASER FRAGMENTATION OF SILVER NANOPARTICLES SYNTHESIZED BY LASER ABLATION OF SOLIDS IN LIQUIDS

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Silver (Ag) colloidal nanoparticles with spherical shape were obtained by the laser ablation of solids-in-liquids (LASL) technique, using a fiber femtosecond laser whit a wavelength of 1030 nm and Polyvinyl Alcohol (PVA) and deionized water were used as liquid medium. Subsequently, the colloids obtained were fragmented with a Nd:YAG laser with nanoseconds pulses and a wavelength of 1064 nm, using an energy per pulse of 15 mJ and varying the exposure time, the main objective of fragmenting the nanoparticles in the colloid was homogenize the size. Homogenization is important within nanoscience since having all the nanoparticles of the same size makes it possible to evaluate specific properties in the different fields of application.
The characterization of the colloids was carried out using ultraviolet-visible spectroscopy (UV-VIS) and transmission electron microscopy (TEM) techniques in order to determine the optical properties, size and morphology. In addition, a theoretical study was carried out using finite element modeling to obtain the theoretical absorption spectrum as a function of the size of spherical nanoparticles. In the results obtained shown that the maximum of the absorption band that is in the interval of 300 to 600 nm presents a shift after the fragmentation towards shorter wavelengths, these results were simulated and suggest that with the different laser fragmentation times used, there was a decrease in the sizes of the nanoparticles starting at 30nm and ending at approximately 5nm, these results were subsequently corroborated by TEM.

Keywords: *Laser ablation of solids in liquids; silver nanoparticles; laser fragmentation.*
Author for correspondence: mariela@cicese.mx
Reference: The effect of laser pulse energy on ZnO nanoparticles formation by liquid phase pulsed laser ablation Suha I. Al-Nassar a, Furat I. Husseinb, Adel K. McJ. materrestechnol . 2 0 1 9;8(5):4026–4031 https://doi.org/10.1016/j.jmrt.2019.07.012
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[NSN-106] MORPHOLOGY EFFECT ON TOXICOLOGICAL IMPACT OF MAGNETIC NANOMATERIALS IN BLOOD THROUGH HEMOLYSIS TEST

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The need to develop specific, fast, and effective means for diagnostics and imaging for aggressive diseases has always been a crucial factor in medicine. That is where nanotechnology has had accelerated research expanding on existing materials providing new and innovative properties or creating materials ab initio improving on their bulk counterparts. On this subject, magnetic nanoparticles (MNP) attracted substantial attention due to their properties allowing them to navigate remotely to specific directions, vibrating with targeting coatings or heating tissue through vibration, among others. However, the toxicological impact these nanomaterials could have inside complex structures like the vascular system must be studied. A hemolysis test was carried out with different morphologies, cubes, and rods, at different concentrations (0.1, 0.3 0.5, 0.7, and 0.9 $mgmL^{-1}$) to accomplish this. Magnetite materials were obtained through chemical coprecipitation (CQ) and chemical reduction (RQ) respectively. Results show that morphology is an essential factor to consider in toxicology. The nanorods showed a toxicological behavior in most concentrations, while magnetite in cubes only showed prominent hemolysis at 0.7 mg. These results show that concentrations are crucial in bulk materials; morphology, at the nanoscale determines certain toxicological impacts on biological systems.

Keywords: Magnetite; Silica coating; Nanorods; Nanobiomedicine; Hemolysis
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[NSN-328] NANOSTRUCTURE FORMATION FROM HIGH POWER INTENSE CAVITATION

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Cavitation has been used in a wide variety of applications, from sample cleaning immersion in liquids, to particle dispersion in colloidal suspensions, among others. Even though, there have been reports of the reduction of the size of the particles, usually the precursors are in forms of compacted pellets, powders or in general soft materials with weak coalescent bonds. We present the results of the studies performed on two materials, titanium and graphite, with completely different properties (mechanical and chemical), that were submitted to intense high power ultrasonic vibration in water. In these experiments, strong bubble cavitation was produced in the liquid medium, this transferred enough energy to the starting materials to produced suspensions of nanostructures. In the case of the Ti, the size distribution and changes of the properties of the nanoparticles were observedby transmission electron microscopy (TEM), such as, mild oxidation and the formation of non-stoichiometric Ti-O core-shell structures. For the graphite, after the cavitation, the observed materials were mainly overly stacked sheets of graphene, confirmed by TEM and Raman spectroscopy. These suspensions were used in spin-coating to produce films on glass, and the electrical conductivity and optical transmittance was measured.

Keywords: nanomaterials, graphene, titanium, cavitation.
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[NSN-16] ORANGE: ULTRA-SMALL GOLD PARTICLES

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Sub-nanostructured systems are the edge of nanoscience and nanotechnology. The application of these subsystems has allowed further progress in studies of nano-bio interactions, size-dependent localization of small clusters inside cancer cells, tuning of surface electronic states, etc. This study aims at the green route synthesis to obtain sub-nanostructured gold species using *Citrus x sinensis* (orange fruit). Chloroauric acid ($HAuCl_4$) by Sigma Aldrich was used as a precursor solution Au^{+3} and *Citrus x sinensis* extract as a reducing and stabilizer agent of the particles. The infusion was kept under magnetic agitation at room temperature for 1 h. The solution was filtered and stored for 24 h. The gold species obtained exhibit localized absorption bands into the Ultraviolet region (338 nm). No evidence of surface plasmon resonance (SPR) was observed. TEM analysis revealed the identification of sub-nanostructured species with predominant sizes of about 0.9 nm. Such systems were tested as SERS substrates using pyridine, with favorable results. The chemical enhancement (CE) mechanism was studied as a leading source of the SERS effect. Complementarily, the structural and optical response to the interaction between gold clusters (Au_{2n}, with n=1-5) and pyridine was modeled using DFT (Density Functional Theory) at the B3LYP (Becke-3-parameter-Lee-Yang-Parr) approximation level in combination with the LANL2DZ (Los Alamos National Laboratory 2-Double-Zeta) basis set. The correlation between adsorption energy and the SERS Enhancement factor was analyzed. The SERS effect depends on the interaction distance between the Py and metal cluster systems, indicating a maximum enhancement close to the experimentally reported value for the N-Au bond.

Keywords: Sub-nanostructured gold particles, chemical enhancement mechanism, *Citrus x sinensis*, SERS effect.
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Reference: Bo Yang, Ju Chou, Xiaoqing Dong, Chengtun Qu, Qingsong Yu, Kerry J. Lee, and Natalie Harvey, J. Phys. Chem. C 121 (2017) 8961–8967.
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[NSN-360] PLASMONIC DISORDERED NANOHOLES INTEGRATED IN A MICROFLUIDIC CHANNEL: TOWARDS AN OPTICAL BIOSENSOR

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A motivation in sensor research is to create sensing platforms compatible with microfluidic systems, for fast and high-sensitivity measurements in diverse applications. Optical sensors based on localized surface plasmon resonance (LSPR) have been demonstrated to be effective platforms for the quantitative monitoring of biological and chemical processes. Plasmonic nanostructures such as nanoholes on metal nanofilms can excite LSPR. Those plasmonic nanostructures have been employed as sub-diffraction optical systems with high aspect-ratio that involves optical transmission and large electric field intensities. However, a low-cost, fast, easy, controllable, and reproducible integration methodology of those nanostructures into microfluidic systems still represents a big challenge for the scientific and industrial community. Here, we describe the numerical investigation of plasmonic nanoholes and the microfluidic channel by a mathematical modeling software as well as the nanofabrication strategy of a sensor, consisting of gold nanoholes integrated in a microchannel. The nanofabrication methodology describes four steps: i) polystyrene nanospheres deposition. ii) Design of the microfluidic mask. iii) Gold and titanium deposit by e-beam evaporation and iv) removal of nanospheres. The resulting sensor platform consists of gold nanoholes of 21 nm of thickness, whose diameter can range from 90 nm to 100 nm with a random distribution integrated in a microfluidic channel of 70 µm of thickness. Therefore, the well-controlled fabrication process of the optical platform with microfluidics provides the possibility to use the sensor in a wide range of biosensing applications.

Keywords: optical sensor, nanoholes, microfluidics, LSPR, nanofabrication
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[NSN-119] QUANTUM TUNNELING BETWEEN PARALLEL SEMICONDUCTOR NANOWIRES

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Vertically aligned arrays are a frequent outcome in the nanowires synthesis by selfássembly techniques or in its subsequent processing. When these nanowires are close enough, quantum electron tunneling is expected between them. Then, because extended or localized electronic states can be established in the wires by tuning its electron density, the tunneling configuration between adjacent wires could be conveniently adjusted by an external gate. By considering the collective nature of electrons using a Yukawálike effective potential, we theoretically explore the electron interaction between closely spaced, parallel GaAs/AlGaAs nanowires while varying the electron density and geometrical parameters [1]. We find that, at a low density Wigner crystal regime, the tunneling can take place between adjacent localized states along and transversal to the wires axis, which in turn allows to create twoánd threédimensional electronic distributions with valuable potential applications.

Keywords: Wigner crystal, quantum tunneling, nanowires.
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Reference: [1] R. Méndez Camacho and E. Cruz Hernández, Tunneling between parallel onedimensional Wigner crystals, Scientific Reports 12, 4470, (2022) 1-10. https://doi.org/10.1038/s41598-022-08367-x
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[NSN-67] RECYCLED POLYSTYRENE COATINGS WITH LOW-LAYER GRAPHENE TO PREVENT DAMAGE TO HISTORICAL MONUMENTS BY ACID RAIN

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ABSTRACT: Acid rain has become a potential problem that damages various materials. The effect caused by this phenomenon in stone monuments has been studied for several years, however, in our country there is little information on how to prevent this damage and keep the materials protected. Coatings can be used as a chemical barrier to protect these monuments, derivatives of acrylic acid are normally used, however, nanomaterials such as graphene, due to their unique and interesting properties, have emerged as potential coating materials since they can be functionalized with low-cost and commonly used materials to give rise to a new one, with improved physicochemical properties depending on the intended application. In this work recycled polymer is functionalized with graphene and proved as coating to protect stone monuments. They recycling of plastic waste is an alternative to reduce pollution, due to the large amount of plastic waste that is produced. An example, thousands of tons of polystyrene are generated per year creating substantial amounts of garbage since this plastic generates many empty spaces, its composition is 98% air and 2% polymer. Although the production od plastics does not represent a major problem, because the do not degrade in their environment, their elimination does, since it is cumulative. During this work, the problems of deterioration of stone monuments caused by acid rain and plastic recycling are considered, a polystyrene coating functionalized with graphene is synthetized and characterized by Raman spectroscopy and contact angle. Afterwards, the functionalized polymer was used as protecting coating of quarry and marble, common materials of stone monuments. Finally, improvements in the properties of the polymer after its functionalization with graphene were observed, such as, enhanced adherence to surfaces and a better protection of stones in acid environments.

Keywords: graphene, coating, polystyrene, acid rain.

REFERENCES: Cui, G.; Zhang, C.; Wang, A.; Zhou, X.; Xing, X.; Liu, J.; Li, Z.; Chen, Q.; Lu, Q. Research Progress on Self-Healing Polymer/Graphene Anticorrosion Coatings. *Progress in Organic Coatings* **2021**, *155*, 106231.

[NSN-355] Synthesis and study of Bismuth nanoparticles in sodium chloride aqueous solution

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Bismuth nanoparticles are characterized by their versatility and multiple applications in science, engineering, industry and medicine.The synthesis of bismuth nanoparticles can be performed by more than one method, so it is important to characterize the crystalline phases of bismuth and the bismuth compounds that can be obtained with each of them, seeking to reduce costs in the synthesis, improve the stability of the crystalline phases or propose new applications based on the morphologies obtained. The synthesis and subsequent oxidation of bismuth particles in an aqueous sodium chloride medium is studied in this work, comparing the oxidation time and the type of bismuth compounds obtained in this medium and in a traditional synthesis in a distilled water medium. Small-sized bismuth particles are prepared by laser ablation of solids in liquids technique using sodium chloride in different concentrations as the aqueous medium. The laser is configured to emit 300 pulses, of 6 nanoseconds duration per pulse, at a wavelength of 1064 nm on a 3 cm diameter disk-shaped bismuth target. The particles have been characterized by UV-Visible spectroscopy, scanning electron microscopy and transmission electron microscopy. It is observed that the bismuth particles have a shorter oxidation time when they are in the sodium chloride aqueous medium, moreover, the oxidation time increases with increasing sodium chloride concentration in the solution.
Keywords: Bismuth, nanoparticles, UV-visible, sodium chloride, SEM.

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[NSN-157] THE USE OF TAGUCHI STATISTICAL TOOL FOR SYNTHESIS OF CARBON NANOSTRUCTURES BY CHEMICAL VAPOR DEPOSITION FROM EPS

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In the search for new alternatives for obtaining carbon nanostructures through more economical, environmentally friendly processes and for move it from laboratory-scale to industrial-scale, chemical vapor deposition is a method that can satisfy these requirements. In the present work we propose the synthesis of carbon nanostructures from expanded polystyrene (EPS) as precursor, with the presence and absence of an AISI 304 metal catalyst, considering the principles of green chemistry. Taguchi's design of experiments was applied, which is a statistical tool that allowed to optimize the chemical vapor deposition process, in order to demonstrate that expanded polystyrene is a sustainable source of carbon. The different flows of carrier gas, times and temperatures of synthesis were used. The obtained samples were characterized by scanning electron microscopy, which determined the spherical morphology of the synthesized nanomaterials. Energy dispersive spectroscopy showed high percentages of carbon and traces of oxygen and iron. Fourier transform infrared spectroscopy showed the presence of the functional groups like -OH, -CH_x, CO, C=C. X-ray diffraction showed certain grade of crystallinity of the obtained carbon spheres. Raman spectroscopy presented the characteristic D and G bands for carbon nanomaterials, with high grade of graphitization. Based on the analysis of characterization of obtained materials Taguchi design was applied and the optimal conditions of synthesis were obtained. The validation of these conditions was realized and corroborated. The obtained carbon spheres can be applied in different fields like electronics, electrodes for different cells, energy storage, drugs vehicles, etc.

Keywords: carbon nanostructures, carbon spheres, design of experiments, chemical vapor deposition, green chemistry.
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[NSN-250] Theoretical and experimental study of optical losses in a periodic/quasiperiodic structure based on Si-SiO2 porous

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In this work, we manufactured periodic/quasiperiodic structures based on porous silicon and Si-SiO_2 porous consisting of two Bragg reflectors and two localized defects between them. The periodic/quasiperiodic structures were fabricated by electrochemical etching and were subjected to two-stage of dry oxidation at 350 °C for 30 minutes and 900 °C for 30 minutes. In this way, we obtained an oxidized periodic/quasiperiodic structure that exhibits two localized modes in the transmission spectra; where porous silicon normally absorbs light making the creation of silicon based photonic crystal devices impossible in that electromagnetic energy region. Moreover, we used the Maxwell-Garnett model and J. E. Lugo model to obtain the refractive index of porous silicon and Si-SiO_2 porous. The J. E. Lugo model predicts that our structures are made almost complete of SiO_2. Furthermore, we calculated the transmission, reflection, and absorption spectrum on periodic/quasiperiodic structure in the UV-VIS range before and after dry oxidation, where we can have observed that a periodic/quasiperiodic structure fabricated of porous silicon absorbs more the light than the periodic/quasiperiodic structure manufactured of Si-SiO_2 porous. In this way, we made a theoretical analysis of absorption and Rayleigh scattering losses, at the wavelength of the two localized modes in the periodic/quasiperiodic structure estimating the photon losses due to Rayleigh scattering before and after oxidation in our samples. So we used the equation of Breit-Wigner modified by Miller to get the lifetime of photons and photon losses at the wavelength of the two localized modes. We found that the lifetime of the photons in the VIS range is smaller than the lifetime of photons in the blue and green range. From these results, we can conclude that dry oxidation helps to reduce absorption and scattering losses in the blue and green region. Optical characterization of periodic/quasiperiodic structure was carried out by UV-VIS-NIR.

Keywords: porous silicon, Si-SO_2 porous, absorption losses, scattering losses, periodic/quasiperiodic structure
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[NSN-120] TOXICITY EVALUATION OF A TIO2/FE3O4 COMPOSITE ON BRACHIONUS CALYCIFLORUS ROTIFERS

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One of the areas most benefited by nanomaterials is water remediation, where nanoparticles such as titanium dioxide (TiO_2) and magnetite (Fe_3O_4) contribute with their photocatalysis and magnetic manipulation properties, respectively, which are appropriate for the removal of contaminants such as dyes or drugs. However, using nanomaterials entails a problem: their incorrect handling and possible introduction into the environment, which can affect various organisms. The objective of this research focuses on knowing the possible adverse effects that various types of nanomaterials such as TiO_2, Fe_3O_4, and a TiO_2/Fe_3O_4 composite may have in a model of aquatic toxicity such as rotifers. These organisms are an essential part of the healthy development of various bodies of water, as well as the toxic effect of a sample of water with paracetamol treated by photocatalysis to evaluate the viability of reinsertion of said treated water to ecosystems inhabited by organisms. Rotifers (*Brachionus calyciflorus*) were subjected to acute toxicity tests in concentrations of 10,20, 40, 80, and 100 ppm of nanomaterials for 48 h, recording the number of living organisms based on their response to light stimulation. On the other hand, the toxicity of water treated by photocatalysis without the presence of nanoparticles was evaluated following the same methodology. The results showed that exposure to synthesized nanomaterials in the concentrations did not mean a reduction in the number of living organisms. Using a paracetamol solution treated by photocatalysis as a medium for developing rotifers did not reduce the number of live rotifers.

Keywords: Nanotechnology, nanotoxicology, titanium dioxide, magnetite, rotifer.
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Reference: R. Valerio-García, I. Medina Ramirez, M. A. Arzate-Cárdenas, and A. Carbajal-Hernández, “Evaluation of the environmental impact of magnetic nanostructured materials at different trophic levels,” *Nanotoxicology*, vol. 15, pp. 1–19, Jan. 2021, doi: 10.1080/17435390.2020.1862335.
This work was supported by: Engineering Faculty-UAQ FIN202106 and FONDEC-UAQ 2021 FIN202115 and FIN202116.

[NSN-290] Î´-BI2O3 HOLLOW NANOPARTICLES OBTAINING BY OXIDATION OF BISMUTH NANOPARTICLES WITH NaClO.

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Bi_2O_3 exhibits polymorphism and exists in six polyforms, including two stable phases (α- and δ-phase) and four metastable phases (β-, γ-, ε-, and ω-phase). Each polymorph possesses different crystalline structures and various electrical, optical and mechanical properties. The FCC structure δ- Bi_2O_3 is stable over a narrow range 729– 825 C. The cooling down of the high temperature δ-Bi_2O_3 phase leads to the formation of intermediate metastable phases such as tetragonal β- Bi_2O_3 and/or BCC γ- Bi_2O_3 before transforming into stable monoclinic α-Bi2O3 at room temperature. δ- Bi_2O_3 could be stabilized at low temperature by doping with different transition metal oxides or rare earth (1).
The present work shows the obtaining of hollow nanoparticles of δ-Bi_2O_3, which were obtained by oxidation of bismuth nanoparticles with NaClO and were stabilized with sodium from hypochlorite at room temperature. The chemical composition of the colloid samples was done in a micro-Raman spectroscopy, the study of their crystal structure, that was carry out by X ray diffraction (XRD), the oxidation state was studied by X-ray Photoelectron Spectroscopy (XPS), the size and morphology of the obtained nanostructures were studied by transmission electron microscopy (TEM) and the optical properties of the bismuth nanoparticles synthesized in water, the mixture of the nanoparticles with NaClO solutions and the resulting nanomaterials after the oxidation by UV-VIS spectroscopy, UV-vis spectroscopy was employed to estimate the band gap energies and to evaluate the photocatalytic activity.

Keywords: δ- Bi_2O_3 nanoparticles, Hollow nanoparticles, oxidation, NaClO.
Corresponding author: mariela@cicese.mx
References: Fan HT, Pan SS, Teng XM, Ye C, Li GH. Structure and thermal stability of δ-Bi2O3 thin films deposited by reactive sputtering. J Phys D Appl Phys. 2006;39(9):1939–43.

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, STM)
- X-ray Photoelectron Spectroscopy
- etc.

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.

[PLV-163] Characterization of hybrid plasma generated by microwave ECR-assisted reactive pulsed laser deposition.

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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 [1]. The aim of this work is to report the study of the combination of continuous nitrogen plasma, formed by a microwave discharge and pulsed plasma of laser ablation of a molybdenum target. The hybrid plasma was created at a working pressure of 6 x 10^{-4} Torr. Plasma parameters were measured using a type specific Langmuir probe, for each plasma source separately. The plasma density and electron temperature were measured using a cylindrical probe, and their dependence on the power is shown. The mean kinetic ion energy and plasma density for the case of PLD plasma were determined using a planar Langmuir probe. Optical emission spectroscopy was carried out to identify chemically active species in the plasma in all cases. In this work, we report the formation of MoN films using the hybrid plasma system. The structure and chemical composition of the nitride MoN films results are reported.

Keywords: microwave plasma, Pulsed laser ablation, kinetic energy, Langmuir probe, molybdenum nitride
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[1] Camps, E., Campos-González, E. & Rivera-Rodríguez, C. Characterization of the combination of microwave and laser ablation plasmas. *Surf. Coatings Technol.* **422**, 127509 (2021). https://doi.org/10.1016/j.surfcoat.2021.127509

[PLV-384] Fabrication of p-type semitransparent conductive BiCuOSe thin films and doped with divalent ions (Mg2+, Sr2+ and Ba2+) by PLD technique

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BiCuOSe oxychalcogenide has attracted much attention. because it exhibits attractive properties that indicate its possible use as a transparent conductor. BiCuOSe consists of alternating layers of $[Cu_2Se_2]^{2-}$ tetrahedra and anti-fluorite $[Bi_2O_2]^{2+}$ distorted tetrahedra in a tetragonal P4/nmm structure. Its p-type conductivity can be enhanced by the substitution of some divalent ion (X^{2+}) for Bi^{3+}. In this work, a ceramic target of BiCuOSe was made in a micro-planetary mill from the solid-state reaction of the precursors Bi_2O_3, Cu_2O, and Se, and was doped with Mg, Sr, and Ba ions. BiCuOSe powders were used as targets in the pulsed laser deposition (PLD) technique to grow BiCuOSe and doped BiCuOSe thin films. XRD patterns for BiCuOSe and doped BiCuOSe targets were indexed concerning PDF#45-0296, and it was found that most of the peaks present belong to the quaternary BiCuOSe. The optical characterization of the films was performed by spectroscopy measurements in the UV-Vis range. The undoped BiCuOSe films have an average transmittance of 30%, when doping with Mg, the transmittance increases to 40%; to 60%, with Sr; and for Ba, the transmittances are 80%. The electrical characterization using Hall effect measurements indicates that for the undoped BiCuOSe films there are carrier densities of $1.5x10^{18}$ cm^{-3}, when substituting with Mg atoms the concentration of carriers was maintained; but, when doing so with Sr and Ba the concentration decreased by two orders of magnitude. Regarding electrical conductivity, there are values of up to 50 S/cm.

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[PLV-383] Fabrication of p-type transparent conductive LaCuOS thin films by PLD technique

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The absence of high-efficiency p-type transparent semiconductor oxides (TSOs) has limited the development of the next generation of optoelectronic devices, including transparent electronics. LaCuOS has the potential to be used as *p*-type transparent semiconductor oxides (TSO), due to 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 interface region between the TSO and the *p*-type layer. In this work, a ceramic target of LaCuOS was made through a two-step route, first the synthesis of $CuLaO_2$ by solid-state reaction and later its sulfurization under a sulfur atmosphere. This is an economical, efficient, and versatile process that eliminates the use of toxic H_2S gases, which are used in the conventional sulfurization process. LaCuOS powders were used as targets in the pulsed laser deposition (PLD) technique to grow LaCuOS thin films. XRD patterns for LaCuOS thin films present the planes (001), (002), and (006). LaCuOS films present optical transmittances between 52-81% in the visible range of the spectrum, which are suitable values for their application in transparent devices. Electrical measurements indicate high values of hole mobility, and carrier densities of up to 10^{19} cm^{-3}, with p-type electrical conductivity of 0.74 S/cm. Such properties ensure that LaCuOS has a high potential to be integrated into devices as transparent electrodes.

The authors acknowledge the technical support of Marcela Guerrero, A. García-Sotelo, from the Physics Department of the CINVESTAV-IPN and Arturo Velasco Hernandez from Universidad Autónoma de Querétaro. The authors acknowledge the partial financial support for this work from CONACyT under Contract No. INFR-2014-01-230183. The authors also acknowledge the financial support for this work from Universidad Autónoma de Querétaro through FONDEC-UAQ 2021.

[PLV-199] INFLUENCE OF Al, Cu, AND GRAPHITE ELECTRODES FOR THE SPATIAL EMISSION OF HOLLOW CATHODE DISCHARGES

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The name hollow cathode is used to describe almost any cathode with a cavity-like geometry, either cylindrical, planar or spherical, as long as the plasma is confined within the conductive walls at the cathode potential [1]. Three types of discharge can exist in a hollow cathode: a typical low-current high-voltage discharge, a resonant discharge with a density of ~10^{17} m^{-3}, and a dispersed arc with a density of ~10^{19} m^{-3}. For certain combinations of gas pressures (*p*), and hollow cathode diameter (*D*), at relatively high applied powers, the negative glow of the plasma almost completely occupies the interior volume of the electrode. This work reports spatial distribution profiles of a hollow cathode discharge by optical emission spectroscopy (OES) using different electrode materials for both resonant and non-resonant discharge source operated in the DC mode. The spatial distribution profiles of Ar I spectral lines at 811.5 and 750.3 nm were analyzed for aluminum, copper, and graphite at different gas pressures. OES results show that in a resonant discharge at a *pD* = 1.3 Torr·cm, there is a significant difference in the emission spatial between Al, Cu, and graphite (keeping constant power and pressure), and the emission intensity of Ar I is higher for the aluminum than for the graphite. In the three materials, the Ar I transitions due to electrons impact excitation occurs mainly at the edges of the cathode, and Ar I transitions due to ions or fast atom impact excitation occurs mostly at the center of the hollow cathode.

Keywords: Hollow cathode discharge, optical emission spectroscopy, spatial distribution profiles.
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[1] S. Muhl, A. Pérez, The use of hollow cathodes in deposition processes: A critical review, Thin Solid Films. 579 (2015) 174–198. https://doi.org/10.1016/J.TSF.2015.02.066.
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[PLV-64] LIBS - IMAGING ON TARGET POISONING DURING REACTIVE MAGNETRON SPUTTERING

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Reactive magnetron sputtering is a commonly used process to fabricate compound thin-film coatings on various substrates. Typically, a too high supply of reactive gas will allow the formation of the stoichiometric composition film but will cause poisoning of the target surface, which may reduce the deposition rate significantly. There may exist optimum processing conditions where both high deposition rate and stoichiometric film composition may be obtained [1]. Thus, we propose to study the target poisoning by Laser Induced Breakdown Spectroscopy (LIBS – imaging).
LIBS – imaging is an all-optical elemental analysis method that can analyze a sample *in situ* as the technique does not require previous preparation; additionally, the sample state of matter and its medium is not fundamental. This technique collects and analyzes the light intensity from an ablation plasma using optical emission spectroscopy (OES) [2].This work mainly aims to determine the spatially resolved composition of the target surface using LIBS - imaging for various poisoning conditions.
Hence, different reactive magnetron sputtering thin-film depositions of silicon oxides and nitrides were made at different poisoning rates and at different working pressures. For each thin-film deposit, the target was mapped step-by-step and in situ by LIBS, starting at the center and ending before hitting the edge of the magnetron shield. Then the spectroscopy data were analyzed to see the behavior between the target's ablated position and the emission lines of its constituents. Principal component analysis (PCA) was performed to see if grouping conditions were plausible to similar conditions.
It was observed that the compound information was contained in the first three laser pulses so that a direct behavior could be observed between the emission lines, the target's position, and its poisoning degree. Therefore, LIBS-imaging proved to be useful to make inferences about the target poisoning.

Keywords: *Reactive magnetron sputtering, Target-poisoning, LIBS – imaging, Principal Components Analysis.*

References: [1] S. Berg and T. Nyberg, "Fundamental understanding and modeling of reactive sputtering processes," *Thin Solid Films*, vol. 476, no. 2. Elsevier, pp. 215–230, Apr. 08, 2005. doi: 10.1016/j.tsf.2004.10.051.
[2] L. Jolivet, M. Leprince, S. Moncayo, L. Sorbier, C. P. Lienemann, and V. Motto-Ros, "Review of the recent advances and applications of LIBS-based imaging," *Spectrochimica Acta - Part B Atomic Spectroscopy*, vol. 151. Elsevier B.V., pp. 41–53, Jan. 01, 2019. doi: 10.1016/j.sab.2018.11.008.

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[PLV-61] OXIDATION OF GaAs BY PLASMA AT ROOM TEMPERATURE

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The floating electrode of a commercial plasma cleaner (model PE-25 from PlasmaEtch Co.) with an operating frequency of 50 kHz and a power of 400 Watts was modified in order to increase the potential difference between the plasma and the electrode. This made it possible to use oxygen plasma for effective ion irradiation of the sample surface. Experimental samples approximately 3x5 mm were cut from a standard commercial GaAs wafer. The time of oxygen plasma irradiation varied from 5 to 30 minutes. Plasma treatments were performed at room temperature. The formation of $GaAs_{1-y}O_y$ film was confirmed by the SIMS and Raman spectroscopies. The $GaAs_{1-}$yOy film thickness grew over time from 15 nm to 65 nm according to the hyperbolic law (~ $t^{1/2}$). The analysis of the surface with an atomic force microscope showed a low roughness of the resulting surface, approximately equal to the initial roughness of the GaAs crystal. The resistance of the oxidized film was measured by a four-point meter. Additional annealing in the RTP system in an oxygen atmosphere at 900°C for 30 minutes led to the growth of a polycrystalline gallium oxide film with a thickness of more than a micron. Based on the results of the study, a conclusion was made about a simple and effective method for obtaining oxide on the GaAs surface.

Keywords: GaAs oxidation, plasma, room temperature.

[PLV-378] Silicon Carbide thin films deposited using laser ablation at different fluence

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Semiconductor electronic devices based on Silicon Carbide (SiC) are commonly used in the industry in high-temperature, high-power and high-frequency applications. Furthermore, Silicon Carbide has a wide band gap energy, high carrier saturation velocity and high-thermal conductivity, which make it interesting for optoelectronic applications. In this work, SiC thin films had been deposited on quartz substrates using laser ablation in vacuum (~ 10^-6 Torr), varying the incident fluence. The plasma parameters (mean kinetic energy and ion density) were estimated for the different fluences. SiC thin films were optically characterized through UV-Vis and photoluminescence spectroscopies; Raman spectroscopy was used to study their structural properties; surface morphology was analyzed by scanning electron microscopy.

Keywords: SiC, laser ablation, photoluminescence, optoelectronics
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[PLV-203] Study of ion species in PECVD (Plasma-Enhanced Chemical Vapor Deposition), using a retarding field energy analyzer (RFEA) and Langmuir probe

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PECVD is a technology in which vast insights have been found in terms of cathode configurations. Basically, there is a configuration of the cathode in the form of a showerhead and another planar, which is only a disk and its connection with the plasma source. With respect to the first mentioned, it has even been modified along with the gas inlet; varying geometry and dimensions of the pipe through which the injection is made. The debate on this topic lies in the density balance with plasma coupling. By directly injecting the gases into the field, the coupling is facilitated and the decomposition of the gases into radicals would be more effective. This leads to denser samples as the gases do not leave the induced field. Therefore, there is no guarantee of homogeneity in the manufacture of the film, due the affectation of the field by the presence of the holes. The foregoing opens the way to the characterization in terms of the distribution of the power induced to the cathode, generation of reactant species and threshold or minimum power that can be coupled. Based on the above, studies of the ion species within the plasma were implemented through two techniques. The first, using a retarding field energy analyzer (RFEA) measuring different ion energy distribution functions. Second, using a Langmuir probe, which allows measurements of electron temperature and density. Results of ion distribution functions, ion density and temperature will be shown, varying gas pressures (Ar, NH3) and applied powers.

Keywords: PECVD, RFEA, Langmuir probe
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[PLV-214] Syntesis and characterizacion of titanium thin films by magnetron sputtering and the effect of the addition of a grapite anode

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Abstract: In this work titanium (Ti) thin films were deposited onto glass substrates using two different techniques: by DC magnetron sputtering [MS] system and with the addition of a graphite anode, which introduces a second anode-type plasma. Films were deposited for a period of 5 min as a function of the argon (Ar) gas pressure (5, 10, 15 mTorr), MS current (50, 64 mA) and voltage applied on the anode (ranging from 80 to 120 V). The changes in the characteristics of the MS plasma was studied using optical emission spectroscopy (OES) and I-V measurements versus the anodic plasma parameters. Additionally, the properties of the films were determined for the different deposition conditions with emphasis on the effect of the anodic plasma. Finally, the film adhesion to the substrate was studied using scratch tests.

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Keywords: Magnetron sputtering; Optical emission spectroscopy; Deposition rate; Adhesion.
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[PLV-259] Synthesis of hybrid compounds of polypyrrole and silver by one step plasma polymerization

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Hybrid compounds would be able to combine the properties of inorganic an organic element in one; improving optical, electrical, and magnetic properties, among others, with a wide variety of applications, for example, in biomedicine, or energy systems.[1]. In this work, polypyrrole-silver (PPy-Ag) compounds were made by plasma polymerization with direct current and radiofrequency electric discharges at 10, 20, 30 W. Pyrrole was used in phase gas and silver from an electrode made of a .925 sterling silver coin (92.5% Ag and 7.5% Cu) and a sheet with a 100% Ag.

The morphology was studied by Scanning electron microscope (SEM), the surface was homogeneous and smooth perhaps a good mix between PPy and silver. The main functional groups of the hybrid PPy-Ag compound were analyzed by attenuated total reflectance (ATR) of infrared spectroscopy. In general, the dehydrogenation of the pyrrole rings and the formation of polymer chains can be observed also it was possible to detect the characteristic Ag-O a which suggests the Ag is oxidized. This opens the possibility of chemical interaction between polymers and metals through oxygen bridges.

The superficial chemical states were studied by X-ray Photoelectron Spectroscopy. The elemental content was analyzed as a function of the erosion time and the energy distributions of the 1s orbitals of C, O, N, and the 3d Ag orbital. The electronic orbital distribution was fitted with Gaussian curves and related to the chemical states of the compounds. The chemical state C-O-Ag was detected at 534.5 eV with an energy formation of 5.2 eV. Finally, conductivity was calculated with the reciprocal of resistivity. The values of conductivity varied in the range of 10^{-8} a 10^{-6} S/m

Keywords: Hybrids compounds, polypyrrole, silver, XPS, IR, conductivity.
Author for correspondence: guadalupe.olayo@inin.gob.mx
Reference: Omastová M., Mosnáková K., Fedorko P., Trchová M., Stejskal J. (2013). Polypyrrole/silver composites prepared by single-step synthesis. Synthetic Metals, 166, 57-62. doi:10.1016/j.synthmet.2013.01.015
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[PLV-121] TiO2-Au THIN FILM COMPOSITES SYNTHESIZED BY PULSED LASER DEPOSITION

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TiO_2 has been widely studied and synthesized by various methods. It is possible to modify the optical properties of TiO_2 by incorporating noble metal nanoparticles in order to enhance the photoresponse in several solar energy applications [1]. In this work, TiO_2-Au thin film composites were grown by pulsed laser deposition technique. Ti and Au targets were simultaneously ablated such that the plasmas combined under a reactive atmosphere containing oxygen at a pressure of Torr. The plasmas were analyzed individually by means of a planar Langmuir probe to calculate the mean kinetic energy and the plasma density of the Ti and Au ions. Ti plasma parameters were kept constant at 196 eV and while the Au plasma density was varied from to in order to change the Au content in each film. Optical properties were obtained by UV-Vis spectroscopy measurements, with which the band gap was calculated by means of the Tauc method, resulting in a value of 2.36 eV for the amorphous TiO_2 thin film, and decreasing at a value of 1.54 eV for the film with the highest Au plasma density. The morphology of the films was studied by scanning electron microscopy. The formation of spherical Au nanoparticles was noticed, whose average sizes increases as the Au plasma density increased, resulting in values to be in the range of 15 to 72 nm, respectively. Finally, the films were calcined and characterized using the same techniques.

Keywords: pulsed laser deposition, composites, thin films, plasmas, titanium oxide

[1] H. Park, Y. Park, W. Kim, W. Choi, Surface modification of TiO_2 photocatalyst for environmental applications, J. Photochem. Photobiol. C: Photochem. Rev. 15 (2013) 1-20. https://doi.org/10.1016/j.jphotochemrev.2012.10.001

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Sesión Oral

[PLV-35] CHARACTERIZATION OF A HYBRID PLASMA SYSTEM

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The hybrid plasma under study in this work was created by combining a stationary microwave ECR (with magnetic field) discharge using nitrogen as the working gas, and the plasma formed during the pulsed laser ablation of an aluminum solid target. The pulsed plasma propagates perpendicularly through the microwave plasma flux. The hybrid plasma was created at a working pressure of 6 x 10^{-4} Torr. Plasma parameters such as density, electron temperature and mean kinetic ion energy were determined using Langmuir probes. The optical emission spectroscopy measurements showed a significant improvement of the excited species present in the hybrid plasma in comparison with the individual plasmas. The intensity of the optical emission can be varied as a function of the deposited power on the target, which in the present work was changed by varying the size of the laser spot on the target. The change of power density produces a laser ablation plasma with different mean kinetic ion energies. The hybrid plasma was used to deposit aluminum nitride (AlN) thin films under different experimental conditions, mainly a laser ablation plasma with different mean kinetic ion energies. The composition of films studied by XPS showed that the oxygen content in the films was as low as 2.5 at%, with most bonds corresponding to that of the AlN compound.

Keywords: AlN thin films, microwave plasma, pulsed laser ablation

[PLV-422] Deposition of ZnO thin films from the laser ablation of a zinc target in leaked ambient air

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Since ZnO is a semiconducting material with lots of different applications, the control and reproducibility of its deposition while reducing costs, is a relevant goal. In this work, ZnO were deposited via pulsed laser ablation of a zinc target, in a system with a base pressure around 5×10^{-6} Torr. Promoting oxidation with ambient air introduced through a leak valve, to increase the working pressure to values up to 10^{-3} Torr, in steps of half order. Plasma kinetic energy and density were analyzed using a Langmuir planar probe, which shall provide the desired reproducibility. Structural, optical, and electronic properties of the samples were analyzed by means of XRD, Raman dispersion, UV-Vis spectroscopy, along with impedance spectroscopy.

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[PLV-380] Influence of nitrogen pressure on carbon thin films deposited by PLD

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Thin films of carbon have been grown by pulsed laser deposition. The ablation of a graphite target under a nitrogen atmospheres were performed on quartz and silicon substrates. The influence of the nitrogen pressure on the plasma parameters (mean kinetic energy and ion density) were studied by measuring the time-of-flight curves obtained from a Langmuir planar probe. It was found that plasma parameters remain unaltered for pressures under 3mTorr values, while a pressure of 20mTorr showed a decrease in both ion density and mean kinetic energy.
The films were structurally characterized by Raman spectroscopy. Optical properties were analyzed by means of UV-Vis spectroscopy. Chemical composition and oxidation states were studied by X-ray photoelectron measurements.

[PLV-247] Investigation of a Ti-25TaxB alloy fabricated through spark plasma sintering

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Ti-25TaxB alloys have been synthetized by spark plasma sintering (SPS) process using a mixture of elemental powders processed by mechanical alloying. The main objective is to analyze the effect generated by the B addition on the sintering kinetics, microstructure and mechanical properties. Samples with 2, 5 and 7 wt.% of B, as well as Ti-25Ta alloy were sintered at 1100 °C with a heating rate of 150 °C-min^{-1} with a constant load of 50 MPa. Sintering kinetics and the in-situ densification were performed by the analysis of the punch displacement during SPS processing. Structural details of consolidated materials were evaluated by the combination of X-Ray diffraction, and scanning electron microscopy. Mechanical properties were evaluated by Vickers microhardness. The results show that samples reached high densification values up to 99.7% of the relative density by using lower sintering temperatures in comparison to conventional sintering techniques. It was also determined an increment in the activation energy as the B addition increased. The alloys showed a lamellar microstructure which is generated by the mechanical alloying. The microhardness was increased up to 45% by the addition of B with respect to the Ti25Ta alloy. It is concluded that B addition has a strong effect on the sintering kinetics, although with a small reduction on the final densification. The microhardness values obtained with 4 wt.% of B were around 1000 Vickers, which is promissory for improving the wear behavior of the Ti25Ta alloy.

Key words: Spark Plasma Sintering, Ti alloys, kinetics, Microstructure, Microhardness.
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[PLV-369] Pulsed Laser Deposition of Thin Films from the Ablation of Cu in Oxygen Containing Atmospheres at Different Pressures

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In this work, a Cu target was ablated under an oxygen atmosphere at different pressures (20,15, 10 and 5 mTorr) to deposit thin films on glass substrates. The generated plasmas were diagnosed by means of time of flight curves obtained from Langmuir planar probe measurements. The incident fluence was changed in order to keep plasma ion density and mean kinetic ion energy constant at 1.6 x 10^{13} cm^{-3} and 135 eV, respectively. The ablation time was 30 min for all the experiments with a target to substrate distance of 5 cm.
Optical properties of the films were studied by means of UV-Vis spectroscopy in wich it was found that at low pressures (5 and 10 mTorr), films are mainly metallic Cu, whilst for higher values (15 and 20 mTorr) copper oxide thin fims are obtained. Surface morphology and topology of the films were studied by means of Scanning Electron Microscopy and Atomic Force Microscopy, respectively.

RENEWABLE ENERGY: MATERIALS AND DEVICES

CHAIRMEN

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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 other topics 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 in catalytic 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.

[RWE-372] A facile one-pot microwave-assisted hydrothermal synthesis of BiVO4 with application in ciprofloxacin photo-degradation

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The water pollution is a problem that has increased in recent years due to many factors as the demographic explosion. Among the principal water pollutants, there is the pharmaceutical compounds e.i. ciprofloxacin, which after the human consume, it is integrated to the water as contaminant agent. This research represents a contribution toward materials development for water treatment. In this work, bismuth vanadate ($BiVO_4$) was synthesized by microwave-assisted hydrothermal method. The present work aims to take advantage of $BiVO_4$ photocatalytic properties and reduce the time of synthesis. $BiVO_4$ was synthesized by microwave-assisted hydrothermal synthesis which allows reaction time reduction to just 30 s. The $BiVO_4$ powders were obtained with microwave hydrothermal reaction carried at 30 s, and characterized via X-Ray diffraction, Fourier-Transform Infrared spectroscopy, N_2 adsorption-desorption test, and UV-Vis-NIR spectroscopy. The results are $BiVO_4$ with 2.4 eV band gap, and photo-degradation of ciprofloxacin evaluated by UV-Vis-NIR spectroscopy reach to be more than 40% in 4 hours. The influence of synthesis parameters in the physical and chemical properties is discussed.

Keywords: microwave-assisted, hydrothermal, ciprofloxacin
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[RWE-8] Ammonia plasma treatment as an effective passivation scheme in black silicon solar cells

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Abstract — 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, the Black silicon solar cells, the passivation scheme on the surface is 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 to form 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-V_{oc} equipment.

[RWE-267] Development of cathode for aqueous aluminum ion battery: Ab initio and experimental study of Mn(1-x)BxAl2O4 (B=Co,Ni)

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Abstract: Aluminum manganese spinels have been proposed as a cathode for aqueous aluminum ion batteries[1], however, the dissolution of manganese in the electrolyte is one of the factors that limits its cycling capacity. In this work it was proposed to study experimentally and theoretically by means of DFT the effect of substitutional doping of manganese in concentrations of 0.125 and 0.25 mol with cobalt or nickel in the $MnAl_2O_4$ cubic spinel phase, in an aqueous aluminum ion battery system with an electrolyte of "water in salt" of $AlCl_3$*$6H_2O$. Theoretical study shows that the $MnAl_2O_4$ phase presents a bandgap of 2.6 eV. When $MnAl_2O_4$ is doped with cobalt from 0.125 to 0.25 mol, the bandgap tends to increase in the order of 0.1 eV, while with nickel, the bandgap value abruptly decreases to 0.638 eV at a concentration of 0.125 and then rise again to 1.8 eV as the doping increases to 0.25 mol by DFT analysis. From the band structure it was found that all phases have a direct band gap in all doped and undoped phases. Experimentally, the phases were synthesized using the modified Pechini method. The doped and undoped phases were indexed to cubic spinel Galaxite $MnAl_2O_4$ phase, showing no secondary phases in the material; thus, indicating the correct insertion of Co and Ni in the manganese sites. The morphology of the doped and undoped phases were characterized by SEM; which showed the formation of single crystals with sizes around 100 µm; which will enable to reduce capacity fade due to low interface defects between particles and slow manganese dissolution. EDS showed the presence of the dopant in the structure. In future, this material will be used to build the complete cell of an aluminum ion battery.

Keywords: Aluminum Ion Battery, Single Crystal Cathode, Pechini, Manganese Aluminate, DFT
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One reference: [1] W. Pan *et al.*, "An Aqueous Al-Ion Battery Boosted by Triple-Ion Intercalation Chemistry with a High-Energy MnAl2O4 Nanosphere Cathode," *Electron. J.*, Apr. 2020, doi: 10.2139/SSRN.3569552.
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[RWE-375] Fabrication and electrical characterization of (Al,Ga)As-based Schottky junctions solar cells grown by molecular beam epitaxy

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Schottky contacts are named also metal-semiconductor rectifying contact and formed when contacting a semiconductor with a metal having a larger work function. It is generally believed that formed Schottky barriers accelerate the separation of photogenerated electron-hole pairs, facilitate electron injection from semiconductor to metal thus improving photovoltaic effect [1]. Molecular beam epitaxy was employed to explore the concept of multi-quantum well Schottky barrier solar cells employing a n-type GaAs (100) substrate. The quantum wells were grown employing AlGaAs as barrier layer. Thus, the (4nm)AlGaAs/(6nm)GaAs/(4nm)AlGaAs quantum structure was embedded into 10^{18} cm^{-3} Si-doped 150 nm GaAs layers. Two samples were grown with quantum a well sequence of 10 and 20 periods, individually. Physical vapor deposition technique was employed to form 500 nm thick Ag(Cu) electrode to form the Schottky(Ohmic) junction. For the front-contact a finger of 0.7 mm thick were deposited. The current-voltage response was measured under AM1.5D spectra with a power density of 550 W/m^2. Modification in the Jsc was observed with the inclusion of quantum wells, increasing with the number wells embedded. Our experimental results have been supported by numerical analysis which is also employed to describe the quantum properties of the devices.

Keywords: Schottky barrier solar cells, Molecular Beam Epitaxy, GaAs.
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[RWE-429] FABRICATION OF A SMALL-MOLECULE ORGANIC SOLAR CELL WITH A NEW STRUCTURAL CONFIGURATION

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Organic solar cells represent an alternative to conventional devices due to their attractive promising characteristics: flexibility, semi-transparency, low cost, and diversity of organic semiconductors. However, these devices have short lifetimes, which has forced the investigation of new different materials used in the layers of the device's structural configuration in order to improve their efficiency and stability. In this work we present the fabrication and analysis of bulk heterojunction inverted organic solar cells (iOSC), fabricated using a small molecule as donor material. The materials used for the fabrication of the active layer of the cell were the donor p-DTS(FBTTh$_2$)$_2$ (small molecule) [1] and the acceptor PC$_{70}$BM (fullerene), being the structural configuration of the device ITO/PFN/ p-DTS(FBTTh$_2$)$_2$: PC$_{70}$BM /MoO$_3$ /Ag. The performance parameters obtained from the illuminated J-V curves of the devices were analyzed and simulated using the equivalent circuit model of three diodes proposed by Roland.

Keywords: organic solar cell, p-DTS(FBTTh$_2$)$_2$: PC$_{70}$BM blend, equivalent circuit model, bulk heterojunction.
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Reference: [1] M. Ramírez-Como, A. Sacramento, J. G. Sánchez, M. Estrada, J. Pallares, V. S. Balderrama, & L. F. Marsal. Small molecule organic solar cells toward improved stability and performance for Indoor Light Harvesting Application. Solar Energy Materials and Solar Cells. 230 (2021) 111265. https://doi.org/10.1016/j.solmat.2021.111265
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[RWE-395] Heterogeneous catalysis of lignocellulosic biomass (corn stubble) for the production of bioethanol

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Abstract: Biofuels are a viable option because they are produced in a renewable way and have a lower environmental impact than conventional fuels. Bioethanol produced from corn stover is a promising option for diversification from fossil fuels due to its high abundance and low cost. Therefore, this work will focus on the greater use of lignocellulosic waste, specifically, corn stover, for which we not only propose obtaining bioethanol but also synthesizing a non-toxic heterogeneous catalyst, both from plant biomass. Where it will be used in the hydrolysis reaction of the lignocellulosic material. The synthesis of the heterogeneous catalyst is carried out from the same biomass, which is subjected to a thermal treatment, proposing a more sustainable process. Subsequently, the resulting carbonaceous material is treated by means of a sulfonation reaction. These catalysts have excellent activity due to their acid character. The catalysts obtained will be analyzed by structural techniques. On the other hand, the biomass will be subjected to chemical treatment (acid hydrolysis) by adding H_2SO_4 to obtain sugars such as cellulose and lignin, the hydrolysate is placed in the presence of a heterogeneous catalyst to obtain reducing sugars. Finally, to produce bioethanol, an alcoholic fermentation of these sugars using the yeast S. cerevisiae is proposed. Likewise, the products obtained from the fermentation process are evaluated using the Fourier Transform infrared spectroscopy technique. The use of bioenergy from biofuels is a very attractive alternative for this 21st century due to its high calorific value and low CO_2 emissions due to being renewable and low cost.

Keywords: Corn stover, sulfonation, catalyst, heterogeneous catalysis, *S. cerevisiae.*
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[RWE-445] Impact of Te layer as part of back contact and their performance on CdS/CdTe solar cells

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CdTe semiconductor is an absorbent material used in “tandem” photovoltaic solar cells. This material is commonly deposited by thermal evaporation presenting electrical resistivity values about of 10^5 W*cm to 10^9 W*cm. CdTe is applied in thin solar cells as p-type layer which is in contact with metal back electrode in solar cells. In the CdTe/metal junction a Schottky barrier exits; and small number of charge carriers have enough energy to get over the barrier and cross to the metal back contact. To solve part of this problem, nanostructured Te thin films were used as intermediate layers between CdTe and metal contact. Te layers whit different physical properties were deposited on CdS/CdTe structure by thermal evaporation employing different growth parameters. The electrical parameters of CdTe solar cells were influenced by p+ Te regions. p+ Te regions used as intermediate layer with large deposition time increases the FF and V_{OC} values from 30% to 60% and 560 mV to 730 mV respectively. Also, the electrical resistivity is reduced from 10^6 W*cm to 10^3 W*cm. In this sense, Te region implemented as nanostructure allows to reduce the series resistance from 99 W to 20 W and increases the shunt resistance from 1445 W to 4424 W; Te region as thin films demonstrated not be adequate.

Keywords: Nanostructured Te, CdS/CdTe Solar cells, p+ region, back contact, CSVT system.
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[RWE-444] INFLUENCE OF CdO AS BUFFER LAYER ON CdS/CdTe SOLAR CELLS

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CdO is an interesting semiconductor material due to widely band gap energy commonly reported in a range of 2.18-2.5 eV and low resistivity. CdO and CdS thin films was grown by chemical bath deposition technique (CBD) on FTO (SnO_2:F) substrate. The morphological, optical, electrical, and structural properties was studied. Band gap energy increase from 2.25 eV for single CdS film to 2.48 eV using CdO/CdS arrangement. CdO films was evaluated on CdTe solar cells obtaining a shunt resistance increment from 2003 Ω to 9362 Ω and corresponding efficiency increase from 8.9% to 14.4% using CdO buffer layer. EQE reveals an increment at 600-800 nm region using CdO/CdS monolayers.

Keywords: Nanostructured CdO, CdS/CdTe Solar cells, Buffer layer, CdO/CdS, CdS/CdO.
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[RWE-129] Joint performance of self-cleaning coatings and natural assisted cleaning methods in solar trackers

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The geographical locations with the greatest photovoltaic potential are mostly deserted and semi-deserted regions where sand accumulates and adheres to the surface of the photovoltaic panels, causing significant losses in energy production efficiency. Conventional solar panel cleaning methods use large amount of water, which is a scarce resource in such areas, and represent a considerable expense in human resources and cleaning products or devices. Previously, the performance of "assisted natural cleaning methods" by control algorithms in solar trackers under favorable weather conditions has been studied, taking advantage of low and medium intensity rains to improve the cleaning effect that it produces in solar panels. As another approach, self-cleaning coatings have been extensively studied for application on surfaces exposed to dirt outdoors and more recently have been implemented for application on the surface of solar panels. These coatings, through the superhydrophobic or superhydrophilic properties, allow to take advantage of rain or dew drops to carry out a self-cleaning process, eliminating the dust accumulated on the surface of the panel. Both assisted natural cleaning and self-cleaning coatings have proven to be viable contributions in photovoltaic installations, however, they are not capable of fully replacing conventional cleaning methods, at least not applying them individually. The objective of this research is to demonstrate superior performance to other cleaning methods through the joint use of self-cleaning coatings and assisted natural cleaning methods, as well as to evaluate the joint performance in laboratory environment and in real environment, evaluating the soiling rate, with and without the use of coatings as well as the natural assisted cleaning techniques.

Keywords: self-cleaning coatings, soiling, cleaning methods, sun tracking.
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Reference: G. A. Cruz, and P. Vorobiev, Dust adhesion physics on photovoltaic surfaces and its application on assisted natural cleaning of solar trackers, J. Phys.: Conf. Ser. 2238 012013 (2022). doi:10.1088/1742-6596/2238/1/012013
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[RWE-9] Molybdenum oxide thin films for heterojunction solar cells

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In the present work, MoOx nanostructures were obtained from Mo seed layers, grown by a sputtering technique. The X-Ray Diffraction (XRD), Atomic Force Microscopy (AFM), UV-Visible (UV-VIS) were applied to investigate the structural, morphological, and optical properties of the samples. By optimizing the different deposition conditions, MoOx thin films were grown from 90 nm to 340 nm. The analysis made using the XRD Spectroscopy showed the presence of matrix MoOx (where x; could vary from 1 to 3). Especially, it was noticed that the samples have an oxidation state value (x = 2) before treatment, whereas it changes to 3 after the treatment. Additionally, changes were found in the photoconductivity response of the thin films because of the heat treatment. Thin films grown in this work could be used for the fabrication of hole collector as well as the back contact region in the p-n type solar cells.

[RWE-376] Numerical and experimental analysis of the front-surface field layer in the performance of (Al,Ga)As-based solar cells grown by MBE

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GaAs solar cells have attracted a lot of attention due to their interesting properties such as crystallinity, reproducibility, and efficiencies above 25%. Furthermore, studies indicate that it can reach efficiency up to 26.8% [1]. Nevertheless, in GaAs-based materials the surface plays an important role and in photovoltaics decreasing the conversion efficiency by the absorption of short-wavelengths. In this work, a doped layer known as a front surface field (FSF) is inserted in an (Al,Ga)As photovoltaic heterostructure with the aim to reduce the effect of surface recombination. First, a numerical study is employed to determine the effect of the AlGaAs layer on the carrier's distribution at surface, being reduced as the Aluminum composition (%Al) is increased. Then, three (Al,Ga)As solar cell samples were grown by molecular beam epitaxy with 40 nm AlGaAs FSF layer where the %Al was set to 0, 15, and 30. The Raman measurement showed that L- and LO vibrational modes intensity changes, suggesting that surface charge density at surface was modified by %Al. FSF layer was studied through the Franz-Keldysh oscillation (FKO) in the photoreflectance spectra, finding a reduction in their period. The optoelectronic properties are explored by current-voltage measurements under AM1.5 illumination spectra with 550 W/cm^2 power density, revealing a increasing in the performance by the improvement on the short-wavelength absorption when the FSF layer is %Al = 0. Thus, surface has an important effect on research of thin-film technology of photovoltaic systems and the FSF layer is a strategy to modulate their impact.

Keywords: Front surface field, GaAs solar cells, Molecular beam epitaxy.
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[RWE-374] Numerical design of GaAs-based Schottky solar cells for multi-photon absorption

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Schottky barrier solar cells (SBSC) are a promising alternative to photovoltaic technology by the lower layer sequence necessary to be manufactured in contrasted with the conventional p-n junction system. Additionally, the SBSC can be employed to develop strategies to overcome the theoretical efficiency limit Shockley Queisser of 33.5% for conventional single-junction cells. In this work, technology computer aided design (TCAD) is employed to develop SBSC. The model employs carriers' generation and recombination process, layer sequence and doping profile, the properties of the electrodes were also considered. First, the metal work-function is explored to produced ohmic and Schottky junctions employing 500 nm of a single layer based on Cu, Ag, In, Sb, and InGa on the $5x10^{18}$ cm^{-3} n-type GaAs. An increasing on the Schottky barrier effect is obtained when the high difference work-function is employed (Ag) in conjunction with the ohmic contact (Cu). Next, the multi-photon absorption mechanism is added to the SBSC by the inclusion of quantum wells. GaAs-wells are embedded in higher bandgap material system. The InAs, InGaAs, and AlGaAs barriers are explored. The numerical results indicated that AlGaAs barriers increases the current-voltage behavior. Thus, the barrier heigh is designed through the aluminum molar fraction, getting the maximum short-circuit current density (J_{sc}) of 135 $\mu A/cm^2$ when the ternary composition is 35%. With the aim to increase the SBSC efficiency the number of AlGaAs/GaAs/AlGaAs layer system was varied, obtaining 20% more efficiency with 20 periods in contrast with the SBSC without quantum wells. This work describes the numerical model and results for the design of photovoltaic cells by means of a Schottky junction, determining the optimum experimentally reproducible layer sequence.

Keywords: Schottky barrier solar cells, technology computer aided design, GaAs-wells.
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[RWE-406] One-pot green synthesis of biodiesel from Ricinus Communis seeds by direct heterogeneous catalysts

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Currently, due to the great use of fossil fuels in the world, an immense emission of greenhouse gases (CO2, NOx, SOx, CO) has originated, which have caused a problem on a global scale, the acceleration of climate change. For this reason, in recent years solutions have been sought to reduce or mitigate these emissions, one of the proposals is the use of biofuels. One of the main biofuels used is biodiesel which is a mixture of monoalkyl esters of long chain fatty acids, this biofuel is sustainable, renewable, biodegradable, non-toxic , helps reduce the emission of carbon dioxide, and completes de carbon cycle. In this work, the catalytic influence of basic laminar oxides on heterogeneous transesterification reaction was evaluated using *Ricinus communis* seeds for the production of pure biodiesel by direct heterogeneous catalysts. This product was used to make diesel-biodiesel blends and perform tests on injection diesel engines for evaluation. The authors acknowledge the support of the SECTEI CM-059/2021 , SECTEI 048/2022 and SIP-IPN 2104 (modulo 20220625) projects and BEIFI scholarship.

Keywords: biodiesel, Ricinus Communis seeds, direct heterogeneous catalysts.

[RWE-181] PHOTOCATALYTIC DEGRADATION OF TURMERIC USING ZIRCONIUM DIOXIDE OBTAINED BY THE SOL-GEL TECHNIQUE

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Zirconium Dioxide is a ceramic material, which has unique characteristics such as porous morphology, biocompatibility and high hardness, also is a candidate material for photocatalysis due to its applications in the medical, chemical and pharmaceutical areas. ZrO_2 is an amphoteric material, which has three phases: monoclinic, tetragonal and cubic; which are achieved at different temperatures and this means that each of them has different properties.
In the present work it is intended to create a ZrO_2-based photocatalyst using Sol-Gel technique. Raman thermal study in real-time was carried out to determine the obtaining temperature for the tetragonal phase, which has been reported to have photocatalytic activity. Additionally, SEM studies were carried out, in order to know morphology and elemental composition of the sample. Optical properties were determined using Diffuse Reflectance Spectroscopy.
In special, it is intended to carry out the photocatalytic degradation of turmeric, despite being a root that has antioxidant, anti-inflammatory and anticancer properties, it has little solubility in aqueous systems, this means that it is limited to being absorbed by the body and in most cases is excreted by the body, so it becomes a pollutant present in waste water

[RWE-266] PRECURSOR INFLUENCE ON THE RAMAN SPECTRUM OF KNNLiTaLa0.01 PREPARED BY TWO DIFFERENT METHODS

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The ceramic $KNNLiTaLa_{0.01}$ with composition $(K_{0.44}Na_{0.52}Li_{0.04})_{0.97}La_{0.01}Nb_{0.9}Ta_{0.1}0_3$ was prepared by two different methods. The first was the classical solid-state reaction technique. The second synthesis procedure included the $NaNbO_3$ compound as a precursor obtained from a topochemical reaction between $Bi_{2.5}Na_{3.5}Nb_5O_{18}$ (BiNN) and Na_2CO_3, using the Reactive-Templated Grain Growth Reaction (RTGG) method. Afterwards, the obtained precursor was made to react with the appropriate carbonates, and oxides through a solid-state reaction to obtain the desired composition. Both materials were characterized by X-ray Diffraction (XRD) and, after analyzing the phase parameters and phases relative content no structural alteration due to the precursor was detected. The Raman spectra of the samples obtained by the classical solid-state reaction consist of four modes, while the spectra of the samples obtained by the two-step method consist of six modes, where the appearance of two new IR modes $F_{1u}(\nu 3)$ and F_{2g} $(\nu 4)$ is associated to oscillations in the perpendicular plane to the basal plane of the structure.

[RWE-425] Rotating cylinder electrochemical reactor for removing Cr (III) from real effluents

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The effluents from the tanning industry are characterized to present Cr(III) and Cr(VI). Nevertheless, the Cr(III) sulfate basic is the most used reagent in the tanning process at the commercial level due to its excellent features to tan the leather and low cost. The treatment methos of wastewater containing Cr(III) include: reverse osmosis, adsorption, bioadsorption, ionic exchange and chemical precipitation. Although these processes can achieve removal efficiencies around 98 %, they present important drawbacks like no combining a low cost along with a high efficiency or a short residence time, besides most of these processes have been developed for synthetic solutions, whence they do not undergo the same challenges as real effluents containing complex matrices inhibiting the removal efficiency of physicochemical processes. Specifically, the electrochemical techniques have been seldom used to remove Cr, membrane electrolysis has been efficiently applied to remove Cr (VI) but this technology is considerably expensive.
In this work, an alternative treatment was proposed for the removal of chromium with an approximate concentration of 3586.25 mg L^{-1} present in effluents from the tanning industry, through the electrochemical precipitation process. A rotating cylinder electrode (RCE) electrochemical reactor was used. The rector was made up of an anode (1018 carbon steel), two different types of cathodes: (1) (TiO_2/RuO_2) cathodes, called dimensionally stable cathodes (DSC) or (2) 316L SS (stainless steel) cathodes and a reference electrode. Stirred at 300 RPM was applied by means of a variable revolution motor. For this type of process, two types of solutions were analyzed: a synthetic solution with an initial concentration of 2700 (mg L^{-1}) and a real solution from the tannery industry with a Cr (III) concentration of 3585 (mg L^{-1}), with a pH of 3.55, and three different current densities (10, 20 and 30 mA cm^{-2}). Finally, the initial pH value was proposed to be increased to values of 5 and 6 for the real solution, since the electrochemical precipitation of Cr (III) was not favorable at the original pH of the wastewater from the tannery industry, approximately at 3.55, in contrast to the synthetic solution with a pH value of 2.8.
Different experimental parameters were calculated, such as: chromium (III) removal, current efficiency and energy consumption during the electrochemical precipitation process, to know the optimal conditions of the electrochemical reactor. Cr(III)-pH fraction diagrams help on understanding that $Cr_2FeO_{4\ (s)}$ and $Cr_2O_{3\ (s)}$ precipitates are the most dominant species at pH > 3.5 in these sulfate solutions, in the absence and presence of Iron, respectively. The influence of the cathode material occurs particularly at current densities below 20 mA cm^{-2}, where Cr removal kinetics proceeds faster on the TiO_2/RuO_2 electrode than 316L SS.Residence times of 80 min and 60 min were necessary to remove all Cr (III) concentration at pH 5 and 6, respectively. The characterizations of the precipitates were carried out by X-ray diffraction (XRD) and scanning electron microscopy (SEM). In the electroprecipitation mechanism, it was confirmed that the precipitates were formed mainly by Cr2FeO4 (Chromite) regardless of the experimental condition used in the Cr (III) removal process. They were developed for the two types of cathodes at a current density of 30 mA cm^{-2} and with the two modifications of the pH value 5 and 6, an elimination of 99.99% in times less than 60 min.

Keywords: Chromium removal, Cr(III), Tanning wastewater, Electro-precipitationIron dissolution.
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[RWE-168] Sb2S3 THIN FILMS ON PLASTIC TAPE SUBSTRATES BY CHEMICAL BATH DEPOSITION FOR FLEXIBLE ELECTRONIC APPLICATIONS

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Antimony sulfide (Sb_2S_3) is an emergent material which belong to chalcogenides semiconductors group with a energy bandgap ranging between 1.56 to 2.25 eV, high absorption coefficient (>10^5 cm^{-1}), the compounds of the material are low cost, earth abundant elements and low toxicity. Due to its properties, Sb_2S_3 has attracted the researchers attention because it is suitable for solar cell applications as absorber layer. There are several methods for its obtaning such as thermal deposition, spray pyrolysis and chemical bath deposition (CBD) among others. In this work, Sb_2S_3 was succefully deposited on plastic tape substrates by CBD in a cooled solution bath (5°C) and thermally treated using a hot plate in air atmosphere for promoting crystallization. Sb_2S_s thin films were characterized by XRD to determines its crystalline structure, optical studies were carried out by micro Raman and UV-vis reflectance-transmittance spectroscopy, SEM and EDS analysis were done to observe the surface morphology and elemental composition.

KEYWORDS: Sb_2S_3, THIN FILMS, CHEMICAL BATH DEPOSITION, PLASTIC TAPE SUBSTRATE
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[RWE-373] Study of GaNAs quantum wells embedded on p-i-n GaAs solar cell for multi-photon absorption

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The development of molecular beam epitaxy (MBE) allows 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. 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 by 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. In this work we analyze a set of p-i-n GaAs heterostructures grown by molecular beam epitaxy where a 10 and 20 periods of GaAs/GaNAs/GaAs quantum wells were embedded. The diffraction of [004] plane obtained by rocking curve method indicated two peaks intensities who dominates the diffractogram which correspond to GaAs and GaNAs, denoting that strain increases with the number of layers by lattice mismatch. Raman spectroscopy was employed to analyses the composition of the photovoltaic structure where modes related to GaAs 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. Photoreflectance spectroscopy was used to determine the effect of tensile strain in the heterostructure where third-derivative lineshapes are found related to E- and GaAs gap. The strain redshifts these critical points. Additionally, the line shape on photoreflectance spectrum indicates that the electric field distribution is also modified by the quantum wells structures.

Keywords: Schottky barrier solar cells, technology computer aided design, GaAs-wells.
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[RWE-125] STUDY OF THE IMPACT OF NANOSTRUCTURES ON KESTERITE SOLAR CELLS UNDER THE RADIATIVE LIMIT

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The nanostructure application to solar cells has been of growing interest in recent years, particularly for less toxic, affordable supply, and high efficiency potential materials. $Cu_2ZnSn(SSe)_4$ (CZTSSe) semiconductor material is presented as a competent candidate, whose properties allow it to advance towards its maximum theoretical efficiency of 28%. In this simulation work, it is shown a comparative analysis between CZTS and CZTSe bulk materials in ideal conditions, varying composition and thickness, obtaining the highest efficiencies with S/(S+Se) = 0.74 and 2μm, respectively. Afterward, at the same ideal conditions, CZTSe quantum wells are incorporated into CZTS material, studying the impact of different well number and width. Based on these results, in a subsequent analysis, the influence of both barrier and well compositions are evaluated and optimized, reaching an efficiency of 37.5%, which is higher than the value obtained for solar cells without nanostructures.

Keywords: $Cu_2ZnSn(SSe)_4$; solar cell simulation; quantum wells.
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[RWE-396] Synthesis and characterization of vanadium oxide by hydrothermal synthesis.

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Vanadium has shown very interesting structural, optical and electrical properties, primarily due to its different oxidation state (+2 to +5). Recently, much research has been done on the synthesis and applications of vanadium oxide in areas like: photocatalysis, solar cells, gas sensors, smart windows, and batteries. In this work, vanadium oxide (VO_x) nanostructures were achieved using a hydrothermal method, the effects of time and concentrations on the purity of the obtained phase were explored in the process. We successfully prepared VO_x, at different ammonium metavanadate (0.015, 0.1 and 0.15M) concentrations in 25 ml of distilled water and stirred for 30 minutes. Hydrogen peroxide was added into the previous solution (10 V:1 H_2O_2) and stirred 15 minutes until the solution turned yellow, then nitric acid was added drop by drop to obtain pH 2 and stirred for 15 minutes until a color change on the solution to orange was observed. Subsequently the solution was transferred to a 25 ml autoclave and heated at 180°. Several experiments were carried out at different temperature ranges (8 to 36 hours). The obtained precipitates were washed with distilled water and ethanol, dried at 150°C and calcined at 500°C for 1 hour. The structural and morphological properties of the VO_x was analyzed via X-ray diffraction (DRX), Raman spectroscopy and Scanning Electron Microscope (SEM), while optical properties were evaluated by FTIR and UV-Vis. The XRD pattern shows that all calcined samples are crystalline, corresponding to orthorhombic phase of V_2O_5 (PDF-00-041-1426) and second phases are not present. Raman and FTIR show the presence of V-O and V=O bonds, which are reported for the V_2O_5 structure. A platelet structure was observed in SEM microscopy. The band gap energy of the samples were calculated by UV-Vis spectroscopy, obtaining values in the range of 2.3-2.4 eV for all samples.

Keywords: Vanadium, hydrothermal method, vanadium oxide, characterization, synthesis.
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[RWE-398] Synthesis and electrical characterization of 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, solar cells and catalysis. In this work, gadolinium doped cerium oxide thin films were prepared by Ultrasonic Spray Pyrolysis. The influence of gadolinium concentrations of 10, 15 and 20%, substrate temperatures of 425, 450 and 475ºC 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 structural, optical and electrical properties 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.

Keywords: gadolinium, characterization, thin, film.
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[RWE-288] THERMAL STUDY OF ZIRCONIUM DIOXIDE TO OBTAIN TETRAGONAL PHASE AND ITS POTENTIAL APPLICATION IN PHOTOCATALYTIC DEGRADATION OF INDIGO DYE

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The last few decades, environmental pollution has demonstrated a world-wide problem. Pollution can present as a solid, liquid and gas or a mixture of them, altering in a negative way to the environment, causing health problems and affecting quality of life. Scientist and environmentalist have been worried by offering effective and progressive solution to solve all these problems. Many oxide-based semiconductors such as TiO_2 , ZrO_2 , WO_3 , etc., have been applied as photocatalyst for photodegradation of organic pollutant. Due to unique characteristic and properties of ZrO_2 , it can be used as photocatalyst or as a support to another catalyst. Tetragonal phase of ZrO_2 has been reported to have exceptional photocatalytic properties. In this work ZrO_2 powders were synthesized using sol-gel technique. Evolution of crystalline phase as a function of temperature and time was done means of in-situ μ-Raman measurements. Optical properties, morphology an elemental composition were determined using DRS, SEM and EDS, respectively. The principal objective of the obtain photocatalyst is to degradation the indigo dye.

Keywords: Photocatalysis, Degradation, Indigo dye .
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Sesión Oral

[RWE-164] 2D MATERIALS: A PROMISING ALTERNATIVE TO ENERGY STORAGE

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Two dimensional materials, such as Graphene oxide (GO), reduced graphene oxide and MoS_2 are used for several applications nowadays. Some of these applications lay in the energy harvesting and storage field. Such materials are of great interest due to their capability to increase the performance of the different energy devices. Those properties relay specially in the combination of their high surface area, electronic properties, electrical conductivity and optical properties. In this work we have studied and compared the performance of different 2D materials and its potential application as energy storage devices. For this study the materials were characterized by means of XPS, FTIR, UV-Vis-NIR and cyclic voltammetry. The results of those analyses are presented and discussed.

Keywords: 2D Materials, Chemical Properties, Optical band gap, Energy Storage.
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[RWE-3] Analysis of anti-reflecting coatings for antimony chalcogenide solar cells

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Antimony chalcogenide thin-film solar cells have been considered as promising candidates in the field of photovoltaics, due to their suitable physical and chemical properties. However, the reported experimental record efficiency is far from the corresponding theoretical value. Multiple works have been directed to increase the value of the efficiency of these devices, but as far as we know, studies related to losses due to the reflection of the incident radiation or the effects of the reticular decoupling of the constituent layers of the solar cells in the formation of interfacial states have not been addressed systematically. Considering these aspects, this work presents a study of reflection losses and a description of the influence of lattice decoupling in the formation of interfacial states that allows improving the efficiency of these devices. The first analysis evaluates the impact on the short circuit current density and the second on the open circuit voltage. Some of the materials traditionally used in these devices are considered as anti-reflective coatings (ARC), and at the same time the formation of interfacial states, derived of their lattice mismatch, evaluating their respective impacts on the electrical parameters mentioned.

[RWE-399] Analysis of combined cycle plants in Mexico for potential adaptation in dual combustion of natural gas with green hydrogen

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Currently, hydrogen technology worldwide has become a great potential as an energy vector. However, most of the hydrogen demand is supplied through natural gas and coal, this production process generates gases, which is known as black or gray hydrogen. An alternative that can combat Climate Change is green hydrogen, produced by water electrolysis, which can be powered by renewable energies and accordingly not generate any polluting atmospheric gas. In addition, Mexico can take advantage of the large number of Combined Cycle Power Plants it has to implement a partial mix between natural gas and hydrogen. In this way, the emissions produced by the combustion of natural gas would be reduced, since hydrogen only generates water vapor. It would also be taking advantage of the country's high potential for the development of photovoltaic solar energy for the use of electrolysis. An intensive search of 84 Combined Cycle Power Plants existing in Mexico was carried out, a comparative table was made that includes the name of the plant, the location, its total capacity (MW), global energy generation (GWh), and type of turbine. gas installed. As a case study in a first stage, the Central Agua Prieta II plant was chosen, to carry out an analysis of implementing hydrogen enrichment to the natural gas line. This plant has a suitable location to take advantage of the solar potential and to install an electrolyser to generate green hydrogen. The available land of the plant itself was considered to size the solar park.

Keywords: Combined cycle plants, green hydrogen.
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[RWE-409] Fast Microwave-Assited Hydrothermal Synthesis Of BiVO4 Microstructures Decorated With Au Nanoparticles For Ciprofloxacine Photocatalytic Degradation

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Bismuth vanadate ($BiVO_4$) is a material which has carried great interest recently due to the photocatalytic activity, oxidative properties and great chemical stability. The $BiVO_4$ 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 electromagnetic spectrum. Nevertheless, the recombination rates of the photogenerated charges restrict its applicability. Therefore, a heterojunction with Au plasmonic nanoparticles (AuNPs) can overcome this issue. AuNPs can work as a tramp for photo-induced electrons. In addition, AuNPs absorbs visible light due to localized surface plasmon resonance (LSPR). The present work aims to take advantage of $BiVO_4$ photocatalytic properties and enhance light absorption with AuNPs nanorods growth on the surface of the photocatalysts for the further formation of an Au/$BiVO_4$ heterostructure. $BiVO_4$ was synthetized by the microwave assisted hydrothermal synthesis which allows reaction time reduction to just 30 s. X ray diffraction demonstrate monoclinic $BiVO_4$ as the main phase. SEM and TEM show nanostructures of ~100 nm long and 50 nm wide, with shape of nanobars and characteristic lattice planes of the $BiVO_4$. On the other hand, AuNPs were synthetized by the seed method to have a better control on shape and size of the nanoparticles. UV-Vis spectroscopy demonstrates AuNRs typical absorption bands due to longitudinal and transverse LSPR. SEM and TEM confirmed nanorods shape. Modification of seed method allowed growth of AuNRs on the surface of the photocatalyst provides a simple and repeatable method for the possible formation of the heterostructure. The absorption spectra showed the absorption bands of AuNRs and BiVO4, and TEM confirms the heterostructure and planes that allow its formation. To determine the improvement of the photocatalytic activity of BiVO4, the photodegradation of ciprofloxacin (CIP), a highly present contaminant in wastewater, was evaluated using the photocatalyst with and without AuNRs decoration illuminated with a visible light lamp (xenon 150 W). The CIP degradation using $BiVO_4$ was 40% after 2 h. The results show that surface modification of photocatalysts with metallic nanoparticles is a potential application for degradation of CIP in wastewater treatment plants, in addition to the use of a green method for the synthesis of the photocatalyst.

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Keywords: $BiVO_4$, Au nanorods, microwave assisted hydrothermal synthesis, $BiVO_4$/Au, photocatalysis.
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[RWE-27] Ge incorporation in kesterite thin films by solution processing route and its use in solar cells

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The substitution of Sn with Ge is one of the promising approaches to fabricate high-efficiency $Cu_2ZnSn_{1-x}Ge_xS_4$ (CZTGS) thin-film solar cells, especially for the multijunction or band gap-graded solar cells. Herein, we report a promising solution-processing deposition method for the controlled incorporation of germanium (Ge) in Cu_2ZnSnS_4 (CZTS) films using a nontoxic molecular ink. The effect of Ge concentration in the precursor solution on structural, optical, electrical and electronic properties of the films were systematically investigated. The successful Ge alloying in CZTS was confirmed by XRD analysis and exploring the sensitivity of Raman scattering. The as-synthesized $Cu_2ZnSn_{1-x}Ge_xS_4$ (CZTGS; x = 0, 0.1, 0.15, 0.2 and 0.25) films exhibit strong absorption in the visible region with the gradual increment in the band gap energy from 1.46 to 1.61 eV by increasing x from 0 to 0.25. A decrease in Urbach energy at higher [Ge]/[Sn + Ge] ratio supports the reduction of overall disorder into the system. The information about the correct oxidation states of the constituent elements and optimal chemical composition of the CZTGS films was obtained from X-ray photoelectron spectroscopy (XPS). The decrease in Sn^{+2}/Sn^{+4} signal ratio with the increase in Ge further supports the suppression of deep-trap Sn_{Zn} antisite defects. The XPS valence band spectra reveal that the position of valence band maximum ascended from 0.09 to 0.15 eV with increasing Ge content in the films. The solar cell was fabricated with a stack structure of FTO/TiO_2/CdS/CZTGS/C. The efficiencies of CZTGS films at the Ge percentages of 0% and 15% were 0.17 and 0.33%, respectively.

[RWE-96] Impedance spectroscopy analysis of semi-transparent inverted ITO/TiO2/P3HT:PCBM/PEDOT:PSS organic solar

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Organic solar cells (OSCs) based on conjugated polymers have drawn a lot of attention in the field of photovoltaic devices, due to some attractive characteristics such as low-weight, low-cost, semitransparency, and the feasibility of being solution-processed. Among these features, semitransparency allows the devices to be integrated into buildings as windows or facades taking advantage of the already available areas, turning semitransparent OSCs into a promising way to harvest solar energy. To achieve this application, spray coating deposition stands as a processing method that meets the requirements of being simple, scalable, and compatible with large area deposition and it can be used to obtain different layers of the OSCs. In these multilayer systems, the electrical properties of the materials and interfaces have a major impact on the performance of the final device. In this study, the spray coating technique was used to obtain deposits of titanium dioxide (TiO_2) as electron transport layer (ETL), regioregular poly(3-hexylthiophene):[6,6]-phenyl-C_{61}-butyric acid methyl ester (P3HT:PCBM) blend as photoactive layer and poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) as the anode to achieve inverted OSCs with the structure ITO/TiO_2/P3HT:PCBM/PEDOT:PSS. Different systems by varying the thickness of each layer were obtained and characterized by I-V curves and impedance analysis under illumination. The I-V characteristics and electrical properties from Nyquist plots of the different devices are discussed. The results show the potential of impedance spectroscopy to characterize OSCs to understand different operating processes and optimize the performance of the devices.

[RWE-431] Indirect electrochemical degradation of acetaminophen: process performance, pollutant transformation, and matrix effects evaluation

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Acetaminophen (ACE) and its toxic transformation products have been found in surface wastewater, and drinking water, which has several environmental concerns, was degraded in aqueous matrices (distilled water and synthetic fresh urine) by reactive chlorine species (RCS) electrogenerated using Ti/IrO_2 electrodes. Initially, the effect of the current (10-40 mA) and ion present in surface water and wastewater (Cl- or SO_4^{-2}) on the electrochemical system was evaluated. Then, the kinetics, and byproducts transformations involved in the elimination of ACE were described. It was found that, in distilled water, the process at 40 mA in NaCl presence led to 100 % of ACE degradation (10 min, 0.056 Ah L-1). Theoretical analyses of atomic charge for ACE indicated that the amide group is the most susceptible to attacks by RCS such as HOCl. On the other hand, degradation of acetaminophen in the synthetic fresh urine was slower (21% of degradation after 60 min of treatment) than in distilled water. This was attributed to the other substances in the urine matrix, which induce a competition for the degrading RCS. Results obtained from this work are promising for practical applications because short reaction times and low current densities are needed for degradation of ACE and its oxidation products.

KEYWORDS: Electrochemistry, Chlorination, Pharmaceuticals, Water treatment.
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[RWE-402] Natural deep eutectic solvents (NADES) in supported liquid membranes (SLM) for CO2 separation.

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Deep eutectic solvents (DES) mixtures have been proposed in the last years as viable and more sustainable solvents, in a myriad of applications. CO_2 capture or adsorption is one of those possible applications, where DES can act as greener alternative to the amine-based solvents that are currently being used in carbon capture and storage (CCS) processes. Deep eutectic solvents are defined as a mixture of two or more components, which may be solid or liquid and that at a particular composition present a high melting point depression becoming liquids at room temperature. When the compounds that constitute the DES are primary metabolites, namely, aminoacids, organic acids, sugars, or choline derivatives, the DES are so called natural deep eutectic solvents (NADES). NADES fully represent green chemistry principles. In this work, different choline chloride DES were prepared, and CO_2 gas transport coefficients were measured. Two types of NADES were prepared by mixing and heating of hydrogen bond acceptor (choline chloride) with either urea, glucose, tartaric and ascorbic acid as hydrogen bond donor. The Fourier transform infrared spectroscopy (FTIR) confirmed the hydrogen bond interactions in the resulting NADES. The NADES based supported liquid membranes were investigated systematically to determine the permeability and selectivity for the mixture of gases at both ambient and elevated temperatures. The DES were immobilized in a TiO_2-rutile macroporous support, and the pure gas permeability of 3 different gases (N_2, CO_2 and CH_4) was assessed, as well as NADES supported liquid membranes ideal selectivity.
The effect of operating temperature on membrane performance was also investigated that makes them an appropriate alternative to the conventional ILs

Keywords: Natural deep eutectic solvents, Membrane separation, CO_2 separation
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[RWE-65] Optimization of SnSe/CdS solar cell: Impact of loss mechanisms using SCAPS 1-D.

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Currently, thin film solar cells (TFSCs) with record efficiencies are based on materials such as cadmium telluride (CdTe), or copper indium gallium selenide (CIGS). However, the use of these materials carries some serious environmental and economic concerns due to the toxicity and scarceness of some of the constituents. The increasing energy demand from recent years arises the need for novel materials for applications in solar cells but without negative effects. Tin selenide (SnSe) is a non-toxic and affordable semiconductor that has drawn the attention of researchers owing to its high absorption coefficient which makes it suitable for solar cell applications. Nevertheless, so far TFSCs based on this material have not achieved efficiencies that can contribute to satisfy the increasing energy demand. Significant effort has been made to tackle the problem of low efficiency in SnSe-based TFSCs which includes theoretical studies and more particularly modeling. In this work, losses due to radiative and non-radiative recombination mechanisms over the photovoltaic characteristics of a solar cell with Au/SnSe/CdS/ITO structure with ideal and non-ideal series and shunt resistances are evaluated using SCAPS 1-D. Additionally, different parameters are varied for optimization employing a previously reported SnSe-based TFSC as the starting point for modeling. The influence of parameters such as absorber (t_{SnSe}) and buffer (t_{CdS}) layer thicknesses, the density of defects at the absorber (N_t) and at the absorber-buffer interface (N_{ts}), as well as shallow acceptor density (N_A) has been taken into account for device optimization. Result of this analysis, it has been shown that non-radiative recombination mechanisms due to volume defects in SnSe have the most detrimental effect on solar cell characteristics including efficiency. Also, for an ideal resistance device with t_{SnSe} and t_{CdS} of 1.7 Micra and 50 nm, N_t, N_{ts}, and N_A around $1x10^{16}$ cm^{-3}, $1x10^{6}$ cm^{-2}, and $2x10^{19}$ cm^{-3}, respectively, it is possible to achieve an efficiency of 21. 89 % under AM 1.5 G illumination at 300 K.

[RWE-167] PHOTOCATALYST FLOATING COMPOSITE USED FOR DYES DEGRADATION

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Floating photocatalysts have caused interest due to the benefits they provide. One of the main advantages of the floating support, is its characteristic lightness and flexibility; while the photocatalyst is able to interact with sunlight without the need of stirring or oxygenation, because the composite remains on liquid's surface. In this work, a floating photocatalyst based on a TiO_2 / agglomerate composite has been prepared. The agglomerate was elaborated using a post-consumer packaging of multilayer containers (i.e. Tetra Pak). The photocatalyst was prepared by synthesizing titanium dioxide powders by sol-gel method. The photocatalyst powder was attached to substrate surface using a varnish obtained by dissolving post-consumer polystyrene containers in toluene. The photocatalyst has different phase A-R (Anatase-Rutile) ratios. Using UV-Vis spectroscopy, the bandgap was estimated between 2.56 eV and 2.90 eV. The agglomerates have a rupture modulus of 14.95 N/mm2 ; they are hydrophobic materials and possess dimensional stability against changes in humidity (length) less than 10%, chemical resistance, are flame retardant. The TiO_2 /agglomerate composite is used for the photocatalytic degradation of a model pollutant (methylene blue) using sunlight.

Keywords: Titanium dioxide, multilayer container, photocatalysis
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[RWE-124] POLY CRYSTALLINE ANTIMONY SULFIDE THIN FILMS BY ULTRASONIC SPRAY PYROLYSIS: CHARACTERISATION AND COMPUTATIONAL ANALYSIS

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Antimony chalcogenides have gained great research interest as photovoltaic absorbers owing to their tunable optoelectronic properties, low toxicity, and high ambient stability. Among them, antimony sulfide (Sb_2S_3) is known to have a relatively lower processing temperature (<550 °C) and can be deposited using solution-based techniques[1]. In this study, we employed the ultrasonically assisted spray pyrolysis technique to prepare Sb_2S_3 in a single step using a non-aqueous precursor solution containing $SbCl_3$ and thioacetamide, a scaling process for a large area. The films deposited on glass substrates kept at 200 °C, by varying Sb/S precursor molarities were analyzed. XRD and Raman spectroscopy confirmed the phase pure films with polycrystalline nature and the crystallinity increased with Sb/S in the precursor solution. Surface morphology revealed uniform and homogenous thin film. The films were photosensitive with an optical band gap of 1.7 eV. The first principles simulation for the Sb_2S_3 unit cell using Vienna Ab initio Simulation Package (VASP) was also performed. Electronic band structure calculations were done using various functionals and potentials. The Raman spectral analysis was also done theoretically. The experimental and theoretical results were compared.

Keywords: Ultrasonic spray pyrolysis, Sb_2S_3, DFT, XRD, SEM,
Author for correspondence: kbindu_k@yahoo.com
Reference: [1] C. Jiang, J. Zhou, R. Tang, W. Lian, X. Wang, X. Lei, H. Zeng, C. Zhu, W. Tang, T. Chen, 9.7%-efficient Sb2(S,Se)3solar cells with a dithieno[3,2-: B: 2’,3’-d] pyrrole-cored hole transporting material, Energy Environ. Sci. 14 (2021) 359–364. https://doi.org/10.1039/d0ee02239j.
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[RWE-358] SENSIBILIZATION OF A Ti/TiO2 PHOTOANODE WITH CARBON QUANTUM DOTS AND SULFUR IONS

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Since the last century, the investigation about the *photoelectrochemical* process have been directed to found a photoanode capable of absorb the greatest amount of light in the spectra, therefore, in this project we work on the sensibilization with quantum dots of carbon and sulfur ions on the TiO_2 semiconductor layer to amplify the absorption spectra from UV to visible. In this work we use the ablation process to create a layer of TiO_2 by the irradiation of a pure Ti foil immersed in a suspension of quantum dots of carbon, and another one with sulfur ions. Also, we measure the optical properties of the after-ablation solution, and the capacity of conversion of photocurrent in the *scanning photoelectrochemical microscopy* (SPECM) technique, to see if the addition of this elements is favorable to the conversion of light in electricity.

[RWE-128] SILVER ANTIMONY SULFO-SELENIDE: GRAPHENE THIN FILM GROWTH USING GRAPHENE-SELENIUM NANOCOLLOIDS AND THEIR INTEGRATION IN SOLAR CELLS

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Silver antimony sulfoselenide ($AgSbS_{2-x}Se_x$) is an emerging absorber material composed of low-cost and earth-abundant elements. The present work is about the synthesis, characterization, and fabrication of graphene integrated $AgSbS_{2-x}Se_x$ absorber material[1]. Graphene -Se nanocolloids were synthesized by laser irradiation of selenium and graphene powders in isopropyl alcohol. Then the graphene-Se nanocolloids were spin-coated over the Sb_2S_3-Ag precursor layers synthesized by chemical bath and thermal evaporation method respectively. These films were heated in a vacuum furnace under different heating conditions. Optical absorption spectra revealed a red shift for graphene integrated $AgSbS_{2-x}Se_x$ films compared to pure $AgSbS_{2-x}Se_x$. Photocurrent response indicated one order increment in the photocurrent value in graphene integrated films. Solar cells were fabricated with a device structure glass/FTO/CdS/$AgSbS_{2-x}Se_x$: graphene/Ag. The device showed a power conversion efficiency of 3.5% which is higher compared to the reference solar cell fabricated with $AgSbS_{2-x}Se_x$. The complete study of structural, morphological, and opto-electric properties of the graphene integrated $AgSbS_{2-x}Se_x$ films and photovoltaic performance of the fabricated solar cells will be presented at the conference.

Keywords: Graphene, $AgSbS_{2-x}Se_x$ films, Se nanocolloid, opto-electric properties, solar cells
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[1] Y. Xiao, C. Li, X. Tan, L. Zhang, Y. Zhong, H. Zhu, Full-Inorganic Thin Film Solar Cell and Photodetector Based on “Graphene-on-Antimony Sulfide” Heterostructure, Sol. RRL. 1 (2017) 1–8. https://doi.org/10.1002/solr.201700135.
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[RWE-50] SOLAR TRACKER INTELLIGENT CONTROLLER: ASSISTED NATURAL CLEANING, INTERNET CONNECTIVITY AND ENVIROMENTAL TESTING

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Soiling is one of the main solar energy generation obstacles, specially in large open field arrays. However, photovoltaic surfaces cleaning technologies were not a popular research topic until recently. Among such technologies, the use of solar tracker's own motorization for the assisted natural cleaning benefit was never studied, until our Industry 4.0-oriented intelligent solar tracker controller was propoused (and briefly covered on XIV-ICSMV-2021). Since its introduction, dust adhesion has been studied in detail specially for this type of application, in order to assess the technology effectiviness. Now, the ongoing enviromental testing, which takes place in the warm semi-arid climate of Monterrey, Nuevo Leon, Mexico, shows first promising results for controller's advantages over it's traditional counterpart, clearly showing energy generation improvements during comparable periods of time. Solar tracker design, control algorithms, assisted cleaning effectiviness, tracker's own power consumption and overall functionality are discussed in this article, including the intent-in-progress of an application of the Taguchi methodology for the experiment design, which has not been used before for photovoltaic installations validation tests.

Keywords: solar trackers, photovoltaic panel cleaning, soiling, precipitation exploitation
Reference: Asl-Soleimani E., Farhangi S., Zabihi M., "The effect of tilt angle, air pollution on performance of photovoltaic systems in Tehran", RenewEnergy, vol 24, pp. 459–468, 2001.
This work was supported by: Fondo Sectorial CONACYT-SENER-Sustentabilidad Energética through Grant 207450, "Centro Mexicano de Innovación en Energía Solar (CeMIE-Sol)", within Strategic Project No. 91 "Desarrollo de un prototipo de seguidor solar inteligente con funciones de comunicación y control estratégico".

[RWE-257] Study on the impact of limiting factors on Cu2ZnGeSe4 solar cells

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Kesterite materials have recently attracted a great deal of attention from the scientific community for solar cell applications. One of the problems concerning this technology is the presence of the multivalence element Sn, which forms oxidation states +II and +IV, where in particular Sn^{2+} results in recombination centers that degrade the open-circuit voltage of the device. The partial or total replacement of Sn by Ge has been proposed as an interesting approach to solving this problem. In particular, the total replacement of Sn by Ge in the $Cu_2ZnSnSe_4$ (CZTSe) compound forming $Cu_2ZnGeSe_4$ (CZGSe) material results not only in the increase of band-gap from 1.0 eV to 1.35 eV but also increases the open-circuit voltage since it inhibits the formation of Sn^{2+} estates. Therefore, CZGSe semiconductor constitutes an attractive material for solar cell application. However, experimental efficiencies reported for this technology are still low. In this work, we present results on numerical calculations on CZGSe solar cells by SCAPS. The purpose of the work is to study the main limiting factors of this technology. The impact of defects at bulk and interfaces on solar cell performance is analyzed and discussed.

Keywords: Kesterite solar cells, CZGSe, solar cell simulation, SCAPS

[RWE-401] Synthesis of bismuth ferrite (BFO) via a solution combustion method and its catalytic evaluation on the sonochemichal assisted degradation of emerging contaminants (EC).

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It is widely known that water is an essential resource indispensable for human life. In fact, water covers at least 71% of the earth's surface, yet only 1% of it is suitable for human consumption. For quite a time now, water shortage has become an alarming issue and it wasn't until recently that efforts have been made to develop and improve technologies to ensure water safety. One of the areas many research has focused in is waste water treatment. Where many chemicals such as medicines, personal care, household cleaning products, agricultural, cosmetics, etc., are making their way "silently" in to water and waste water sources mainly because the consequences of such presence, have not yet been fully noticed (or were previously found in lesser concentrations). We refer to these compounds as emerging contaminants (EC) and due to the difficulty of removal in water treatment plants they represent an important environmental problem and health risks.This study explores the synthesis, characterization and catalytic evaluation of a bismuth ferrite (BFO) catalyst prepared via a solution combustion approach using bismuth nitrate $Bi(NO_3)_3 \cdot 5H_2O$, ferric nitrate $Fe(NO_3)_3 \cdot 9H_2O$, HNO_3 as precursor salts and urea as a fuel. The effect of different metal nitrate/ organic compound molar ratios has been studied in order to evaluate their suitability in obtaining pure BFO powders. The obtained powders were characterized by X-ray diffraction (XRD), infrared spectroscopy and scanning electron microscopy (SEM). The band gap and surface area of the catalyst was also determined using a Uv-Vis Nir spectrophotometer and the N_2 adsorption and desorption isotherms were obtained using BET analysis. The catalytic activity of the synthesized BFO powders was evaluated on the sonochemical assisted degradation (SAD) of EC under various conditions including photo catalyst concentration, initial EC concentration and pH variation. The results reveal that a BFO photo catalyst was successfully obtained in 2.5h at 550 ºC. The powders obtained showed high BFO phase content and smaller crystallite size.

Keywords: BFO, sonochemestry, emerging contaminants, water remediation, solution combustion.
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[RWE-443] Tetrapods based Smart Materials for Advanced Technologies

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Considering the size-dependent utilization complexities of nanoscopic dimensions for real applications, the focus of the nanomaterials community is merging to three-dimensional (3D) forms of materials that are built out of interconnected nanostructures. This talk will briefly introduce the importance of complex shaped nanostructures toward smart 3D nanomaterials structuring. A simple flame-based single-step approach was developed for synthesizing zinc oxide tetrapods which demonstrated many applications in different technologies. These tetrapods have been used as building blocks to construct highly porous interconnected 3D nanonetworks in form of flexible ceramics which offer further new application avenues. Additionally, these 3D networks have been utilized as sacrificial templates to develop hollow tetrapodal 3D networks from almost any desired material, carbons, nitrides, oxides, polymers, hydrogels, etc. The sacrificial template-based strategy offers new and unique opportunities in the direction of 3D nanomaterials engineering and accordingly advanced technological applications. Some examples of 3D nanomaterials engineering will be demonstrated along with their applications [1-10]. The scopes of 3D nanostructuring-based smart materials in sensing, electronics, optoelectronics, energy, and biomedical engineering will be briefly highlighted in the talk.

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ACS Nano 15, 8069, 2021 Materials Today 6, 631-651, 2018
Advanced Functional Materials 1909725, 2020 Materials Today 32, 108 -130, 2020

[RWE-403] The effect of the donor/acceptor ratio on organic solar cell performance

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The active layer of the organic solar cells comprises an interpenetrating network with nanoscale phase separation between a donor and an acceptor materials. This architecture is known as bulk heterojunction (BHJ) and creates a larger interface area than in a planar heterojunction, so that an electric field in the vicinity of the interfaces of donor and acceptor materials is distributed throughout the volume of the active layer and a more effective charge separation is achieved. Due to the deposition method, BHJ architectures with irregular morphologies are obtained since the random mixing nature of the donor and acceptor during solution processing [1]. In order to understand and improve the performance of organic solar cells, here we propose an approach that uses an algorithm to generate BHJ architectures with irregular random disordered morphologies [2] to theoretically analyze the effect of the donor/acceptor ratio on device performance. The power conversion effciency is obtained as a function of donor/acceptor ratio for arbitrary semiconductor materials to illustrate our approach.

Keywords: Organic semiconductor, bulk-heterojunction, irregular morphology, solar cells
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References: [1] F. Zhao, C. Wang, and X. Zhan, Morphology Control in Organic Solar Cells, Adv. Energy Mater. 8 (2018) 1703147. https://doi.org/10.1002/aenm.201703147.
[2] I.C. Flores-Contreras, V. Cabrera-Arenas, and L.M. Reséndiz-Mendoza, An algorithm to generate two-dimensional morphologies of organic solar cells, 19th International Conference on Numerical Simulation of Optoelectronic Devices, Ottawa, Canada, MPDP3 (2019). https://www.nusod.org/2019/MPDP3.pdf
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[RWE-388] Use of cerium oxide thin films in the electrocatalytic water splitting process

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In this work, nanostructured cerium oxide thin films were grown over FTO, titanium and steel substrates by ultrasonic spray pyrolysis varying the carrier and director gas flows, which were air in all cases. Cerium acetylacetonate as a metallo-organic precursor dissolved in anhydrous methanol at 0.02 mol/L were used, the substrate temperature was set at 475 °C and the deposition time was 30 min. 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. Thin films were electrochemically characterized by chronoamperometry, impedance spectroscopy, cyclic and linear voltammetry measurements, all of them, except that one's grown over Titanium, showed that films can be used in water reduction process applying a potential of -1.5 V vs Ag/AgCl. As the potential increases the current density increases, and when it reaches -2.0V vs Ag/AgCl films grown over FTO suffers an excessive loss of oxygen, due to this the CeO_2 loses crystallinity. Measurements indicate that the films are suitable for use as catalyst in the photoelectrocatalytic water reduction process.

Keywords: Hydrogen, Ceria, Thin films.

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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 collaborationshas 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
- 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.

[SEM-309] (Fe2O3)x(ZnO)1-x Thick Films obtained by Ultrasonic Spray Pyrolysis

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$(Fe_2O_3)_x(ZnO)_{1-x}$ composite thick films were prepared by Ultrasonic Spray Pyrolysis on a glass substrate. at 450°C. using 0.1 M aqueous solutions of $FeCl_3$ $6H_2O$ and $ZnCl_2$ anhydride compounds. To obtain different elemental concentration of Fe and Zn, we varied the volume of each aqueous solutions. The samples were characterized by X-ray photoelectron spectroscopy (XPS), The X-ray diffraction, Raman spectroscopy and optical transmission. The XPS results shown that x values were varied from 1 to 0.87. The X-rays diffraction caractherization revealed that the films were composed of different phases corresponding with common stable iron oxides ($ZnFe_2O_4$ - α, -Fe_2O_3) and zinc oxide (ZnO). Results from raman spectroscopy indicate that Fe_2O_3 vibrational modes are accompanied with new modes due to the presence of additional phases ZnO compounds. The band gaps were evaluated with the help of the experimental transmittance datas using the Tauc model, the results shown a modulation of the band gap values with the incorporation of ZnO. Theorical transmittance curves were obtained using the effective medium theory, using the Bruggeman model, the results showed a good agreenment with the experimental transmittance curves.

This work was supported by SIP-IPN 20221355

[SEM-152] A NOVEL BISMUTH OXYCHLORIDE /OXYIODIDE PHOTOCATALYST AND EFFICIENT DEGRADATION OF ORGANIC POLLUTANTS UNDER VISIBLE LIGHT

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Today, water pollution is generated mainly by the paper industry, the textile industry, and the paint industry. This water has as final disposal rivers, seas, and lakes. However, all these contaminants are treated in wastewater treatment plants through primary and secondary methods, without achieving their complete mineralization. For this reason, it is necessary to implement new techniques and materials to achieve the complete mineralization of these organic contaminants. In this work, binary solid solutions of bismuth oxyhalides of chlorine and iodine of different compositions ($Bi_4O_5Cl_XI_Y$, X+Y=2) have been easily obtained through the synthesis method by precipitation at room temperature using non-toxic precursors. The effect of the composition has been studied through different characterization techniques, such as SEM, EDS, DRS and XRD. These binary solid solutions have been found to exhibit photocatalytic activity under visible light. The results confirm the successful obtaining of the binary solid solution, and not a mixture of phases. In addition, the compounds showed band gap energies from 2.40 to 2.85 eV and an absorption edge shift from 391 to 501 nm, making their activation possible under visible light. Depending on the application, the modulation of its band gap is possible, therefore, it could be applied to many organic pollutants.

Keywords: Bismuth Oxyhalide, Bismuth Oxyiodide, Bismuth Oxychloride.

[SEM-209] Analysis of ZnO co-doping with Sb and Teflon

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ABSTRACT: Optic, structural and electric properties of Zinc Oxide (ZnO) has been studied because of its application for optoelectronic and spintronic devices. Achieving stable *p*-type conductivity of ZnO has been a difficult challenge in recent years due to the low solubility, low energies of formation of the donor levels compared to the acceptor levels, and self-compensation, which causes the conductivity to revert to *n*-type within days, even hours, being this phenomenon the most challenging issue. In the present work the possibility of controlling the physical properties of ZnO by means of diffusion process was studied. Single crystal wafers of ZnO with orientation (001) growth by hydrothermal method were subjected to solid diffusion process with Antimony and subsequently subjected to thermal treatment with Teflon, seeking to achieve the diffusion of Fluorine and/or Carbon. In this way, a codoping of two or three elements is attempted to study their behavior and optic properties of ZnO. Characterization of physical properties of samples was performed using Photoluminescence (PL), optical transmittance and Raman microscopy. Structural characterization was performed by High Resolution X-Ray Diffraction (HRXRD) analysis. In PL analysis, the goal is to understand the contribution of Antimony and Teflon, as well as the characteristic defects play in ZnO optoelectronic properties and important changes in PL signal about band associated to defects of Zn anti-sites. In Raman microscopy analysis, finding the bonds present in the ZnO crystal lattice, looking for signs of bonds with foreign elements and understanding their influence is of great importance. In HRXRD analysis, the changes in crystal quality and the lattice constant are looked for to determine the presence of impurities in the lattice. Impurity diffusion process produces alterations in crystal lattice, associating to deeper diffusion.

Keywords: Zinc Oxide, co-doping, Antimony, defects, Teflon.
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[SEM-370] Annealing effects on the optical properties of thin films GaNAs:Sn layers grown by MBE

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One of the most interesting highly mismatched alloys is the GaN_xAs_{1-x} where the addition of nitrogen atoms leads to division of conduction band in two sub-bands know as and , so that the alloy can be employ in the development of intermediate band photovoltaic devices [1]. Nevertheless, the adding of nitrogen atoms to GaAs compound changes their optical, structural, and electronic properties toward reduced values. Thus, the study of mechanism to improve the optoelectronic properties of the GaNAs alloy by in-situ and ex-situ techniques is imperative. In this research, $GaN_{0.02}As_{0.98}$ layers were grown by Molecular-Beam Epitaxy on intrinsic GaAs(100) substrate. The addition of tin atoms was controlled by the tin effusion cell temperature (T_{Sn}) in the 700 to 850 °C range. With this n-type doping strategy the in-situ optimization of the ternary is searched. Additionally, Rapid Thermal Annealing (RTA) was applied for 60 seconds at 800 °C to modify the structural properties of the sample as ex-situ scheme. The behavior of the GaNAs properties before and after the RTA was analyzed by Raman spectroscopy, where an increase on the relation was observed, indicating an improvement on the carrier concentration for T_{Sn} > 750 °C. The LO mode presents a redshift related with a strain state on the lattice, increasing with the RTA. The effect of annealing in the band structure of the alloy was also analyzed by photoreflectance spectroscopy where a redshift of the transition related was measured. Additionally, the spectral region of Franz-Keldysh oscillations was modified toward higher frequencies, as an indicative of modification on the carrier distribution of the samples. Through this research project, both in- and ex-situ methods are proposed to optimize GaNAs alloy to their application in the photovoltaic devices.

Keywords: GaNAs, Rapid Thermal Annealing, Photoreflectance, Raman.
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[SEM-153] BAND GAP VARIATION AND CHARACTERIZATION OF THIN FILMS OF THE TERNARY SEMICONDUCTOR CDSXSE1-X GROWN BY LASER ABLATION.

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Using a laser ablation system, thin films of the binary semiconductors CdS and CdSe were prepared, as well as the ternary semiconductor CdSxSe1-x with compositions at x= 0.25, 0.5 and 0.75. In this way, we went from the CdSe (x= 0) to CdS (x=1), analyzing the optical and structural properties. The bandgap was obtained by UV-Vis spectroscopy, and related to x-ray diffractometry in which cubic and hexagonal phases were observed.

Keywords: CdS_xSe_{1-x}, laser ablation, thin films
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[SEM-400] Characterization of the InxSey and CuInSe2 layers

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The objective of this work was to study the In_xSe_y and $CuInSe_2$ layers for their possible application in solar cells or charged particle detectors.The scientific community has made efforts to find new materials that are friendly to the environment. Among these materials, In_xSe_y is an n-type semiconductor with a bandgap of 1.8-3.2 eV, which is very promising to replace CdS. On the other hand, $CuInSe_2$ is a highly studied semiconductor, which can be used as absorbing layers in photovoltaic devices, showing great promise for charged particle detectors. In_xSe_y and $CuInSe_2$ thin films were synthesized in a multisource thermal coevaporation facility using a Knudsen cell, where the substrate temperature was maintained between 300 and 400 °C, and the Knudsen cell temperature was deposited depending on the material. The In_xSe_y film is deposited on the conducting oxide of SnO_2:F and the $CuInSe_2$ layer on the In_xSe_y film.The structural and morphological properties of each In_xSe_y and $CuInSe_2$ layer were investigated by X-ray diffraction (XRD), Raman spectroscopy, and scanning electron microscopy (SEM). From the results obtained, gamma and beta phase bands can be observed in the In_xSe_y Raman films. As for $CuInSe_2$, a mixture of CuSe and InSe binary phases was identified by XRD, and binary bands were observed by Raman. In conclusion, it is possible to study the morphological and structural layers of In_xSe_y and $CuInSe_2$, obtaining favorable results for their application in charged particle detectors.

Keywords: layers, In_xSe_y,$CuInSe_2$, morphological and structural.
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[SEM-434] CHARACTERIZATION OF THERMAL PROPERTIES OF InP QUANTUM DOTS FOR APPLICATIONS AS INFRARED PHOTODETECTORS

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Semiconductor quantum dots (QDs) have been the subject of extensive research in the last decades due to their great importance in the development of new devices in areas such as semiconductor lasers, photodetectors, solar cells, optoelectronics, and recently in areas such as biomedical devices. These QDs can be fabricated by sophisticated and expensive growth techniques such as MBE and MOCVD, and also by more simple and less expensive methods such as chemical synthesis and sputtering. In this work we report on the synthesis of indium phosphide (InP) QDs by means of the one-pot chemical synthesis process without injection of hot precursors; these InP QDs are obtained in colloidal solutions and the QDs sizes are controlled by adjusting the synthesis parameters such as temperature, precursors concentrations and the pH of the solution. Because of the quantum confinement effects, the bandgap energy of the QDs will depend on the QD size, in such a way that the fluorescent wavelength of the InP QDs can be controlled by their size. In their application for infrared photodetectors, we make use of the electron intraband transitions in the conduction band whose energy separation will depend on the QD size. In this work we report on the characterization of the structural and optical properties of InP QDs and their variation with QD size; also, we show results on the variation of the QDs thermal conductivity with QD size, since this parameter is important to obtain good eficiency in the infrared photodetectors.

Keyword: Quantum dots, Semiconductors, Thermal properties, Photodetectors
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[SEM-137] Comparison of thermodynamic stability of the GaSb substrate in contact with Ga(Al)-rich and Sb-rich AlGaSb liquid phases

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In this work a comparative analysis of the thermodynamic equilibrium at the liquid-solid (L-S) interfaces formed by a GaSb substrate in contact with either, a Ga(Al)-rich and Sb-rich liquid phases of AlGaSb ternary system was carried out. Estimations were made using the CALPHAD method and SGTE data. Initially, it is shown that the saturated ternary AlGaSb liquid phase of any composition becomes overheated when it is brought in contact with the GaSb substrate. The overheating temperature increases with the Al concentration in the two types of liquid phases and reaches slightly higher values for Sb-rich liquid phases. Overheating of the liquid phase causes dissolution of some quantity of the substrate and results in the supersaturation of the liquid phase leading to the deposition of some quantity of a solid phase forming an epitaxial layer. The relationship between the quantities of dissolved and deposited materials permits to estimate the thermodynamic stability of the substrate. The thermodynamic stability of the GaSb substrate decreases monotonically in contact with the Sb-rich liquid phase as the Al content increases. In the case of Ga(Al)-rich liquid phase, the thermodynamic stability has a well-defined minimum at some Al concentration that decreases noticeably and shifts towards the GaSb rich side at higher temperatures but it never exceeds the values achieved by the Sb-rich liquid phase. From these results we can conclude that the GaSb substrate is more thermodynamically stable in the case of contact with Ga(Al)-rich AlGaSb liquid phase as compared with a Sb-rich liquid. This fact can be used in liquid phase epitaxy (LPE) processes to form heterostructures with sharper boundaries between epitaxial layers.

[SEM-285] EFFECT OF SOL-GEL PROCESS PARAMETERS ON QUALITY AND PROPERTIES OF SNS THIN FILMS

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In the present work, SnS thin films were deposited by dip-coating method. Precursor films were coated onto glass substrates using a stable solution of SnCl2·2H2O and thiourea were used for Sn2+ and S2− ion sources respectively in the solution. Following the deposition, films were annealed at different temperature in the range of 200–300°C for 30 min and cooled down inside of muffle under air atmosphere. The surface morphology was modified by the annealing temperature. The crystalline properties of the material were investigated using XRD. The effect of annealing temperature on the optical properties of SnS films was also investigated using UV–Vis spectroscopy.

Keywords: SnS thin films; XRD; UV-Vis spectroscopy; sol-gel.
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[SEM-105] GaAs LAYERS ON GRAPHENE GROWN BY CSVT

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Epitaxy is one of the most widely used techniques for the growth of III-V semiconductors. An epitaxial growth allows obtaining crystals of very high quality. In recent years, the discovery of graphene (G) has innovated many aspects of science and technology. Van der Waals (VdW) epitaxy was developed by studying the behavior of bonds that exist in two-dimensional materials. In this work, the use of quasi-Van der Waals (qVdW) epitaxy is reported, which consists of depositing a bulk material on Graphene [1]. The objective is to study the structural, surface, and vibrational properties of GaAs layers grown on G/GaAs(100) and G/Si(100) by the closed space vapor transport technique (CSVT). Graphene was obtained by chemical vapor deposition (CVD) on copper, then it was transferred on Si(100) and GaAs(100) substrates. The graphene was analyzed with Raman spectroscopy. The characteristic G and G' peaks of a graphene bilayer (G) were found at 1569 and 2709 cm^{-1} respectively. The GaAs layers grown on G/GaAs(100) and G/Si(100) substrates were characterized using Raman, X-ray diffraction and scanning electron microscopy techniques. Finally, we found the LO and TO modes of GaAs at 292 and 269 cm^{-1} respectively. This is a growth of GaAs cheaper.

Keywords: GaAs, CSVT, Graphene, Quasi Van der Waals epitaxy, Graphene on silicon, Heteroepitaxy

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[SEM-262] GAAS LAYERS ON SI(100) GROWN BY CLOSE-SPACED VAPOR TRANSPORT

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The main impediment to using a single crystal GaAs wafer as a substrate is its high cost and the epitaxial growth of the device structure. A solution is a layer device approach on a low-cost substrate. The CSVT method has been successfully used to grow a variety of semiconductor materials including homo-and hetero-epitaxial GaAs layers. This technique has some advantages compared to the other ones as they are a low-cost manufacturing technique that allows the deposition of layers at atmospheric pressure and moderates temperatures. Here, it is reported, GaAs layers grown via CSVT. GaAs layers were grown varying the deposition time (5 and 13 min), the substrate (Si and quartz) and the substrate chemical cleaning (RCA or HF). Under these conditions and through morphological, structural and topographic characterizations, the GaAs layer grown on a Si (100) substrate previously subjected to RCA chemical cleaning for 13 min stood out. By XRD, three major diffraction peaks at 27.29° 45.36° and 53.70° were observed, with the peak at 27.29° being the most intense. Regarding the chemical composition, 53.5% of Ga and 46.5% of As in at% were determined by EDS analysis. An increase in grain size was noted in the SEM micrographs as the growth conditions were optimized. Meanwhile, in the Raman spectrum of the GaAs layers, both TO and LO vibrational modes were presented. However, as the growth parameters were varied, the intensity of the LO mode exceeded the intensity of the TO mode, indicating fewer defects in the material. This was confirmed by determining the FWHM, which changed from an initial value of 6.56 cm^{-1} to a value of 3.80 cm^{-1}.

Keywords: Low-cost substrates, GaAs, CSVT
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Reference: [1] J.J. Cruz Bueno, G. García Salgado G, R. Balderas Valadez, et al. Effect of the Gaseous Atmosphere in GaAs Films Grown by Close-Spaced Vapor Transport Technique. *Crystals*. 2019;9(2):68. doi:10.3390/cryst9020068
This work has been supported by CONACyT.

[SEM-79] IMPLEMENT DIFFERENT DOPANTS ON THE PROPERTIES OF MATERIALS WITH STRUCTURE TCO/CDS/C AND TCO/CDS:M/C

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A metal-semiconductor interface is an integral part of numerous electronic devices such as Schottky barrier diodes, photodetectors, and photovoltaic cells, amongst other applications. This study presents the synthesis of semiconductor thin films of pure cadmium sulfide and doped with metals by the chemical bath deposition technique. XRD, SEM, EDS, XPS, UV-Vis spectroscopy, I-V, and photocurrent measurement were used to analyze these thin films. Afterwards, the synthesized materials were applied to Schottky diodes. The doped CdS thin films reveal differences in the size of the crystallite, differences in morphology, and the energy bandgap shows a shift. The implementation of dopants allows the design of materials, this enables the design of window layers by choosing the suitable dopant for the CdS. Due to the incorporation of determinate dopants, the photoresponse of the doped CdS Schottky diodes improved.
The Schottky diodes manufactured in this work show variation in height of the potential barrier. These results demonstrate the impact of dopants on the characteristics of craft materials and photodiodes elaborated, exhibiting an enhancement in their photoresponse. Overall, our extensive study reveals that there is great potential in the design of affordable multifunctional optoelectronic devices depending on the dopants applied.

[SEM-23] Influence of Ni2+ impurities in the physical properties of CdS thin films

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Cadmium sulfide layers prepared by chemical bath synthesis on glass substrates at 80 °C were doped with Ni^{2+} impurities. $Cd_{1-x}Ni_xS$ samples, with Ni atomic percentage (at%) in the $0.0 \leq x \leq 0.74$ interval, were grown with average crystallite size (CS) in the 18-20 nm range. Presence of Ni^{2+} ions in CdS lattice alters interplanar spacing (IS) and CS, which in turn introduce changes in the energy band gap (E_g), phonon modes (PM), photoluminescence (PL), dark electrical conductivity (σ), among other properties. Changes are due to the relatively high ionic radius (R) difference between Cd and Ni (R_{Cd} = 78 pm, R_{Ni} = 54 pm). IS increases and CS decreases as Ni^{2+} concentration rises to x ~ 0.4, afterwards the behavior is inverted up to x = 0.74. This result is due to the incorporation of Ni^{2+} in Cd^{2+} sites for low x values, and in interstitial sites for higher ones. As consequence, the vibrational longitudinal optical (1LO) mode frequency first diminishes up to x ~0.4 and then increases for higher x values. Similar dependence is observed for direct band gap (E_g) of CdS films. PM-1LO and E_g versus x behavior, both, follow an inverted function than expected, which is explained in accordance with results found in literature.

[SEM-385] Influence of Cu and substrate temperature on CIS thin films processed by thermal coevaporation

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The CIS films were deposited with different growth parameters by thermal coevaporation technique: Cu temperature variation and substrate temperature variation. X-ray diffraction analysis was performed on the CIS films, revealing the presence of the chalcopyrite phase of the CIS ternary in all the films. The EDS results of the CIS films, the presence of the elements copper, indium, and selenium was confirmed, probing that at high temperatures, there is a higher atomic percentage of copper in the films. From the images obtained by Scanning Electron Microscopy (SEM) for the In_2S_3 thin films, it was impossible to observe the films' morphology since their thicknesses are less than 100 nm. For samples rich in copper, columns of hexagonal flakes are obtained and for those with a higher percentage of selenium, they are characterized due to the presence of columns of cauliflowers, being both morphologies of the CIS. In copper, it is present stacked hexagons forming columns on its entire surface, and agglomerations of cauliflower columns, both morphologies distinguish the CIS.

Keywords: CIS, THERMAL, COEVAPORATION, Cu-In-Se, TEMPERATURE, SEMICONDUCTOR
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[SEM-12] Joule Heating and Nonlinear Charge Transport in Bipolar Semiconductors

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Joule heating of a homogeneous bipolar semiconductor leads to the appearance of nonequilibrium spatially inhomogeneous current carriers. Both energetic and concentration nonequilibrium states arise. Temperature and concentration gradients at the boundaries always have opposite signs. The concentration will become lower in heated regions, while it will become higher in less heated ones. Moreover, the spatial distributions of concentrations have one minimum in thin samples and two minimums and one maximum in thick samples. As a result, the current–voltage characteristic can take superlinear and sublinear forms.

[SEM-86] LO phonon-plasmon coupling in n-type InGaAsSb alloys, a tool to estimate carrier concentration.

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Plasmonics has been growing exponentially in the later years due to the uses and applications of surface plasmon polaritons (SPP) and localized surface plasmons (LSP). Nonetheless, there is another form of plasmons in certain materials: the bulk plasmon. These plasmons are described as oscillations of free carriers into the material; for this reason, they can be excited by long-wavelength radiation (red wavelength). Also, they can be coupled to another quasiparticle, phonons. The oscillating nature of bulk plasmons (longitudinal), allows them to couple with longitudinal optic (LO) phonons, creating two modes known as L- and L+ coupled modes. The L- mode presents the same frequency as the transversal optic (TO) mode [1]. Therefore, the vibration detected at the TO frequency is a contribution of two effects, the TO and the L- mode, a compound mode very difficult to separate. On the other hand, the L+ mode varies with carrier concentration as does plasma frequency. Thus, if the L+ mode is found, the carrier concentration can be estimated. This work proposes a method to estimate the carrier concentration using the L+ coupled mode in n-type $In_{0.14}Ga_{0.86}As_{0.14}Sb_{0.86}$ layers. By studying the dielectric function, the Raman shift frequencies of the coupled modes were calculated and, Raman spectroscopy was used to determine the vibrational and coupled modes in the samples in the range 160-1000 cm^{-1}. In order to verify the carrier concentration found in n-type $In_{0.14}Ga_{0.86}As_{0.14}Sb_{0.86}$ layers by Raman, photoluminescence spectroscopy (PL) was employed to estimate these concentrations; both techniques gave the same results. The methods presented here are alternatives to the Hall effect technique and are non-invasive, non-destructive, and cheaper.

Keywords: phonon-plasmon coupling, plasma frequency, Raman spectroscopy, carrier concentration.

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[SEM-6] MBE growth and characterization on InGaAs /GaAs metamorphic layers

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The materialization of heterojunctions (HJ) and heterostructures (HS) has conducted to the development of a wide variety of semiconductor devices, like semiconductor lasers for communications and printers; light emitting diodes for illumination and flat panel displays; p-n junctions in solar cells; high mobility transistors used in mobile phones, radar, imaging, as well as radio astronomy, among many other current applications. The band gap engineering is the basis that confers the advantageous properties of HS. However, the experimental realization of these structures faces several problems such as differences in atom's electronegativity and lattice mismatch. The former is the main responsible for the generation of dislocations due to strain relaxation, defects that reduce the performance of the devices, and that strongly depend on the composition of the HJ and HS layers. In this work, the authors explore the structural and optical properties of metamorphic compositional graded layers of InGaAs grown on GaAs by molecular beam epitaxy (MBE). X-ray diffraction patterns (HRXRD) showed diffraction peaks associated with GaAs, In concentration alloy at which the graded samples started at, and a wide plateau associated with the graded metamorphic layer. It is found that the gradual accumulation of strain is suddenly relieved at ~540 nm when reached a nominal concentration of In=42%. The thickness matches the fastest change in In concentration within the film, as experimentally determined by spectrometry of masses (SIMS). Photoluminescence spectroscopy showed intensity lines at 0.58 and 0.82 eV associated with band-to-band transitions from the dislocation free zone, assisted by the relaxation of photoexcited carriers close to the near-surface band bending of the graded concentration layers. Finally, the strain promoted the generation of dislocations, In segregation, and surface roughness. But, conversely to linear or step-graded layer profiles, for metamorphic layers these phenomena depend on the strain direction (tensile or compressive), and alloys hardening occurs provoked by In in the region of the larger positive gradient in composition.

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[SEM-218] NANOSTRUCTURED CU-CR-O POWDERS: COMBUSTION SYNTHESIS AND CHARACTERIZATION

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The synthesis and characterization of nanostructured copper-chromium-oxide powders is presented in this work. The powders were synthesized by the combustion technique from copper and chromium nitrates using the glycine nitrate route (GNR). The powders were characterized by HR-SEM, EDS, XRD, Uv-vis spectroscopy, Raman spectroscopy, and Impedance Spectroscopy. The as synthesized powders consisted mainly of a mixture of CuCrO2, Cr2O3 and CuO nanocrystals, according to XRD and Raman spectroscopy. The electrical properties of the powders was carried out by impedance spectroscopy, considering effective medium models.

Keywords: Combustion synthesis, Glycine-Nitrate-Route, Impedance Spectroscopy, Cu-Cr-O powders
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This work was supported by Secretaría de Investigación y Posgrado, Instituto Politécnico Nacional, México

[SEM-340] OPTICAL AND ELECTRICAL CHARACTERIZATION OF ORGANICS PHOTODIODES WITH POLYMER P3HT AND FULLERENE PCBM C61 SENSITIVE IN NIR

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The new technologies of flexible electronics allow to have synthetics materials such as poly(hexylthiophene) and carbon derivatives as an option in the design and building of optoelectronic devices. The purpose to have such options of optical sensors on this work is to introduce a bulk heterojunction for building organic sensors in the NIR constructed from this bulk heterojunction on flexible substrates of indium tin oxide, using polymeric materials as a semiconductors and low melting point metal contacts such as indium gallium (InGa) alloy and some metals as Ag, Ni. The performance of organic photodiodes of poly(hexylthiophene) P3HT and fullerene phenyl-C61-butyric acid methyl ester (PCBM) can be determined by its optical and electrical characterization, which are carried out using I-V curves and UV VIS spectroscopy on these devices to observe the displacement of the curve as well as the average transmittance to visualize the possibility of obtaining a sensor in the near infrared region. The optical behavior of the polymer is discussed in the visible spectrum as well as the dark electrical response of the bulk heterojunction and as a function of the incident wavelength above the device. We can observe that the P3HT transmits from the infrared up to about 600nm while the $PC_{61}BM$ has not contribution on the visible spectrum. regarding the electrical characterization I-V, we can find that the photogenerated currents has a lineal shift when the incident wavelength increases, and we approach to the near infrared region. We conclude that the organic photodiodes constructed with these materials serves as optical sensors in the NIR, since their transmittance increases from 600nm to the near infrared region, as well as the shift in the photogenerated current in the I-V curve is lineal as the wavelength approaches to that region.

Keywords: Bulk Heterojunction, Organic Photodiodes, Polythiophene, Photogenerated Currents, Near Infrared

Hrostea, L., Girtan, M., Mallet, R., & Leontie, L. (2018, June). Optical and morphological properties of P3HT and P3HT: PCBM thin films used in photovoltaic applications. In IOP Conference Series: Materials Science and Engineering (Vol. 374, No. 1, p. 012015). IOP Publishing.

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[SEM-249] Optical and Structural analysis of ZnO under influence of gamma radiation

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ZnO thin films deposited on silicon and glass, with sputtering technique, for differen power deposition, have been exposed to gamma radiation from a 137 Cs source, in a large exposition time. Important effects on the structural and optical properties has been observed by XRD and UV-Vis and Raman spectroscopy. Changes on band gap energy from typical values (3.3 eV for no treated ZnO) has been detected, obtaining values around 3.9 eV in the most of the cases, and apparently a predominant crystalline orientation (222) has been caused in the typical hexagonal structure for this material. Previously these effects has been observed for ZnO nanoparticles exposed to these type of radiation.

[SEM-253] Optical and structural calculations of Ba ZrO(1 âˆ’ x)Sx by AB Initio.

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AB Initio calculations for BaZrO3(1−x)S3x has been realized to determine the band structure. The initial crystalline structure proposed was cubical for BaZrO3, and later this structure was doped with sulfur for different concentration. In other direction, the BaZrS3 was considered too, using the orthorrombic structure, and under the same procedure, it was doped with oxygen. There were decisive changes in the crystalline structure (lattice constants) as the dopant is integrated, and in turn, this is observed in the corresponding band structures. A comparative analysis was made using pseudopotentials HSE and PBE, which, as expected, for the PBE case, values below those reported experimentally for the band gap case are obtained.

[SEM-371] Optical characterization of Sn-doped GaNAs thin film grown by Molecular Beam Epitaxy

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Epitaxial growth methods such as molecular beam epitaxy (MBE) allow the synthesis of semiconductor compounds and heterostructures which are applied to the obtention of intermediate band (IB) solar cells. In this task, the GaNAs material is used as IB material for the behavior that its electronic structure of bands acquires, being the division of the conduction band into two energy levels called E- and E+ the most interesting properties for photovoltaics [1]. However, both the lattice mismatch between GaAs and GaNAs and the carriers' mobility are degraded by increasing the nitrogen molar concentration percent (%N). In this work, the authors explore the grown process and the optical characterization of GaNAs layers where tin is employed as donor atoms with the aim to increase the optoelectronic response of this material. MBE is utilized to obtain 500 nm wide GaNAs layers grown on GaAs (100) with two different %N around 0.2 and 2, labeled as A and B set of samples, respectively. The n-type doping level was controlled by the tin effusion cell temperature, exploring the range from 700 to 850 °C. The high-resolution x-ray diffraction spectra of the [004] plane obtained by rocking curve shows %N values of 0.12 and 1.9%, for samples A and B, respectively and indicating an appropriated grown process. Additionally, the crystallinity of the material is not degraded by the addition of Sn, obtaining an unexpected result. Raman spectra exhibits modifications in vibrational modes related to both the %N and Sn incorporation in GaNAs. L- and LO phonon integrated intensities were employed to determinate the donor atoms concentration by the depletion layer estimation, showing the range from $6x10^{16}$ to $6x10^{18}$ cm^{-3}. For similar Sn effusion cell temperature, the B set of samples exhibits a higher donor concentration in contrast with the A series. These results were corroborated by four-point probe method, demonstrating the change in conductivity for the samples with tin atoms concentration. With this study the authors show by first time the employment of Sn as donor element in the GaNAs alloy.
Keywords: GaNAs thin doped, Raman Spectroscopy, HRXRD, Molecular Beam Epitaxy.
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[1] https://doi.org/10.1063/1.4709405
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[SEM-307] Optical, structural, and surface chemical characterization of In2O3 nanoparticles and quantum dots of InP@ZnS.

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Abstract: This work describes the synthesis and characterization of In_2O_3 nanoparticles and InP@ZnS semiconductor quantum dots (QDs). The absorption spectra present a primary shoulder around 380 nm for the InP and 440 nm for the case of InP@ZnS. Using this wavelength the band gap energy of the InP and InP@ZnS QDs was determined. It can be observed that the diffractograms present a typical form of a nanostructured material. Diffraction peaks are identified with the crystalline phase of the InP. ZnS offers zinc blended (FCC) type, located in the planes (111) and (311). In addition, the phases of In_2O_3 can be observed in the planes (211). From the photoluminescence spectra, we observed QDs emission peaks at 2.1 eV for InP; and from 1.9 eV to 2.2 eV for InP@ZnS QDs; also, we observed a decrease in the PL emission due to defects generated by the In2O3 formation. Charge carrier lifetime measurements for the nanoparticles of In2O3 were achieved, obtained with the time-resolved photoluminescence technique, indicating that the dominant mechanisms for recombination are the non-radiative recombination processes.

Keywords: Quantum dots, InP, InP@ZnS

[SEM-389] Photocatalytic degradation of bisphenol A by HAp/TiO2 composite

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Bisphenol A (BPA) is a compound used in the production of many common materials that can harm both humans and other organisms when released into the environment. BPA is of particular interest due to its use in the plastic industry and its capacity to act as an endocrine disruptor. Hydroxyapatite (HAp) has been widely studied due to its similarity with bone tissue and its biocompatibility. However, recent investigations have shown its potential use in adsorption and photocatalysis of emerging pollutants. In the photocatalysis field, TiO_2 has been widely researched for this purpose. For these reasons, the HAp/TiO_2 composite was synthesized by a mechanical method and tested in the photocatalytic activity against BPA. The HAp/TiO_2 composite was analyzed by X-ray diffraction (XRD), Raman spectroscopy, and diffuse reflectance spectroscopy (DRS). During the photocatalytic experiments, UVA light was used (λ=350 nm). The HAp/TiO_2 composite showed 92% of BPA total removal after 4 hours. Furthermore, the reusability of the composite was tested for 5 cycles. In these experiments, the composite showed a decrease in the photocatalytic activity, where 30% of total BPA removal was achieved in the last cycle after 3 hours of experiment. Finally, radical trapping experiments were conducted using isopropanol (IPA), p-benzoquinone (BQ), ammonium oxalate (OA), and silver nitrate ($AgNO_3$). Radical trapping experiments revealed that the superoxide radicals (O_2^-) were the major active specie responsible for BPA degradation. The present work shows that the HAp/TiO_2 composite is a promising material for photocatalysis.

Keywords: Photocatalysis, bisphenol A, hydroxyapatite, TiO_2, UVA light.
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[SEM-280] PROPERTIES OF CERIUM DIOXIDE THIN FILMS PREPARED DIP COATING METHOD

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Cerium dioxide thin films were deposited on corning glass substrates by dip coating method. The precursor solution was prepared by dissolving cerium nitrate in ethanol with lactic acid as stabilizer at room temperature. The as-deposited films were annealed at different temperatures from 250, 350 and 550 °C, in open atmosphere. The properties of cerium oxide thin films were studied by X-ray diffraction, UV-vis absorbance spectroscopy, and scanning electron microscopy. X-ray diffraction shows that all films annealed exhibit fluorite cubic structure. The UV-vis spectra show that all the films have high optical transmittance, ~75% in the visible region. The SEM image of the film annealed at 250 °C showed a smooth surface, homogeneous, and cracks free. When annealing temperature was increased at 550 °C the films exhibited a granular morphology.

Keywords: cerium dioxide, thin films, properties, dip coating.
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This work was supported by: NanoBiotechnology and Photocatalysis Laboratory (FI-UAQ).

[SEM-282] SOL-GEL PREPARED Cu2ZnSnS4 (CZTS) SEMICONDUCTOR THIN FILMS BY DIP-COATING

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The situations beneathneath which skinny movies are deposited (dip-coating approach) are the maximum essential parameter figuring out the bodily overall performance of devices. In this work, we gift the impact of preheating temperatures at the first-rate of Cu2ZnSnS4 (CZTS) skinny movies. Herein we're interested by the structural, morphological, and optical traits of CZTS layers, synthesized the usage of the sol-gel approach. CZTS layers have been deposited at preheat temperatures a 1-h. XRD outcomes affirm the dependence of the crystallite length on temperature. All the deposited layers are in stannite phase, the approach proposed right here may be used to deposited excessive first-rate absorber layers of CZTS for sun cells applications.

Keywords: CZTS thin films; sol-gel; annealing temperature; solar-cell.
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[SEM-343] Solvothermal synthesis of Zn0.5Hg0.5S, for reagent selection on the synthesis of the solid solution

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The ternary sulfide of zinc and mercury ($Zn_xHg_{1-x}S$), is a promising material that could be useful in a wide range of the electromagnetic spectrum (from 0.5 to 3.7 eV), with potential for several optoelectronic applications. Unfortunately, it has barely been studied, presumably due to the difficulties involved on its synthesis. The hydrothermal processing of different mixtures of the binary compounds, ZnS and HgS, varying nominal compositions, was reported in 1960, by Kremheller *et al.* (J. Electrochem. Soc. 107, 12). In this work, we propose a solvothermal process in methanol-water mixtures, using different combinations of reactant sources for zinc, mercury, and sulfur; and mixing the binary compounds, for comparison. Crystalline structure, morphology, and optical properties are explored, to determine the best suited reagents, for the synthesis of the full compositional range.
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[SEM-69] Structural and electronic properties of (CdTe)1-x(In2Te3)x films grown by RF sputtering *

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CdTe is a semiconductor widely employed in the production of solar cells and gamma ray detectors. Alloying with elements like sulphur, manganese, zinc, mercury, indium allows tailoring many of its electronic properties because the existence of their respective tellurates. In particular alloying CdTe with indium made possible to modify the band gap in the infrared range [1].
the compounds In_2Te_3 and $CdIn_2Te_4$ are compounds related to CdTe with a crystallographic structure in which sites in the structure have been identified as ordered vacancies.
$(CdTe)_{1-x}(In_2Te_3)_x$ thin films with a nominal composition in weight between $0 < x < 1$ have been deposited employing RF sputtering. Ten sputtering targets were produced mixing CdTe and In_2Te_3 in the right proportions. The films were deposited on glass substrates at 180 C using argon as working gas.
the produced $(CdTe)_{1-x}(In_2Te_3)_x$ thin films are uniform and were characterized to obtain chemical composition and structural and electronic properties.
Xray diffraction results indicate the presence of amorphous and crystalline phases which are associated with the incorporation of In in the CdTe structure. Transmission spectroscopy shown a band gap modulation between 1.1 and 1.46 eV.

[1] Zapata-Torres, M., et al. "Structural transition from CdTe to $CdIn_2Te_4$ in films grown by close paced vapor transport combined with free evaporation." *Thin solid films* 358.1-2 (2000): 12-15.

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[SEM-42] STRUCTURAL AND OPTICAL CHARACTERIZATION OF ZNO FILMS WITH TIO2 NANOPARTICLES DEPOSITED BY SCREEN-PRINTING.

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ZnO and TiO2 are metal oxides widely researched, produced, and consumed in various industrial sectors: food, health, electronics, and energy, but they are still materials of interest for their different properties such as n-type semiconductors with a favorable bandgap energy (ZnO: 3.37 eV and TiO2: 3.2 eV), thermal and chemical stability, biocompatible and non-toxic, accessible, abundant, and low cost. The screen-printing technique consists of transferring the material through a screen with small openings to deposit it on the substrate surface. Moreover, it is an easy, economical, and flexible production option in terms of design and materials used. The work aims to obtain ZnO films with different percentages (3%, 5%,10%) of TiO2 nanoparticles by screen printing to make it an easy, economical, and scalable option for the industrial sector. The paint is prepared by mixing ZnO with ZnCl2 both in powder form with a 12% W/V polyvinyl alcohol (PVA) solution, then this paint is deposited by screen-printing technique on Corning substrates and heat-treated at 500°C for 2hrs. The morphological and structural characterization was carried out by FESEM, and X-ray diffraction. The spindle and cuboidal morphology is observed and the crystalline phases present in the films are anatase and zincite. The measurement of the absorbance of the films allows to obtain the band gap energy value between 3.09 - 3.15 eV, the tendency is observed the higher the quantity of TiO2 nanoparticles the lower the band gap energy value.

Keywords: screen-printing, ZnO films, semiconductor.
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Reference: Adem Screedha et al., Novel composite ZnO/TiO2 thin films photoanodes for enhanced visible-light-driven photoelectrochemical water splitting activity. J. jelechem. 804 (2017) 92-98. http://dx.doi.org/10.1016/j.jelechem.2017.09.045.
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[SEM-391] STRUCTURAL AND OPTICAL PROPERTY CHARACTERIZATION OF CBD-CdS THIN FILMS STIMULATED BY DOPING WITH (Cu2+, Ag+, Au+) METAL IONS

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In this work, the modified crystalline structures of the cadmium sulphur nanostructured semiconductor (CdS) stimulated by doping with (Cu^{2+}, Ag^{+}, Au^{+}) metallic ions are studied. Thin films of good crystalline quality were obtained by chemical bath deposition, which were doped in synthesis without the need for additional steps with controlled thicknesses around 100 nm that were measured by ellipsometry. The binding energies of the CdS semiconductor compound and its interactions with the different transition metal ions were determined by X-ray photoelectron spectroscopy. The crystalline quality and phase of the CdS thin films were studied by X-ray diffraction, which were confirmed by Raman spectroscopy, obtaining that the dominant crystalline phase is zinc blende in the crystalline direction (111). By XRD, a change from monocrystalline structure to polycrystalline structure was observed in the doped CdS thin films, maintaining the zinc blende crystalline phase as dominant; this behaviour was confirmed by HRTEM micrographs in addition to the different levels of quantum confinement promoted by each incorporated transition metal. By Raman scattering confirmed the zinc blende crystalline 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.

[SEM-144] Synthesis and Characterization by Colloidal and Microwave process on MnSb2O6 nanoparticles.

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Trirutyl-type manganese antimonate ($MnSb_2O_6$) has been the subject of studies for many years, due to its excellent and interesting physical and chemical properties. However, recent investigations have been presented with this material for gas sensors. In this sense, the synthesis by means of a trirutyl-type $MnSb_2O_6$ with a solidified obtaining is carried out. The characterization and obtaining of its crystalline structure. Based on results obtained to give it a future application function in a gas sensor for medical applications. The method of colloidal sintering (sol-gel) during periods of 24 hours of agitation in a magnetic stirrer and in turn assisted to evaporation by microwave radiation (MW) at low power, based on economical experimentation with the use of tools. With the proper management of heating and homogeneous mixing in the nitrates used as precursors, a drying at different temperatures (210 °C and 150 °C) since different syntheses were carried out to observe changes. Subsequently, X-Ray Diffraction analyses were performed. The characterization was obtained by scanning electron microscopy (SEM) and transmission (TEM) studies.

Keywords: Trirutyl, MnSb2O6, precursors, crystalline structure, homogeneous mixing.

Reference: [1] A. Casillas-Zamora et al., "Synthesis of MnSb2O6 powders through a simple low-temperature method and their test as a gas sensor," Journal of Materials Science: Materials in Electronics, vol. 31, no. 10, May 2020, DOI: 10.1007/s10854-019-02700-3.

[SEM-77] Synthesis and characterization of Cr-doped TiO2 by sol-gel process

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Abstract: Undoped TiO_2 and Cr-doped TiO_2 thin films were prepared by the sol-gel dip-coating method using a titanium isopropoxide precursor and chromium (III) chloride hexahydrate as a source of Cr. Chromium concentrations varied for different molar ratios ranging from 2, 4, and 8 %. After thin film depositions on glass substrates at room temperature, the samples were post-annealed in the air at 450 °C for 60 min. The samples' structural, optical, and surface chemical properties were characterized by several techniques, including E.D.S., XRD, SIMS, Raman, UV-Vis, RT-PL, and XPS spectroscopies. The XRD patterns showed that all the films are polycrystalline with pure anatase structure and the crystallite sizes decrease with chromium doping.

Moreover, the anatase phase formation was confirmed from Raman spectra analysis. Concerning the optical properties of the samples, the UV-Vis absorption spectra showed a red shift in the absorption edge in the visible range, following the doping concentration of Cr. In addition, the RT-PL study revealed that the dopant incorporation causes a decrease in the P.L. intensity. The E.D.S. and SIMS analysis associated with the elemental composition of the samples showed that Ti, O, and Cr elements are present in the sample. On the other hand, from XPS measurements, the Ti^{4+} oxidation states of Ti 2p evidenced the formation of TiO_2.

[SEM-151] SYNTHESIS AND CHARACTERIZATION OF MgSbâ,,Oâ,† NANOSTRUCTURES BY COLLOIDAL METHOD ASSISTED BY MICROWAVE RADIATION.

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Currently, a large number of semiconducting oxides have been an interest of research as potential gas detectors, however, recent reports published highlight semiconducting oxides with trirutile-type structure as a strong candidate because of their chemical stability, physical characteristics and the temperature at which they can be handled. It is of great importance to control the size and shape of the trirutile particles for the response of different gases. Thus, it is necessary to study new synthesis techniques for more efficient microstructure control. The Chemical methods as sol-gel, bio-assisted synthesis, among others, are less expensive and allow better control of size and shape. In the present investigation, it was proposed to synthesize and characterize magnesium antimony (MgSbO) following a synthesis process using the colloidal method and the microwave radiation (MW) assisted solution route, since it is a fast, uniform and effective method, which allows increasing the kinetics reaction by one or two orders of magnitude. The Colloidal nanoparticles are synthesized from metal precursor salts dissolved in homogeneous solutions ranging from 2 ml to 5 ml of Ethylenediamine (CHN), with a drying of the solution at 200 °C and subsequently calcined, to analyze and compare by X-Ray Diffraction, the pattern of the MgSbOO oxide powders. The morphology and size of the nanoparticle was verified by scanning electron microscopy (SEM) and transmission (TEM).

Keywords: gas detectors,the MgSbO oxide powders colloidal method, trirutile structure, sencivity.
Corresponding author: andrea.gallegos4732@alumnos.udg.mx
Reference: [1]Alex Guillén Bonilla1*, Héctor Guillén Bonilla2, Verónica María. Rodríguez Betancourtt2, José Trinidad Guillen Bonilla3, Juan Pablo Morán Lazaro1, Mario Martínez García1, Juan Reyes Gomez4, Lorenzo Gildo Ortiz5.(2017)Síntesis y caracterización de nanoestructuras del mgsb2o6 para su potencial aplicación como detector de atmósferas de propano. Recuperado desde: https://iydt.files.wordpress.com/2018/02/4-5_sc3adntesis-y-caracterizacic3b3n-de-nanoestruc turas-del-mgsb2o6-para-su-potencial-aplicacic3b3n-como-detector-de-atmc3b3sferas-de-prop ano.pdf [2] Magaña R., J. Luis; Torres R., Ernestina; Martínez G., Martín T.; Sandoval Juárez, Carmen; Hernández Cantero, Rosalía (2006) Producción de Biogás a Nivel Laboratorio Utilizando Estiércol de Cabras. Recuperado desde: http://www.redalyc.org/articulo.oáid=41616204

[SEM-122] Synthesis and characterization of nanostructured barium antimoniate powders prepared by a wet chemical method.

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In recent years, nanomaterials have gained relevance due to their wide applications in science and industry. This work describes the preparation of barium antimoniate ($BaSb_2O_6$) nanostructures using a microwave assisted wet chemical method. To synthesize this semiconductor oxide, the reagents —antimony trichloride ($SbCl_3$) and barium nitrate ($Ba(NO_3)_2$)— as well as the chelating agent (ethylenediamine), were dissolved in ethyl alcohol. From this, three solutions were obtained, which were then mixed and left stirring for 24 hours at room temperature. Afterwards, the solvent was evaporated using low-power microwave radiation until a precursor paste was obtained, which was then dried at 200 °C for 8 hours [1]. The product was subsequently calcined at 800 °C and characterized using X-Ray diffraction. This analysis led to the discovery of an hexagonal crystal structure with cell parameters a = 5.303 Å and c = 5.758 Å, and a P-31m (162) space group. By scanning electron microscopy (SEM) and transmission electron microscopy (TEM), there were also discovered nano-plates (0.70 – 4.00 µm) and particles with a medium size of 2.00 ± 0.704 µm. In conclusion, the synthesis method used was successful for obtaining micro and nanometric-sized particles.

Keywords: trirutile; $BaSb_2O_6$; nano-plates; semiconductor.

Reference: [1] V. M. Rodríguez-Betancourtt, and H. Guillén-Bonilla, and J. T. Guillén-Bonilla, and Y. L. Casallas-Moreno, J. A. Ramírez-Ortega, and J. P. Moran-Lázaro, and M.L. Olvera-Amador, and A. Guillén-Bonilla, *Synthesis, characterization, and sensitivity tests of a novel sensor based on barium antimonate powders*, J. Materials Today Communications. 31. (2022). https://doi.org/10.1016/j.mtcomm.2022.103579

[SEM-382] Synthesis of MoS2@TiO2 heterostructures and study of photocatalytic activity under visible light irradiation

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The photocatalysis mechanism is an important method that helps remove organic compounds from dyes in contaminated water. A semiconductor that has potential properties to make the photocatalytic mechanism is titanium dioxide (TiO_2). However, the material has limitations. In this work the authors develops a synthesis route based on TiO_2@MoS_2 coupled heterostructures through the hydrothermal technique. The main objective is the study of the effect of MoS_2 on TiO_2 in the photocatalytic activity with different concentrations 0,25% , 0.5%, 1.5%, 2.5% by weight. The samples were characterized by Raman spectroscopy, X-ray diffraction (XRD), Fourier-transformed infrared spectroscopy (FT-IR), UV-vis-NIR spectroscopy. The results of the X-ray diffraction were analyzed by the Rietveld method, and the data from the UV-vis diffuse reflectance spectroscopy were analyzed using the tauc graphic method to obtain the concentration correlation with the band gap in each sample. Photocatalytic activity was measured under visible light irradiation.

Keywords: Semiconductor, TiO_2, photocatalysis, visible ligth, hydrothermal.
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[SEM-367] Synthesis of chalcogenide-based nanocomposite thin films by combining laser ablation of solids in liquids and chemical bath deposition

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In the present work, the development of a novel thin film deposition technique based on the combination of the laser ablation of solids in liquids and chemical bath deposition is presented. Colloidal nanoparticle suspensions synthesized by laser ablation of solid semiconductor or metallic targets in water are used as solvent in chemical bath solutions for the deposition of chalcogenide nanocomposite thin films.

Two different systems were studied; CdS-n-Si and Sb_2S_3-n-Cu, where n-Si and n-Cu stand for silicon and copper nanocrystals respectively. CdS and Sb_2S_3 are well known for their use as window (CdS) or absorber (Sb_2S_3) layers in thin film solar cells. Thus, combining these chalcogenides with nanocrystalline particles can result in enhanced physical properties for the nanocomposite systems.

The physical properties of the fils were studied by UV-Vis and Raman spectroscopies, X ray diffraction, Transmission Electron Microscopy, Photoluminescence spectroscopy. Results indicate that Si or Cu nanocrystals can be succesfully introduced to the chalcogenide matrix enhancing their properties. Results are discussed as a function of the volume fraction content of the colloidal suspentions in the aqueous bath solutions.

[SEM-4] SYNTHESIS OF TUNGSTEN TRIOXIDE BY THE MODIFIED COMBUSTION METHOD WITH POTENTIAL APPLICATION IN THE ADSORTION OF COLORANTS

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Tungsten trioxide (WO_3), also known as tungsten oxide (VI) or volphramic anhydride, is a naturally occurring material in the form of hydrates, which include minerals such as tungstite (WO_3H_2O), meymacita (WO_3)$2H_2O$) and hydrotungstite (of the same composition as meymacita). WO_3 has several uses, among which it stands out as a pigment in the ceramic and paint industry, in the manufacture of tungstates for X-ray screens, as a gas sensor, as a photocatalyst for degrading dyes in wastewater, among other applications.

Due to the diverse applications of WO_3, the synthesis of this material consist in the recovery of tungsten from incandescent waste bulbs. The filament of the bulbs is made of pure tungsten, it is possible to recover it and at the same time it contributes in the decrease of the waste of bulbs disposed in landfills which contaminate the water, soil and air. The conventional industrial method to obtain WO_3 uses dangerous reagents and long reaction times. Here, we report a novel method called Gelification-Modified Combustion, which is a simple method that does not use hazardous materials since they are used as organic acid fuels (urea, alanine and glycine) and metal nitrates to synthesize metal oxides, this method also uses short reaction times (approximately 5 minutes).

The material obtained was a lemon-yellow powder, which presented the physical appearance of the material of interest. The powders obtained were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). X-ray diffraction (XRD) technique was used to determine the molecular structure of the crystals and identify the various phases obtained, we also performed a scanning electron microscopy (SEM) analysis to obtain information about the morphology and surface texture of the particles, the size distribution of the crystals and the composition of the samples synthesized.

Keywords: Tungsten Trioxide, Modified Combustion Method, Synthesis.

[SEM-146] SYNTHESIS OF ZINC ALUMINATE OXIDE (ZnAl2O4) BY METHOD OF MILD CHEMISTRY AND ITS MICROSTRUCTURAL CHARACTERIZATION.

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In this work, spinel-type zinc aluminate oxide nanoparticles $ZnAl_2O_4$ [1] were synthesized for subsequent application as a sensor for propane (C_3H_8) and carbon monoxide (CO) polluting gases. This compound was synthesized through a simple and economical synthesis method, colloidal (sol-gel) assisted by microwaves (MW). In this case, zinc nitrate hexahydrate $Zn(NO_3)_2{\cdot}6H2O$ and aluminum nitrate nonahydrate $Al(NO_3)_3{\cdot}9H2O$ were used as precursors for the synthesis of the compound. The material obtained was dried and calcined at different temperatures in order to evaluate the crystalline evolution of the $ZnAl_2O_4$ compound. Subsequently, a microstructural analysis was carried out using scanning electron microscopy (SEM) and transmission electron microscopy (TEM), as well as the determination of the value of the band gap by ultraviolet visible spectroscopy (UV-vis). In any case, the microstructural characteristics and the nanometric size of the particles give it sensing properties so that the $ZnAl_2O_4$ material can be applied as a detector of polluting atmospheres.

Keywords: The $ZnAl_2O_4$; Spinel-type; Sensor; Microwaves MW; Nitrates.

References: [1] S. Battiston *et al.*, “Synthesis of zinc aluminate (ZnAl2O4) spinel and its application as photocatalyst,” *Materials Research*, vol. 17, no. 3, May 2014, doi: 10.1590/S1516-14392014005000073.

[SEM-149] The oxide NiSb2O6 applied to develop a new digital propane detector

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In this work, the NiSb2O6 powders were prepared through the microwave-assisted colloidal method. In the synthesis was used 1.4560 g de Ni(NO3)2•6H2O (Mallinckrodt Beker, 99%), 2.2802 g of SbCl3 (Sigma-Aldrich ≥ 99%) y 0.5 mL of ethylenediamine (Sigma-Aldrich ≥ 99%). The procedure was done based on the reference [1]. The Pellet was built using the NiSb2O6 powders and the following were electrically characterized through static test. During the characterization, the operating temperature was of 200oC and the propane concentration was of 1, 5, 50, 100, 200, 300, 400 and 500 ppm.

Analyzing the electrical response was built a Wheatstone bridge whose output voltages were connected to the analog input of a PIC16F887A. The digital device was programmed to detect the propane concentration of 5 ppm but the detection concentration can be changed using a keyboard. Whereas, a LCD display is used to indicate that the sensor detected the presence of propane gas in atmosphere.

Our device possesses low cost, versatility, high sensitivity, good performance, fast response, selectivity, adaptability, propane (C3H8) concentration detection between 1 and 500 ppm and operating temperatures of 200oC.

Keywords: The NiSb2O6 powders; Propane concentration; Digital device; High sensitivity; Fast response.

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Reference: [1]. V. M. Rodríguez Betancourtt, H. Guillen Bonilla, M. Flores Martínez, A. Guillen Bonilla, J. P. Moran Lazaro, J. T. Guillen Bonilla, M. A. González and M de L. Olvera. Gas sensing properties of NiSb2O6 micro- and nanoparticles in propane and Carbon monoxide atmospheres. Journal of materials, Vol 2017, Article ID 8792567, 9.

[SEM-338] THIN FILMS ZnO NANOPARTICLES PREPARED BY COLLOIDAL ROUTE AND ITS OPTICAL AND STRUCTURAL PROPERTIES STUDY.

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We investigate the morphological, structural, and optical properties in thin film ZnO prepared by colloidal synthesis. The samples were prepared at different crystal growth temperatures (~60-210 °C ± 4°C), maintained the parameters constant in the crystal growth. The ZnO nanoparticles size/shape evolution were systematically studied by Scanning Electron Microscopy (SEM), X-ray diffraction (XRD), Photoluminscence (PL). SEM images show crystalline and disperse agglomerates associated with the temperature of crystalline growth. XRD measurements confirm the hexagonal phase wurtzite type and crystallite size average of ~4.2-6.3 nm. The transmittance studies display ~80% of transmission and a relative maximum shift located at ~402-378 nm. The band gap obtained using Tauc model, is evaluated at ~3.08-3.26 eV. PL signals show emission bands with different intensities: blue (YB), green (GE), yellow (YE) and red (RE) bands, situated at vis-region, and commonly associated with color points produced by vacancies and interstices crystalline.

Keywords: ZnO, thin films, visible emission, colloidal synthesis, crystalline defects.
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[SEM-351] Towards optoelectronics based on transition metal dichalcogenides produced by liquid exfoliation

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Two-dimension materials such as graphene or transition-metal dichalcogenides (TMDs) are strong candidates for optoelectronic applications due to their exceptional properties. TMDs monolayers are direct semiconductors, a few atoms thick, chemically stable at room temperature, they have very strong optical absorption, and possess electronic degrees of freedom not available in regular semiconductors such as spin coupling to the wavevector, unrestricted capabilities to form heterostructures from the point of view of lattice matching (since the 1D layers couple to each other only through van der Waals forces, not covalent bonds), wide tunability of their bands due to strain and due to the formation of microscopic moiré patterns. They seem thus to be ideal to be the main components of ultra-compact optoelectronic devices with novel functionalities working at room temperature. In this work, we demonstrate the efficient production of TMDs monolayers of high crystalline quality and size of a few hundred nanometers by liquid exfoliation (LE) using a solution of ascorbic acid and water. LE is suitable for applications where it is necessary to cover large substrate areas with material. While other techniques such as to CVD or mechanic exfoliation, for example, can produce monolayers of tens or even hundreds of micrometers, LE is a much simpler technique which allows to deposit the active material on any substrate simply by drop-casting. An inherent drawback of LE is the presence of solvent residues which are difficult to remove and affect the electronic properties of the material or post-fabrication processes. Our technique based on the use of ascorbic acid, water and ethanol allows to completely get rid of such residues. This opens the way to the use of TMD obtained by liquid exfoliation in optoelectronic applications such as microcavity-based devices.

Keywords: 2D materials, transition-metal dichalcogenides, liquid exfoliation
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[SEM-329] VERTICALLY STACKED MoS2-ReS2 AND ReS2-MoS2 HETEROSTRUCTURES FOR BROADBAND PHOTODETECTION

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Molybdenum disulphide (MoS_2) and rhenium disulphide (ReS_2) are members of transition metal dichalcogenides (TMDs) family which has shown great potential for diverse applications in electrical, optical and quantum devices due to its intrinsic mobility, direct band gap and electronic structure. We present a study of the structural and optical properties of vertical MoS_2-ReS_2 and ReS_2-MoS_2 heterostructures (HS) grown by chemical vapor deposition (CVD) for broadband photodetection. A two-step CVD process was used to form the HS: first, MoS_2(ReS_2) monolayer crystals are grown in a CVD chamber at 750 °C on SiO_2/Si substrates, then the sample is introduced in a second CVD chamber to perform ReS_2(MoS_2) growth. Optical and SEM images show the formation of vertical MoS_2-ReS_2 and ReS_2-MoS_2 HS. Raman spectra performed on the vertically stacked HS show the typical A_{1g} and E' Raman bands of both materials with any significant shift suggesting a strong interlayer coupling. Moreover, photoluminescence measurements reveal the presence of both materials only when MoS_2 is stacked on ReS_2. Finally, the optoelectronic characterization was performed to understand the band structure with carrier migration mechanism of both heterojunctions. We demonstrate that for ReS_2 on MoS_2 the responsivity reaches 80 A/W for visible light illumination, whereas the responsivity drops to 14.12 A/W when MoS_2 is on top of ReS_2. These measurements along with UPS complementary data, indicate that ReS_2 stacked on MoS_2 results in a type I heterostructure with efficient light adsorption and rapid charge transfer. The responsivity of these devices fabricated with materials grown by CVD is reasonably high compared with devices using low-end technique.

[SEM-336] ZnO NANOPARTICLES SYNTHESIS BY ASSISTED MICROWAVE IRRADIATION AND ITS APPLICATION IN PHOTOCATALYSIS.

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In this work, a microwave system was used to synthetize ZnO nanoparticles trough colloidal route. Several microwave irradiation times were chosen (2, 3, 4 min) to study its influence on the structural, optic, and morphological characteristics. These nanoparticles exhibited a hexagonal structure wurtzite type with a crystallite size of 5 nm. SEM images showed the agglomerates (2, 3 min), agglomerate/threads (4 min) formation. EDS analysis revealed oxygen excess for the nanoparticles obtained after 2 and 4 min of reaction, which are according with the PL results. After synthesis and characterization, the ZnO nanoparticles were used to study the methylene blue dye photocatalytic degradation under direct sun. The nanoparticles photocatalytic activity was monitored by UV-Vis absorption spectra. The results exposed high efficiency (95 %) in methylene blue degradation after 70 min for the nanoparticles synthesized at 4 min. This degradation percentage was associated to the high surface defects presented on the nanoparticles (i.e.; O_i, Vo) which are direct responsible to the emission and absorption in the visible range as it is observed in photoluminescence spectrum (PL). These defects can be increased simply by controlling the nanoparticle size, which can be confirmed by XRD and correlated to the PL measurement.

Keywords: ZnO, photocatalysis, sun-irradiation, nanoparticles, microwave system.
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Sesión Oral

[SEM-174] BISMUTH OXYHALIDE SEMICONDUCTORS (BIOX, X = Cl, Br, I): PHYSICAL PROPERTIES AND VISIBLE-LIGHT PHOTOCATALYTIC DEGRADATION OF RHODAMINE B

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Recently, bismuth-based semiconductors have gained attention as photocatalytic materials with extremely low toxicity and good chemical and physical stability. They have been used in many applications, including water splitting, degradation of organic and inorganic pollutants, and even in solar energy conversion. In particular, bismuth oxyhalides (BiOX, X = Cl, Br, I) are a new kind of layered materials promising to work under visible light in photocatalytic processes [1]. In this work, we present the synthesis and characterization of BiOX, (X = Cl, Br, I) through precipitation method. Their structural properties were studied by X-ray diffraction, and Raman spectroscopy. Morphology properties were studied by electron microscopy and their optical properties were analyzed by UV-Vis spectroscopy. In addition, we studied the photocatalytic activity in degradation of rhodamine B (RhB) under visible light conditions. Results showed that our BiOX compounds were successfully synthesized (no secondary phases detected). The as-prepared samples exhibited high photocatalytic activity for the degradation of RhB dye.

Keywords: photocatalysis, bismuth semiconductors, rhodamine B
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Reference: [1] V. Meng, and Z. Zhang, Bismuth-based photocatalytic semiconductors: introduction, challenges and possible approaches. *J. Mol. Catal. A: Chem 423* (2016) 533-549. http://dx.doi.org/10.1016/j.molcata.2016.07.030
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[SEM-59] Cu-Sn-(S,I) thin films via rapid iodization of hybrid stacked Cu/SnS layers for photovoltaic applications

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Thin films of the Cu-Sn-S system have been investigated for photovoltaic applications due to their properties and abundance of their elements. In this work, we synthesized Cu-Sn-(S,I) thin films (CTSI) by iodization of hybrid Cu/SnS layers. Cu layer was thermally evaporated on chemically deposited SnS thin films, annealed in vacuum atmosphere and finally subjected to rapid iodization. Structure, morphology, chemical composition, optical and electrical properties were evaluated using XRD, Raman spectroscopy, XPS, X-EDS, SEM, AFM, UV-Vis-NIR spectroscopy and hall effect measurements. X-ray diffraction analysis revealed highly crystalline nature of thin film. Raman spectroscopic analysis was employed to detect amorphous phases in the films. Compact uniform surface morphology reveled by scanning electron microscopic imaging and atomic force microscopy. Synthesized films exhibited high absorption in visible region and suitable bandgap for photodetector and solar cell applications. Photo response behavior under light source of different wavelength were assessed in order to evaluate suitability for photodetector applications. Photovoltaic structure of FTO/CdS/CTSI/Ag was fabricated, and photovoltaic parameters were evaluated. Cu-Sn-(S,I) thin films can produce profound advances in low cost, stable, earth abundant and non-toxic materials for optoelectronic applications

Keywords: CTSI thin films, Novel seminconductors, photovoltaics

[SEM-441] Development of a solvent detector based in a MIS capacitor of mesoporous silica.

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Currently, there is an emergent necessity to develop devices for solvent detection such as toluene, benzene, acetone, ethanol, and dimethylformamide, in other words, substances that could have been the origin of industrial accidents or contamination. Numerous materials are reported in the literature for the solvent's detection as carbon nanostructures and porous materials as MOFS (metal-organic-frameworks). In this research work, a MIS capacitor structure based on mesoporous silica (MCM-41) is used to detect protic, aprotic polar solvents, and nonpolar solvents. The detection of the solvents was made through the evaluation of capacitance-voltage characteristics. Our results correlated with molecular simulations using density functional theory (DFT) and electrical parameters. The surface of the MCM-41 is more sensitive to methanol than the other nonpolar solvents. These results suggest that it is possible to develop a solvent sensor using this low-cost MCM-41 MIS capacitor.

Keywords: MIS capacitor, mesoporous silica, detector, solvents

[SEM-145] Evaluation of InGaN/GaN heterojunction photo detection obtained by PEALD

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A good performance of n-GaN/n-Si y n-InGaN/n-Si heterojunction photodetector was investigated. Both semiconductors materials, InGaN and GaN ultrathin film heterostructure, were growth at 300 °C on Si substrates using atomic layer deposition. The band gap and crystal structure were analyzed by Uv-Vis spectroscopy and XRD technique, the InxGa1-xN and GaN optical band gaps were calculated 3.15 eV and 3.35, respectively. The rise time device exhibit high photoconductivity and responsivity 0.238 W/cm and 706 W/cm respectively and short rise/fall time of this InGaN and GaN thin film photodetector has potential application in photoelectronic devices.

Keywords: Photodetector, ultrathin film, heterostructures, atomic layer deposition
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[SEM-13] Evaluation of nanoindentation characteristics of cubic InN epilayer 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 paper, the load-displacement curves of cubic indium nitride (c-InN) obtained during the nanoindentation with a Berkovich indenter were investigated. c-InN was 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 properties of the material studied. The c-InN thickness is around 180 nm. The reflection high energy electron diffraction and the X-ray diffraction results show that the c-GaN buffer and c-InN grown layers had a high cubic zincblende phase with more than 99%. The obtained values of the hardness are 12.5 ± 0.4 GPa, and the values for Young's is 365.5 ± 7 GPa with a Poisson's ratio of 0.3.

[SEM-324] Monolayer MoS2/SnS2 QuantumDot-Based Mixed-Dimensional Photodetector

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In this work, a mixed-dimensional 0D/2D SnS2-QDs/monolayer MoS2 hybrid is fabricated for high-performance and broadband (UV−visible−near-infrared (NIR)) photodetector. Monolayer MoS2 is deposited on SiO2/Si using chemical vapor deposition (CVD), and SnS2-QDs are prepared using a low-cost solution-processing method. The high performance of the fabricated 0D/2D photodetector is ascribed to the band bending and built-in potential created at the junction of SnS2-QDs and MoS2, which enhances the injection and separation efficiency of the photoexcited charge carriers. The mixed-dimensional structure also suppresses the dark current of the photodetector. The decorated SnS2-QDs on monolayer MoS2 not only improve the performance of the device but also extends the spectral range to the UV region. Photoresponsivity of the device for UV, visible, and NIR region is found to be ~278, ~ 435, and ~189 A/W, respectively. Fabricated devices showed maximum responsivity under the visible region attributed to the high absorbance of monolayer MoS2. The response time of the fabricated device is measured as ~100 ms. These results reveal that the development of a mixed-dimensional (0D/2D) SnS2-QDs/MoS2-based high-performance and broadband photodetector is technologically promising for next-generation optoelectronic applications

Keywords: MoS2 monolayer, 2D-0D integration, broadband photodetector
References: ACS Appl. Mater. Interfaces 2022, 14, 13, 15415–15425
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[SEM-379] Nanostructured antireflective coatings for GaAs solar cells

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Nanostructured antireflective coatings for GaAs solar cells

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The solar cells based on gallium arsenide have achieved historical high efficiencies, among the current solar technologies. This material presents a direct band gap which enables a larger conversation efficiency, which is directly related to the Shockley-Queisser recombination's processes. However, this material is more scare and costly than silicon, which is nowadays the most mature and commercialized technology on the market. For this reason, the optimization of the solar absorption using less amount of GaAs material, is a key issue to move this technology towards real markets. Optical engineering tools, such as the use of antireflective coatings remains a strategy that could increase by huge amounts the GaAs solar cells' performance. However, careful design of them is required to guarantee a proper performance. In this study, the author numerically evaluates the optical properties of nanostructured GaAs surfaces, with the aim to optimize its shape and size for antireflective purposes [1]. In this study, the very basic concepts of TE and TM polarization modes of these types of nanostructures are addressed, to design a correct antireflective coating for the GaAs surfaces. GaAs exhibit an optical anisotropy (related to the TE to TM modes) which cause huge losses of the unpolarized solar irradiation, mainly caused by the TE mode. A full study of the nanostructure dimensions is performed to quench such optical anisotropy. Numerical results unveil that the losses induced by the TE mode can be drastically vanished.

Keywords: antireflective coatings, moth-eye nanostructures, technology computer aided design
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Reference: [1] S. A. Boden, and D. M. Bagnall, "Tunable reflection minima of nanostructured antireflective surfaces," Appl. Phys. Lett. 93, 133108 (2008).

[SEM-7] Novel THz emitters based in InGaAs graded layers grown by MBE for telecommunication applications

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Communications have been the basis of great technological advances, without which the world of today would be completely different. This area has rapidly evolved over the years becoming faster and more effective. However, the increasing and incessant requirements for instant information have forced worldwide researchers to develop new technologies that may allow access to information of any kind at the instant. In this direction, THz technologies have been envisioned with the potential to provide the new devices working at higher communication speeds in the near future, and to achieve this goal novel THz radiation emitters are demanded. This work presents novel THz emitters based on InGaAs/GaAs alloys grown in gradual concentration steps by the molecular beam epitaxy (MBE) technique. It is demonstrated that these devices exhibit higher emission compared to those emitters based on photo-conductive antennas. The two main effects responsible for the emission are the ballistic transport of the carriers which acquire the kinetic energy from the energy difference between the excitation radiation and the band-gap, and the second effect is the acceleration of the electrons, which is improved by the modification of the surface electric field caused by the band-bending in the metamorphic layer. To assure the ballistic transport it is important to maintain high crystalline quality throughout the growth of the layer, and it implies having a low density of dislocations, which is not an easy task considering the 7% mismatch between the materials InAs and GaAs. Consequently, MBE appears as the preferred technique to synthesize these samples. Additionally, to prompt carriers' acceleration, we propose novel designs on the emitter structure comprising concave and convex concentration profiles. We observe that the emission of these devices is twice higher than the conventional GaAs THz emitters.

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[SEM-44] Quantification of wz-inclusions in zb-GaN grown by PAMBE on GaAs by x-ray pole figures

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The group of III-nitride semiconductors in the zincblende (zb) phase is a promising alternative to solve the problems in optoelectronics caused by polarization fields across devices fabricated using the more common wurtzite (wz) phase. However, zincblende nitrides suffer from wurtzite inclusions due to their metastable nature. It is therefore essential to quantify the amount of these inclusions if highly crystalline zincblende films are to be obtained. X-ray diffraction (XRD) allows quantifying the volume ratio between two phases by analyzing the intensities of reflections from the two said phases. Although this is mainly used for randomly oriented samples, it can also be applied to single-crystalline materials through the measurement of pole figures [1]. This work analyzed zb-GaN samples grown through molecular beam epitaxy (MBE) on (001)-GaAs substrates with XRD. Pole figures of the wz-(103) and zb-(113) were taken from each sample in a Rigaku SmartLab multipurpose system using the in-plane geometry. The figures obtained were corrected for absorption and background using the Rigaku 3D Explore software. Additionally, defocus corrections were carried out using a Si-powder reference sample. Once corrected, the integrated intensity was computed from the figures, and the ratio between the two was obtained, considering the structure factor, multiplicity, and diffraction angles for each reflection. The patterns of the pole figures obtained categorically confirm the presence of the zincblende phase in all samples when compared to simulations. However, the wurtzite phase is also shown to appear in varying percentages across the different samples. XRD pole figures have been proven as a powerful technique to analyze wz inclusions in zb-GaN samples grown by MBE on GaAs. They allow qualitative analysis using the pattern. Additionally, quantitative studies can be carried out to analyze phase ratios in a mixed crystal.

Keywords: XRD, Phase purity, Pole figure, Zincblende GaN, MBE growth
Reference: [1] M. Frentrup, L.Y. Lee, S.L. Sahonta, M.J. Kappers, F. Massabuau, P. Gupta, R.A. Oliver, C.J. Humphreys, D.J. Wallis, X-ray diffraction analysis of cubic zincblende III-nitrides, J. Phys. D. Appl. Phys. 50 (2017). https://doi.org/10.1088/1361-6463/AA865E.

[SEM-103] SIMS ANALYSIS OF METAL-HALIDE PEROVSKITE

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Despite the results already obtained on the efficiency of perovskite solar cells exceeding 20%, there remains the problem of high instability of perovskites in contact with air and ultraviolet radiation. The solution of this problem and the improvement of the electrical and optical characteristics of thin films of perovskites is impossible without a comprehensive analysis of the material, including chemical and structural analyses. In this paper, we performed a three-dimensional analysis of thin films of $CH_3NH_3PbI_3$ perovskite using a time-of-flight mass spectrometer. Perovskite films with a thickness of about 200 nm were grown by spin-coting on glass substrates under different growth regimes. Depth profiling analysis showed a uniform distribution of the main elements over the thickness of the film, except for a thin near-surface layer (about 10-20 nm). We did not find diffusion of any elements from substrate for all analyzed samples. The analysis of the mass spectrum allows us to conclude about the ionic nature of the bond in perovskite. Herewith the formation of secondary ions is described within the framework of the bond breaking model. With an increase in the annealing temperature above 100°C the appearance of a second chemical phase in perovskite, defined as PbI_2, is observed in the surface chemical map analysis mode. The formation and growth of the relative concentration of this phase was confirmed by XRD as well. It looks the detected phase separation is one of the reasons for the instability of perovskites over time. Analysis of the mass spectrum in the region of light ions showed that the interaction of accelerated ions with perovskites does not occur the same way as with silicon-type semiconductors: an additional mechanism of ion sputtering (additional to cascade sputtering) is observed, which has yet to be clarified.

Keywords: Perovskite, Spin Coating, TOF-SIMS, Phase Separation
Authors thank to M.Sc. Adolfo Tavira Fuentes (SEES, Cinvestav) for XRD measurements.

[SEM-272] SYNTHESIS AND CHARACTERIZATION OF ZrO2 THIN FILMS WITH HYDROPHILIC PROPERTIES

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ZrO_2 films were prepared by sol gel-dip coating method, the solution was prepared using zirconium n-propoxide $Zr(OCH_3)_4$ as precursor and ethanol as the solvent. The deposited films were then annealed at 250 °C, 450 °C, and 550 °C for 1 h. The influence of annealing temperature variation on the hydrophilic properties of the thin film was characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR); and Photoluminescence (PL). X-ray diffraction results reveled that ZrO_2 films annealed at 450 °C and 550 °C show the formation of tetragonal phase, with layers constituted by nanoparticles with average particle size of 21 nm and 25 nm, respectively. All deposited ZrO_2 thin films presented a high optical transparency, with an average transmittance above 70% in the visible range (400–700 nm). The hydrophilic properties of ZrO_2 films were characterized by means of the measurements of the contact angle. When theZrO2thin films; hydrophilicity; annealing temperature; sol-gel sample was annealed at 550 °C, the hydrophilicity reached the best behavior, which was explained as an éect of the structural and morphological change of the films.

Keywords: ZrO_2 thin films; hydrophilicity; annealing temperature; sol-gel.
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[SEM-26] OPTICAL AND ELECTRICAL CHARACTERIZATION OF ORGANICS PHOTODIODES WITH POLYMER P3HT AND FULLERENE PCBM C61 SENSITIVE IN NIR

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The new technologies of flexible electronics allow to have synthetics materials such as poly(hexylthiophene) and carbon derivatives as an option in the design and building of optoelectronic devices. The purpose to have such options of optical sensors on this work is to introduce a bulk heterojunction for building organic sensors in the NIR constructed from this bulk heterojunction on flexible substrates of indium tin oxide, using polymeric materials as a semiconductors and low melting point metal contacts such as indium gallium (InGa) alloy and some metals as Ag, Ni. The performance of organic photodiodes of poly(hexylthiophene) P3HT and fullerene phenyl-C_{61}-butyric acid methyl ester (PCBM) can be determined by its optical and electrical characterization, which are carried out using I-V curves and UV VIS spectroscopy on these devices to observe the displacement of the curve as well as the average transmittance to visualize the possibility of obtaining a sensor in the near infrared region. The optical behavior of the polymer is discussed in the visible spectrum as well as the dark electrical response of the bulk heterojunction and as a function of the incident wavelength above the device. We can observe that the P3HT transmits from the infrared up to about 600nm while the $PC_{61}BM$ has not contribution on the visible spectrum. regarding the electrical characterization I-V, we can find that the photogenerated currents has a lineal shift when the incident wavelength increases, and we approach to the near infrared region. We conclude that the organic photodiodes constructed with these materials serves as optical sensors in the NIR, since their transmittance increases from 600nm to the near infrared region, as well as the shift in the photogenerated current in the I-V curve is lineal as the wavelength approaches to that region.

Keywords: Bulk Heterojunction, Organic Photodiodes, Polythiophene, Photogenerated Currents, Near Infrared

Hrostea, L., Girtan, M., Mallet, R., & Leontie, L. (2018, June). Optical and morphological properties of P3HT and P3HT: PCBM thin films used in photovoltaic applications. In IOP Conference Series: Materials Science and Engineering (Vol. 374, No. 1, p. 012015). IOP Publishing.

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TRIBOLOGY, SURFACES AND INTERFACES

CHAIRMEN

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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.

[SIT-56] AlN THIN FILMS DEPOSITED BY A HYBRID PLASMA SYSTEM

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A hybrid plasma resulting from a combination of a stationary microwave ECR (with magnetic field) discharge, and a pulsed laser ablation plasma was used to deposit aluminum nitride (AlN) thin films. The hybrid plasma was created at a working pressure of 6 x 10^{-4} Torr. The use of the hybrid plasma allowed efficient laser ablation at low working pressures. Different samples were deposited varying the laser power density on the aluminum target. The variation of this power produced ions of different mean kinetic energy (E_k) of the laser ablation plasma. The values of the mean kinetic ion energy were determined using a Langmuir planar probe and was used as the working parameter. The composition of the AlN thin films was measured using the XPS technique. The measurements showed that the oxygen content in the films was as low as 2.5 at%, and most of the bonds between Al and N corresponded to that of the AlN. The band gap of the samples was determined as a function of the E_k of the laser ablation plasma and was observed to vary between 5.4 and 5.85 eV. Nano indentation measurements showed a variation of the hardness of between 23 and 30 GPa as a function of E_k. The wear rate and friction coefficient were evaluated on samples deposited under different values of E_k, using a reciprocating tribometer.

Keywords: AlN thin films, microwave plasma, laser ablation, mechanical properties, tribological properties

[SIT-76] Duplex Boriding-Nitriding treatment on AISI 8940 steel

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Using an AISI 8940 steel used for engineering components in the metal-mechanical, aeronautical, naval and automotive industries; a novel surface coating is formed by means of a duplex Pack Boriding-Gas Nitriding treatment. The characterization of the obtained coating was performed by optical microscopy, Vickers Microhardness test and X-ray diffraction (XRD). Then, by means of Three-point bend test, the effect of the coating formed on the steel under study was evaluated. The results showed a duplex coating type Fe_3N/FeB+Fe_2B. The microhardness measured on the Fe_3N/FeB+ Fe_2B coating shows microhardness change on iron nitride and iron borides. This innovative study by boriding pack-nitriding gas evidences a duplex coating for possible engineering applications.

Keywords: Boriding, nitriding,duplex treatment.

[SIT-75] Evaluation the mechanical properties of nylon-carbon fiber filament.

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3D printing has represented a technological breakthrough for the manufacturing industry, generating the search for new materials with variable internal geometries and different percentages of filler that can be used in the creation of functional parts, currently there are 3D printers capable of processing materials for industrial use, highlighting materials with carbon fiber, Peek, among others. In the present work, the behavior of the Nylon-carbon fiber material subjected to tension under ASTM D63802a standard is studied, the samples were printed on a flashforge creator 3 machine with extrusion temperature of 270°C, bed temperature of 120°C, printing speed of 50 mm/s. In filling conditions 20% of material with a 3D filling pattern and with samples with moisture, oven dried samples at 3h at 80°c and oven dried samples 3h at 80° coated with primer. The tests were performed on a Shimadzu Authograph AG-100K universal testing machine with a speed of 5mm/min.

[SIT-225] Initial stages of the oxidation of manganese

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Manganese and its oxides are widely applied in surface-engineered materials for catalysis and corrosion. It is well known that these materials have unusual chemical and physical properties. Although XPS is the technique of choice for these surface-related applications, very few studies have been done on metallic manganese and its oxides using this spectroscopy. This is probably due to the high level of complexity of the Mn 2*p* spectra caused by the asymmetry of its signals, intricate multiplet splitting, and strong background. In this work, Angular Resolved X-Ray Photoelectron Spectroscopy (ARXPS) data from Mn 2*p* and O 1*s* of the early oxidation stages are analyzed. Metallic manganese deposits were carried out by sublimation on a clean silicon wafer in UHV conditions (1.0×10^{-7} Torr) and oxidized by a controlled flow of ultra-high purity oxygen for set times. To reproduce the angular dependence, it was necessary to extend the oxidated layer model to include protrusions. The Mn 2*p* metallic spectrum was fitted using a double-Lorentzian asymmetric line-shape for the principal peak and Gaussian line shapes for the multiplet satellites and plasmons.The analysis of the oxidized samples was based on the *Block Approach* which allows for the subtraction of the metallic contributions of the spectrum, and, by consequence, the robust identification of the doublets associated to the oxide. Gaussian line shapes were employed for the peaks in the Mn 2*p* spectra related to the oxide. We found that, for very low exposure to oxygen, about two monolayers of oxide grows in a fraction of the surface, while the rest remains metallic. As it could be expected, the depth of the protrusions increases, and its surface coverage increase with the oxidation level. The oxide corresponds to Mn^{+2}.

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[SIT-316] Insight into the physical origin of the Shirley background and the peak asymmetric through the analysis of the 3d core level of the 5th-period elements

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Peak-fitting of the 3*d* core level from the 5th-period elements is challenging due to the high asymmetry of the main peak, the complex multiplet structure including plasmon and satellite peaks, and the intense Shirley-type background. This work presents 3*d* X-ray photoelectron spectra from pure elements ranging from Sr(Z=38) to Te(Z=52). These were analyzed using the DoubléLorentzian lineshape to account for the asymmetry of the main photoemission line, the branching ratio was forced to the theoretically expected value from the Scofield tables. It was possible to quantify the modulation with Z of the asymmetry of the $3d_{3/2}$ and $3d_{5/2}$ main peaks. It is remarkable that, for elements with completely filled 4*d* orbitals, the Double-Lorentzian asymmetry tends to be roughly equal between the two 3*d* branches. The background was modeled as a combination of a Shirley-type background, SVSC, a baseline, and, in some cases, a Slope background. The Shirley parameter decreases from a high value for Sr to a local minimum for Mo, to a local maximum for Rh. How this behavior sheds light on the physical origin of Shirley's background will be discussed. The fitting parameters employed in the analysis has been published in https://xpsoasis.org/

Keywords: asymmetry, Double-Lorentzian line-shape, Shirley background, plasmon and satellite peaks, 5th-period elements.
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Reference: Kaga, Y., Abe, Y., Yanagisawa, H., Kawamura, M., and Sasaki, K. Ru and RuO2 Thin Films by XPS. *Surf. Sci. Spectra* **6**(1999) 68-74. https://doi.org/10.1116/1.1247890

[SIT-228] Mechanical Behavior of Boriding Microalloyed Steels Immersed in Diesel

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In this work is examined, the mechanical behavior of boriding microalloyed steels subjected to diesel immersion. The growth of the iron boride layers was obtained by the boron dehydrated paste process using the temperature of 1273 K for 6 h. the first part consisted in the determination of FeB/Fe_2B phases obtained by boron dehydrated paste, identified by scanning electron microscopy (SEM), energy dispersive spectrometry (EDS) and X-ray diffraction (XRD). The second part; the boriding specimens are immersed for one year, after tensile test to observe the effect of mechanical behavior of each study material. This work contributes mechanical characteristics of innovative coatings for potential applications in the storage of fuels, oils and biofuels

Keywords: Boriding, Microalloyed Steels, Diesel, mechanical behavior

[SIT-234] Protrusion-like oxidation mechanism from metallic aluminum

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Aluminum is one of the most common materials used in many industries. As metallic aluminum is highly reactive to oxygen, it is important to learn about how oxidation works in films and/or interfaces when is applied in ultra-thin films. This can be done properly with X-ray photoelectron spectroscopy (XPS). The surface chemistry of materials is the point of interaction with the environment and with other materials. Its chemical composition influences how it interacts with its surroundings.

We present the quantitative analysis for chemical assessment of the initial stages of aluminum oxide thin films as well as its oxidation mechanism. The metallic films were obtained through sublimation employing a tungsten filament with a metallic aluminum pellet (99.999% pure Sigma Aldrich). The background pressure in the processing chamber was 1.5×10^{-7} Torr and the pressure during sublimation was 1.1×10^{-6} Torr. The film was characterized with an XPS instrument employing a monochromatic x-ray aluminum source (XR5, from ThermoFisher) and a 7-channeltron hemispherical spectrometer (Alpha110, from ThermoFisher) assembled by Intercovamex.

Oxidation were done under an oxygen-controlled environment at different oxygen exposures (1 kL, 10 kL, 100 kL, 1 ML and 10 ML). Advanced techniques for fitting the Al 2*p* and O 1*s* spectra were used, such as the block method [1], the background active approach, the SVSC background and the simultaneous fitting method. The chemical composition and thickness calculation of the aluminum oxide was done quantitatively from angle-resolved XPS data (ARXPS) analyzed under the multilayer method (MLM). We found that the oxidation kinetics is carried out by the formation of an Al^{3+} oxide layer with protrusions into the metallic substrate but with an Al^{2+} interface layer.

This work was partially financed by Proyecto Fronteras 58518, Conacyt, Mexico.

[1] A. Herrera-Gomez, F. S Aguirre Salgado, Y. Sun, P. Pianetta, Z. Yu, D. Marschall, R. Droopad, W. E. Spicer, “Photoemission from the Sr/Si(001) interface”, Journal of Applied Physics, Vol. 90, 12, p. 6070, 2001

[SIT-57] Surface modification of zinc oxide nanoparticles with amino groups for adsorption of methylene blue

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The lack of water is a problem that affects us worldwide. In some cities, industries and urban settlements discharge polluted water into rivers or lakes, some of the most toxic and difficult to remove pollutants are dyes, which cause adverse consequences for the environment and human health. In the present research work, zinc oxide nanoparticles with amino groups were superficially modified using ultrasound tip of 750 W at 50% wavelength at different reaction times, and to see their adsorption efficiency they were evaluated before the dye of Methylene blue. For the evaluation of the modified ZnO nanoparticles, FTIR, DRX, TGA, SEM and methylene blue adsorption percentage were performed. Through FTIR, DRX, TGA and SEM it was observed that the sample modified by ultrasound at a time of 60 min gave better results, showing a significant change and the appearance of amino groups compared to the unmodified ZnO nanoparticles. The results of the adsorption test showed that the nanoparticles modified with amino groups at 60 min achieved a removal percentage of 97% of the methylene blue dye, improving this property, adjusting to a Langmuir isotherm. Therefore, zinc oxide nanoparticles have a good potential for the removal of methylene blue in aqueous solution.

Keywords: zinc oxide; ultrasound; energy; adsorption.
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Reference: Andrade-Guel, M., Cabello-Alvarado, C., Romero-Huitzil, R. L., Rodríguez-Fernández, O. S., Ávila-Orta, C. A., Cadenas-Pliego, G., ... & Cepeda-Garza, J. (2021). Nanocomposite PLA/C20A Nanoclay by Ultrasound-Assisted Melt Extrusion for Adsorption of Uremic Toxins and Methylene Blue Dye. Nanomaterials, 11(10), 2477.. https://doi.org/10.3390/nano11102477
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[SIT-276] TERNARY COMPOUND THIN FILMS PRODUCED BY A NOVEL CYLINDRICAL HOT REFRACTORY ANODE VACUUM ARC SYSTEM (CHRAVA)

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Vacuum arc deposition systems have been widely used by the wear and protective coatings industries, mainly because its high deposition rates which can greatly reduce productions costs in the long term. But vacuum arc deposition is also known to have a major drawback, the incorporation of non-vaporized material, known as macro-particles (MPs). Several approaches have been taken to address this issue, such as: physical blocking, magnetic filtering or anodic arcs, among others, all of which result in a decrease of the deposition rate. In the late 1990s, Boxman [1,2] proposed a system with a refractory anode arc, to minimize the production of MPs. We have previously reported [3] a novel concentrically oriented electrode configuration. This combined the cathodic and the anodic modes of the electrical discharge, to maximize the extraction of ionized material to produce aluminum coatings with deposition rates up to 4 nm/s and surface roughness (Ra) as low as 25 nm. In the present work we will show the results of the latest modification of the cathode, to be able to produce ternary compounds, such as Ti-Al-N or Cr-Al-N. The produced films have been studied by profilometry to obtain deposition rates and roughness (Ra); XRD, SEM-EDS and XPS to verify structure and composition; scratch test, pin-on-disk and reciprocating tribometer to study, the adherences and the wear resistance, respectively; optical emission spectroscopy (OES) was performed to study the plasma and determine the presence of excited and ionized species.

Keywords: vacuum arc, plasma characterization, thin films, mechanical properties, tribology.
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References: [1] J. Phys. D: Appl. Phys. **28(2)** (1996) 353
[2] Surf. Coat. Technol. **133-134** (2000) 91
[3] Sci. Rev. Instrum. **89(9)** (2018) 095109
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[SIT-132] Tribological characterization of the TiAlON coating deposited on H13 steel

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This research was performed to study the tribological properties of the Titanium Aluminum Oxynitride (TiAlON) coating, deposited on AISI H13 tool grade steel substrates, by cathodic arc physical vapor deposition (PVD) method, in order to understand the mechanical and tribological properties of the material and apply it in cutting tools to increase their lifetime. By scanning electron microscopy and contact profilometry, the thickness of the coatings was determined, on average a 5.9 µm thickness was obtained. By X-ray diffraction (XRD) it was observed that the material has a face-centered cubic crystalline structure. Furthermore, it was determined that the material is composed of a solid solution, where oxygen replaces nitrogen atoms in the crystalline structure. Surface hardness was obtained using microindentation and nanoindentation, with average values of 6.85 GPa and 21.7 GPa for steel and coating respectively. Adhesion tests, performed using the dynamic scratch method, showed critical adhesive loads higher than 17 N, with failures related to chipping. Pin-on-disk wear tests were performed, finding coefficients of friction between 4.5 and 5.5 for the TiAlON substrate and coating respectively. With scanning electron microscopy, the wear mechanisms present for the TiAlON coating were observed, such as the formation of cracks and the accumulation of debris (debris), large areas of plowing and scratching were also found, which are characteristics of the formation of hard particles. These wear mechanisms are generated by reciprocating sliding contact, when debris forms between the two surfaces and there is 3-body abrasive wear.

Keywords: arc-PVD, tribology, thin films, wear
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[SIT-353] Tribological study of 410 SS in different work environments.

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In a tribological operation, the work environment plays a high role in the performance of the surface. One example is the variation of the wear (W) and friction force (Ff) produced in a reactive and no reactive atmosphere. This work presents the tribological changes made in a sliding-contact system of a disk of 410 stainless steel and balls of 5100 steel with 1/8 inch diameter. The 410 SS disks were obtained commercially and polished to bring high-quality finish surfaces (mirror quality). These were cleaned with Extran® and distilled water, acetone and isopropyl alcohol in the ultrasonic bath for 10 min each. The discs' crystalline structure and surface topography were measured using XRD and stylus profilometer, and the elemental composition was determined using EDS. The tribological tests were carried out in a customized tribometer, and assembled in a vacuum system, in atmospheric pressure, 0.6 Pas and 266 Pa of Ar atmosphere. The race tracks were analyzed using SEM, EDS, stylus profilometer and Raman spectroscopy. The Ff values produced in atmospheric pressure and 266 Pa of Ar were similar, with Cof values of 0.49 ± 0.21 and 0.56 ± 0.04, respectively. While in a vacuum atmosphere, the Ff value decreases to obtain a CoF of 0.27 ± 0.04. The wear track presented the wear mechanism of abrasion and adhesion, with the presence of iron oxide in the wear track of atmospheric pressure tests.

[SIT-18] Wet Chemical Etching of Austenitic 316L Stainless Steel for the Characterization of Bulk and Surface Properties

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Metallic biomaterials are widely used in orthopedic implants for hard tissue healing. In view of their significance, the characterization of bulk and surface properties of biomaterials are fundamental for proper uses in the human body. In this work, we identify and characterize the surface of commercially available 316L stainless steel rods used in previous studies on the surface texturization by MeV ion irradiation [1]. Knowing the surface of the material can help in determining the role of its physical properties involved in the formation of nanostructures, and successful applications in both industrial, and medical fields. The disk samples were prepared from 1-cm diameter rod sliced with a 3mm thickness, and polished to mirror-like finished. To characterize the grain structure of the prepared samples, these were subjected to wet chemical etching using Marbles's reactive solution (HCl, H2O and CuSO4) with respect to etch times. Subsequently, the surface morphology and topography were studied with surface techniques including optical and electronic microscopes (SEM, and AFM). The bulk properties of 316L were also studied with a Vicker's hardness tester. An increase of the surface roughness, with an enhanced visualization of crystallographic phases of the processed substrates have been obtained. A comparison is made with other etching techniques that allow visualization and study of crystallographic phases. Finally, information of the surface and bulk properties of the metallic biomaterial 316L stainless steel accentuates appropriate uses for industrial and medical fields.

[1] de la Vega, L. R. et al. Surface Texturization of 316L by Ion Implantation. XI International Conference in Surfaces, Materials and Vacuum, 2018, SIF-176.
This work was financially supported by Dirección General de Asuntos del Personal Académico (DGAPA) of Universidad Nacional Autónoma de México (UNAM) grant PAPIIT IN-114120. M. A. Garcia acknowledges additional support from CONACyT under "Estancias Posdoctorales en el Extranjero Vinculadas a la Consolidación de Grupos de Investigación y Fortalecimiento del Posgrado Nacional".

Sesión Oral

[SIT-173] ADHESION ISSUES IN THE SPUTTER DEPOSITION OF THE Ti-Al-Mo-N COATINGS ON D2 STEEL

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Current research on nitride coatings involves the optimization of properties to improve corrosion resistance and/or the mechanical and tribological performance through multi-alloying. In this industry, dry conditions are commonly required, so solid lubrication is a good option. It is reported that Mo can form oxides that reduce the friction coefficient of the coatings [1]. However, the deposition of multicomponent systems on steel leads to adhesion issues that can prevent the potential application. In this work, we synthesized the Ti-Al-Mo-N system by reactive magnetron co-sputtering on steel D2, using two different bonding layers on the substrate prior to Ti-Al-Mo-N deposition to achieve good adhesion and study the effect on their properties. Using a metallic bonding layer of Ti-Al-Mo, poor adhesion was reached in the system. Such a situation leads to gross spallation at very low critical loads and poor protective character in corrosion because of the detachment of coating once the solution reaches the substrate. Even the mechanical properties were compromised, possibly because of the residual stresses that reach the interface with a weak bonding layer during the nanoindentation test. Once the Ti-Al-N bonding was used, enhanced adhesion was achieved where critical loads were found at higher values. The anti-corrosive character of the Ti-Al-Mo-N system was improved, showing a better performance in the electrochemical test. These results could have a significant impact on the design and optimization of more complex systems, suggesting other applications, for example, anti-corrosive coatings.

Key words: Ti-Al-Mo-N, hardness, corrosion, adhesion.
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Reference: Sergevnin, V. S. *et al.* Hardness, adhesion strength, and tribological properties of adaptive nanostructured ion-plasma vacuum-arc coatings (Ti,Al)N–Mo2N. *Russ. J. Non-Ferrous Met.* **57**, 572–579 (2016).

[SIT-198] Analysis of the mechanical properties and tribological behavior by FEM of a Ti-Al-N thin film

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Nowadays, thin films have a wide range of applications, such as in the automotive and aeronautical industries as hard coatings. One of the most widely used methods for depositing this type of film is using the sputtering technique. A Ti-Al-N thin film was deposited using the magnetron sputtering using Al target power of 80 W. The superficial roughness and the thicknesses obtained were 0.94 nm and 800 nm, respectively. Hardness and young´s modulus were determined by instrumented nanoindentation, using a Berkovich diamond tip. The tests were performed within the quasi-static range, consisting of a loading time of 10 s, a dwell time of 3 s at maximum load, and an unload duration of 10 s. In addition, the samples were analyzed by scratch test, indicating the appearance of failure mechanisms at different critical loads Lc1-4 in whole residual imprint. The FEM simulation of the scratch test was necessary for understanding and quantifying the maximum principal stress in-situ during the experimental deformations. A comparative between the experimental and the simulated parameters as the normal and tangential force was required for ensuring that the stress-strain field produced is as close to reality as possible. Finally, it should be noted that the feedback from the FEM results, allowed us to understand that the stress concentration in the back-tail region at the border of the scratch groove and the region ahead of the contact is in a tensile and compression deformation, respectively, being a crucial behavior which is the responsible of the thin film delamination.

Keywords: Nanoindentatión, Mechanical properties, Scratch test, Failure mechanisms, FEM.
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This work was supported by: CONACYT Grant

[SIT-263] Developing a database for the assessment of the composition of multilayer nanofilms employing XPS or ARXPS data

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Through X-ray photoelectron spectroscopy (XPS), which is a highly surface sensitive technique, it is possible to determine the elemental composition and the structure (i.e., layers' thicknesses) of the top few nanometers (10 nm) of a material's surface, even if it has a multilayer arrangement. It has become synonymous of surface analysis, with many industries and academic institutes regularly using XPS as a qualitative tool.
Quantitative XPS analysis relies on robust fitting analysis with the subsequent assessment of chemical compositions and structures. Although there is no consensus in the XPS community on how to calculate surface composition from the peak intensities, there are highly accepted publications where physical parameters, such as the effective attenuation length (EAL) and the photoelectric cross-section, are employed instead of empirical sensitivity factors. It is also too common the use of the maximum entropy method with algorithms that do not allow for the use of EALs corresponding to each material of the multilayer film.
The MultiLayer Model MLM is a self-consistent analysis method for multilayer films. The MLM employs physical parameters such as photoelectron cross-sections, electron effective attenuation lengths, the transmission function, and, of course, the take-off angle. The analysis is done individually for each species and allows for a meaningful assessment of the uncertainties on the structural parameters (thickness and composition of the layers).
In this work, we present the development of a physical parameters database embedded in software that assesses the composition of a multilayer film employing XPS or ARXPS data. Embarcadero's C++ Builder platform is used because it allows for building a friendly user interface and databases. This tool will be offered free with an open code.

[SIT-162] Hardness of MoxNy thin films deposited by microwave ECR assisted reactive pulsed laser deposition

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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 to deposit MoN thin films. The deposit was formed on quartz substrates at a low deposition temperature (300 °C). The hardness values of the MoN films show a specific dependence on the plasma parameters (mean kinetic energy (E_k) of the ions) that could be varied depending on the power density applied on the target. Plasma parameters were measured by Langmuir probe. The structural characterization of the films performed by X-ray diffraction showed the presence of the δ-MoN (hexagonal) phase in all cases. The XPS analysis showed that the nitrogen content decreases as an effect of the increase of the kinetic energy of the ions, which could explain the increase of hardness of the samples with the ion energy.

Keywords: mechanical properties, microwave plasma, pulsed laser deposition, kinetic energy, molybdenum nitride
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[SIT-114] STUDY OF Mg/Ti MULTILAYERS DEPOSITED BY LASER ABLATION

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The increase of density of interfaces present in coatings has shown a drastic reduction in damage to the properties of the substrate material, when exposed to different processes: physical, mechanical, chemical, and most important ionizing radiation. This last has led to design, generate, and carry out an extensive study of interfaces obtained by combining materials with different structures in the form of multilayers, for example: titanium and magnesium, which combine hexagonal structures (HCP/HCP). The present work was focused on the optimization of the films properties as a function of the experimental parameters and for that purpose, at first Ti and Mg thin films were deposited using the pulsed laser ablation technique and were characterized by XPS, XRD and nanoindentation techniques. In a second step the multilayer system Mg/Ti with different thicknesses was deposited on silicon, quartz, and stainless-steel substrates, using the same deposition technique. The characterization of the multilayers showed that the properties of the individual films are conserved in the multilayer system.

[SIT-303] The 4f photoemission spectra of the sixth period transition metals

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The resulting peak fitting parameters obtained from analyzing the 4*f* core level of the 6th period, from Hf (72) to Hg (80) of the transition metals, have a well-defining behavior as a function of the atomic number. Assessing this dependence is a difficult task that requires state-of-the-art fitting methods because the spectra show complex asymmetry shapes, multiplet structure, plasmons, and satellites; besides, in some cases, they overlap with Auger peaks. Through the use of the empirical double-Lorentzian lineshape, it was possible to very closely reproduce the asymmetry for all the elements, suggesting that it could bear a fundamental basis. A combination of Shirley-type (SVSC) and Tougard-type backgrounds was necessary to reproduce the data. The SVSC parameter decreases from a value of 0.0504 eV^{-1} for Hf 4*f*, with a local maximum for Os (0.029 eV^{-1}). This resembles the behavior of the 2p spectra for the fourth-period and the 3d spectra for the fifth-period elements for the corresponding group elements."The fitting parameters employed in the analysis has been published in https://xpsoasis.org/".

Keywords: photoemission, transition metals, XPS spectra,(SVSC) background, double-Lorentzian asymmetric line
This work was partially financed by Proyecto Fronteras 58518, Conacyt, Mexico"

[SIT-197] Tribological assessment of water-based nanofluids prepared with ceria nanoparticles supported on carbon nanotubes

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Nanofluids have gained popularity in the last decades thanks to their enhanced performance in many applications compared to conventional fluids. Due to its exceptional mechanical and thermal characteristics, carbon nanotubes are of great interest in tribology. The use of nanotubes as a support for substances like metal nanoparticles is a novel application. Despite the wide employment of water lubrication in numerous industrial applications, more research is required to develop new, more efficient water nanofluids. In this work we report the synthesis of ceria nanoparticles supported on multiwalled carbon nanotubes by a microwave method and their use as additives to prepare water-based nanofluids. The tribological performance of this nanofluid was investigated using a pin-on-disk tribometer on steel-steel contacts at a constant load (10N), sliding distance (3.6 m), entrainment speed (60mm/min), fluid temperature (300 K) and additive concentrations (0.01, 0.05, 0.10% wt). The results show that the tribological behavior of nanofluids can be improved by adding the appropriate additive at the optimal concentration. Compared to pure water, ceria nanoparticles supported on carbon nanotubes showed a good performance at 0.10% wt. The lowest friction coefficient (~0.10) was achieved with this additive. The synthesized additive were characterized by high-resolution transmission electron microscopy (HR-TEM), Raman spectroscopy and X-ray diffraction. In order to explain the wear results, the worn surfaces were analyzed by means of scanning electron microscopy (SEM), Raman spectroscopy.

Keywords: Carbon nanotubes, nanofluid, metal nanoparticles, water-based lubricants
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[SIT-134] TRIBOLOGICAL BEHAVIOR OF Nb-DOPED OXYNITRIDES FOR HIGH TEMPERATURE APPLICATIONS

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Titanium aluminum oxynitrides (TiAlON) and titanium aluminum oxynitrides doped with niobium (TiAlNbON) Coatings were deposited on AISI D2 steel substrates by the reactive cathodic arc technique. Structural characterization was performed by X-ray diffraction (XRD), finding for TiAlON crystallographic orientations similar to those of titanium aluminum nitride (TiAlN) and for TiAlNbON the separation of the titanium aluminum oxide phase (Al2TiO5), which makes it a polycrystalline and polyphase coating. This was confirmed by transmission electron microscopy (TEM) analyses. The morphology of the surfaces showed macroparticles or "droplets" characteristic of cathodic arc films, increasing the roughness of the substrate by approximately 50%. A nanohardness of 12.85 ± 2.85 GPa was obtained for the coatings, with an increase in the modulus of elasticity and the resistance to plastic deformation for TiAlNbON. This led to an increase in adhesion for the Nb-doped coating of up to 80%. The tribological analysis performed by pin-on-disk at temperatures of 25 °C, 500 °C, 700 °C and 900 °C showed that when the combination of oxidation and tribo-oxidation affects the wear process, the ability of Nb to modify the diffusion of oxygen and stabilizing the oxides makes it possible to reduce wear, passing through abrasion mechanisms at low temperatures to combined abrasion-adhesion mechanisms at high temperatures.

This work was supported by CONACYT (Consejo Nacional de Ciencia y Tecnología), through project Fronteras de la Ciencia program No: 2015-02-1077, and the support provided through the FORDECYT projects 297265 and 296384. Thanks to the CENAPROT National Laboratory for facilitating the installations and use of the PVD-arc unit and the CIDESI characterization facilities. Juan Manuel González Carmona & Guillermo César Mondragón Rodriguez appreciates the financial support provided through the CONACYT investigadores por México program.
Keywords: arc-PVD, tribology, tribo-oxidation, thin films

THEORY AND SIMULATIONS OF MATERIALS

CHAIRMEN

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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

[TSM-178] A MOLECULAR DYNAMICS SIMULATION OF THE INTERACTION BETWEEN SIO2 NANOPARTICLES WITH STEARIC ACID AND BISPHENOL A MOLECULES IN AQUEOUS SOLUTION

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Different nanoparticles have been applied in catalysis, computer systems, new materials, and biomedicine. In particular, SiO2 nanoparticles have been used in many industrial applications to improve the fundamental properties of complex systems. For instance, in the enhanced recovery in oil wells, or to improve the elasticity of interfacial layer and to increase the stability of foams prepared with surfactant mixtures. Also, these nanoparticles have been used in biomedical applications, to encapsulate drugs and improve their transport in the cellular environment. Due to its wide applications, it is important to study the molecular interaction between nanoparticles and different molecular species such as surfactants or polymeric materials to observe the variations in the physical properties of the systems. At an experimental level, different techniques have allowed to determine the modification of these hybrid systems and obtain their resulting morphology. The use of molecular simulation techniques to understand the nature of the interactions in these systems at the microscopic level is an essential complement to experimental advances. In the present work, the molecular interactions between spherical SiO2 nanoparticles with stearic acid and bisphenol A were studied using molecular dynamics (MD) simulations to study the different molecular interaction present between these species in a solvent. Nanoparticles, stearic acid, bisphenol A and solvent molecules were described with the CHARMM36 and TIP3P force fields, respectively used to estimate the forces between atoms within molecules and between molecules. All the MD simulations were developed with a duration of 100 ns using the NVT type assembly and the GROMACS-2019.2 software. The evaluation of the molecular interactions was carried out through the study of the radial distribution function (RDF) and the calculation of the interaction energy between the characteristic groups of the involved species. These simulations allowed us to determine the surface interaction mechanism of this type of spherical cristobalite nanoparticles with the selected organic molecules.

Keywords: Nanoparticles, Molecular Interactions, Molecular Dynamics Simulations

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[TSM-394] Band structure and partial DOS of graphene-Nitrogen (Boron) layer.

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Since the discovery of graphene in 2004, various technological applications of this material have been reported; among wich stand out its use as a material conductive of electricity, or its use for hydrogen storage. In this theoretical work we do applications of graphene for hydrogen storage, wich we do through molecular modeling of a layer of graphene. First we build the layer of graphene whose structure is optimized. Then we introduce nitrogen (or boron) atoms to substitute some carbon atoms of the lattice. With the modules Castep and DMol3 we report the results of the change in the hexagonal structure of graphene layer, before and after it was doped. Also, we report the results of band structure or HOMO (highest occupied molecular orbital) and LUMO (lowets unoccupied molecular orbital) values and partial density of states.

Keywords: band structure; graphene-N doped; graphene-B doped; partial density of states; homo-lumo orbitals.
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[TSM-81] CHEMICAL INTERACTION BETWEEN NITROGEN-DOPED GRAPHENE DEFECTS AND A COPPER (111) SURFACE

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The electronic properties of nitrogen−doped graphene (pyridinic, pyrrolic and graphitic defects) supported by a copper substrate have been studied by applying density functional theory, together with the vdW−DF correction. We discovered that pyrrolic and pyridinic defects strongly interact with the copper substrate due to covalent chemical bonds between the nitrogen atoms and the underlying metal. The binding energy and charge transfer from the copper to nitrogen atoms induces a formal oxidation state in the copper [copper (I) or copper (II)], depending on the type of defect which interacts. A simple method was applied to synthesize large areas of NG grown on copper foil, via chemical vapour deposition (CVD).

[TSM-107] CO ADSORPTION AND HYDROGENATION ON SRTIO3(001) A DFT STUDY

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Density Functional Theory (DFT) calculations were performed to investigate the adsorption and hydrogenation of carbon monoxide (CO) on strontium titanate ($SrTiO_3$) surface (001). Calculations were performed using PWscf code of the quantum ESPRESSO package. CO adsorption study is relevant because CO is a dangerous pollutant gas. Actually, pollution is an important global problem and studying systems that could help to remove and transform dangerous substances is relevant. This work focuses in CO adsorption, which is useful for removing it, and hydrogenation. Adding hydrogen atoms will transform the CO into industrial valuable substances motivating CO transformation. Adsorption energy, formation energies, structural and electronic properties of selected systems are reported and compared. Understand the mechanism in chemical processes can help to propose improvements that lead to more efficient catalyst materials.

Keywords: carbon monoxide, strontium titanate, hydrogenation, DFT.
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[TSM-318] Effective properties of laminated micropolar nanocomposites under imperfect contact conditions

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The development of efficient theoretical models that describe the effective behavior of micro/nano-structured materials is essential to making and transforming new nanotechnological applications. These theoretical models support the design of experiments in the search for better materials with desired and optimized properties as a guide to improvement. In this work, the heterogeneous elastic micropolar problem subject to imperfect contact conditions is addressed by the two-scale asymptotic homogenization (AHM) method. The imperfect interface is described as a generalization of the interface spring model reported for linear elasticity, that is, the imperfect interface is assumed by the following conditions: the coupled tractions and stresses are continuous, but the displacements and microrotations are discontinuous along the imperfect interface. The jumps of displacements and microrotations are considered proportional to the interface traction and coupled stress components, respectively. In particular, the effective stiffness and torque properties for micropolar bi-laminated nanocomposites with centro-symmetric isotropic components and imperfect contact conditions are determined by AHM. Numerical results are shown and discussed. The effects of the imperfection parameters and the cell length in the y_3-direction on the effective properties are studied. All effective stiffness and torque properties are susceptible to the imperfection effects and the cell length provokes changes in the effective properties behavior when an imperfect interface is assumed.

Keywords: micropolar media, asymptotic homogenization method, centro-symmetric materials, Cosserat laminated nanocomposites, imperfect interface
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[TSM-89] ELECTROMAGNETIC SIMULATION OF BIMETALLIC NANOPARTICLES OPTICAL PROPERTIES

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Bimetallic nanoparticles, composed of two different metals, are of considerable interest and application in diverse fields; these types of NP have a diversity of properties depending on their morphology, material, and size, among which are electrical, catalytic, and optical properties [1].
In this work, we present electromagnetic simulations using the finite element method (FEM) of bimetallic nanoparticles composed of Au/Ag to observe the dependence of optical parameters like absorption and dispersion as a function of size and material proportion. These simulations allow us to have a better approach for a correct synthesis and characterization of our bimetallic nanoparticles for future applications, mainly in the biomedical field as a substrate for Raman signal amplification of biological samples.

Keywords: Bimetallic nanoparticles; Optical properties; FEM.
Reference: [1**]** Loza, K., Heggen, M., & Epple, M. (2020). Synthesis, structure, properties, and applications of bimetallic nanoparticles of noble metals. *Advanced functional materials, 30*(21), 1909260. https://doi.org/10.1002/adfm.201909260

[TSM-148] FIRST STEPS STUDIES OF THE BORON PHOSPHIDE EPITAXIAL GROWTH ON ALUMINUM NITRIDE SUBSTRATES

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First steps of the cubic boron phosphide (BP) epitaxial growth on the aluminum nitride (AlN) (0001) surface are investigated using first principles total energy studies. Calculations are performed within the density functional theory (DFT) as developed in the quantum ESPRESSO package. The modeling considers the experimental evidence of the cubic BP(111) epitaxial growth on an AlN(0001) substrate. In this way studies invoke the hexagonal nitrogen terminated AlN (0001)- surface. The first boron (B) layer is deposited on top of the structure following the hexagonal arrangement. After that, phosphorus (P) atoms are accommodated accounting for the hexagonal sequence. This facilitates the subsequent P-B bilayer formation, which in turn allows the formation on top of the structure the P-B bilayer in two different high symmetry sites: one on the T4 and the other on the H3. Energetics indicate that the H3 configuration is the one with the lowest total energy 0.125 eV smaller than the T4 geometry. This result yields the conclusion that the BP (111) epitaxial layer is formed in the cubic phase as experiment dictates. Studies include calculations of the density of states (DOS) and projected density of states (PDOS) to show the surface metallic behavior.

[TSM-5] First-principles approach to study the electronic and magnetic properties in ferromagnetic RNi2 Laves phases (R = Ho, Er)

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In this work, the magnetic orderings in RNi_2 Laves phases (R = Ho, Er) were simulated by the density functional theory (DFT) as is programed in CASTEP package. The density of states (DOS) and partial density of states (PDOS) are obtained using the generalized gradient approximation (GGA), under the revised-Perdew-Burke-Ernzerhof (RPBE) functional with spin-polarized calculations. Some physical properties, like magnetization and electron population by orbitals at Fermi energy level (E_f), are calculated and discussed. The major electronic contribution to magnetic properties in $HoNi_2$ and $ErNi_2$ structures comes from electrons located at *d* and *f* orbitals, as is reported in scientific literature. Also, the X-ray diffraction patterns are simulated. The simulation results are compared with experimental reports.

[TSM-397] Induction of Electromagnetic Force in a 3D Photonic Crystal

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For this work, the induction of electromagnetic forces in three-dimensional photonic crystals made up of artificial opals based on SiO2 microspheres was theoretically studied. When light is a normal incidence on the crystal, electromagnetic forces generate self-oscillations of these structures resulting in mechanical and electrical energies.
We works with the model of electromagnetic propagation using the scalar wave approximation theory, along a direction of high symmetry of the crystal, specifically in the [111] direction. It was observed that the radiation pressure can be obtained by the Maxwell stress tensor (which makes use of the analytical expressions of the reflection and transmission coefficients obtained by the scalar wave approximation with help of the transfer matrix) and also with the Lorentz volumetric force density. With these approximations, it is determined that the radiation pressure in these structures can be as high as 1.33×10^{-4} N/m², when the laser power is 60 mW and with a spot size of approximately 3 mm2. .
The results provide an innovative method of analyzing the change in electromagnetic forces for 3D dielectric photonic crystals.

Keywords: 3-D Photonic crystals, Synthetic opals, Electromagnetic forces, Radiation pressur, Maxwell stress tensor

[TSM-58] Propiedades electrónicas y estructurales de la willemita bajo presión hidrostática

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En este trabajo se presentan las propiedades electrónicas y estructurales de la willemita (Zn_2SiO_4) bajo altas presiones. La energía total de la celda se calculó asumiendo once estructuras cristalinas hipotéticas: R$\underline{3}$, I$\underline{4}$2d, Imma, Fd$\underline{3}$m, Pnma(1), Pnma(2), Pbca(1), Pbca(2), $P2_1/c$, Cmcm y Fddd, sometidas a una presión hidrostática de hasta 100 GPa. Todas las estructuras fueron relajadas y completamente optimizadas, los resultados fueron ajustados con la ecuación de estado de Birch-Murnaghan de tercer orden. Los cálculos se realizaron dentro del marco de la Teoría del Funcional de la Densidad, utilizando el método de ondas planas aumentadas y linealizadas con potencial completo implementado en el código Wien2k. Hemos incluido en nuestro estudio la aproximación de gradiente generalizado de PBE para el termino de intercambio-correlación.

[TSM-200] SnS-Bi2S3 AS A TERNARY ABSORBER COMPOUND FOR SOLAR CELLS APPLICATIONS: A THEORETICAL STUDY

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Photovoltaic energy is having an increasing impact on power generation. But at the same time, the properties of the materials used for its manufacture are reaching their limits, being the absorber materials the most important component, so it is in search of new absorbers that come from abundant sources and at the same time are economical. Several binary compounds such as SnS, PbS, and Bi_2S_3 implemented in photovoltaic devices have provided acceptable results; however, some of their characteristics as binary compounds, such as their bandgap energy or their layered structure, make them limited, trying to maximize these properties PbS-Bi_2S_3 combinations have been worked for the formation of ternary compounds, with the same intention, but trying to change the lead, it is proposed to know the optical properties of an SnS-Bi_2S_3 configuration as a ternary compound and determine whether it has suitable characteristics for its application in photovoltaic devices.
In this work, we present Ab-initio calculations of the electronic band structure, density of states, and optical properties for different configurations of SnS-Bi_2S_3. We use Density Functional Theory (DFT) approach by using the ultrasoft pseudopotential approximation for the electron-ion interaction and a plane wave basis set for the wave functions with the PWscf code Quantum Espresso. Optimization calculations of lattice parameters and atomic positions were carried out, for the configurations used plane-wave cutoff energy of 680 eV was used. In addition, the calculations were performed considering the spin-orbit coupling (SOC) for which the use of fully relativistic pseudopotentials is required, being for all cases, Perdew-Burke-Ernzerhof (PBE). From our theoretical study, we determine optimal properties for the desired application, such as suitable absorption values and bandgap energy values between 0.8 and 2.4 eV.

Keywords: emerging solar absorber, SnS-Bi2S3, Ab-initio, DFT.
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[TSM-300] Stretching bond force constants of boron nitride nanomaterials: A DFT study

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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. Nanomaterials such as boron nitride nanotubes, chains, fullerenes, and planar arrangements, are just a few examples that demonstrate the structural versatility of this composite, which can form a wide variety of nanostructures. 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, fullerenes and planar structures of boron nitride using density functional theory were compared and discussed.

[TSM-295] STRUCTURAL SIMULATION OF INGAASSB QUATERNARY ALLOYS DEVELOPED FROM EXPERIMENTAL DATA.

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The antimonide family-based compounds have demonstrated to be a viable alternative for the development of new infrared optoelectronic and semiconductor devices. Among some of their principal characteristics and which makes it possible for these materials to be considered as a solid option for the application in optoelectronics devices is a direct band gap energy that covers from the near infrared (1.7 μm) up to the mid infrared (3.5 μm) at room temperature. An important member of this family is $In_xGa_{1-x}As_ySb_{1-y}$ quaternary alloy. Besides sharing some of the main characteristics of the antimonide family, this compound allows to tailor its band gap in accordance with the content of the precursor elements that conform it. In order to being able to visualize some of the main characteristics of this material, having in consideration the multiple possible contents of the $In_xGa_{1-x}As_ySb_{1-y}$, moving from x= 0 and y= 0 for GaSb to x= 1 and y= 1 or InSb, a simulation was developed using MATLAB computational software, which is mainly based on the results of different chemical, structural and optical characterizations performed on $In_xGa_{1-x}As_ySb_{1-y}$ quaternary alloys grown by liquid phase epitaxy. The simulation is deployed upon a graphical user interface, where it is possible to observe some data computed as a function of the x and y contents of the alloy, which are: Lattice constant and bond length, Varshni's parameters and band gap energy for a hypothetical temperature, 2θ peak position for an XR diffractogram and a graphical visualization of the structure, in which one may see the accommodation of each different atom from different directions.

Keywords: Structural simulation, Antimonide Family, InGaAsSb quaternary alloy
Reference: M.A. González-Morales, J.J. Cruz-Bueno, G. Villa-Martínez, M. Ramírez-López, D. Flores-Ramírez, P. Rodríguez-Fragoso, J.L. Herrera-Pérez, Y.L. Casallas-Moreno, and J.G. Mendoza-Álvarez, Importance of liquid phase epitaxy on achieving near-lattice-matched growth of In0.145Ga0.855As0.132Sb0.868 layers on GaSb(100) substrates, Superficies y Vacío 35 (2022), https://doi.org/10.47566/2022_syv35_1-220601
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[TSM-281] Structural, vibrational and electronic properties of limonene

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Limonene, a chiral aliphatic hydrocarbon, is the major component in the oil of citrus fruit peels and is already used in mostly agronomy related applications as well as in the food industry. The availability of limonene among the increasing amount of urban waste and the fact that it does not increase pollution, has made it very interesting. In this work we use first principles calculations based on the density functional theory to study the structural, vibrational and electronic properties of both enantiomers of limonene.

[TSM-319] Studies of the half-metallicity in reconstructed CrN (111) surfaces

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Transition metal nitrides (TMNs) have recently attracted the attention of the scientific community because of their excellent mechanical, optical, and magnetic properties. Among TMNs, chromium nitride (CrN) has been investigated recently due to its interesting structural and magnetic properties, that makes it ideal for data storage and memory devices, i.e., spintronic applications. On the other hand, it has been demonstrated that surface properties can be different from those of bulk. In addition, these properties depend on the thickness, orientation, strain, and defects at the surface. Therefore, it is important to study the physical properties of different CrN surfaces for practical applications, such as in spintronic. Taking into account the above mentioned, we perform spin-polarized first-principles calculations to study the electronic and magnetic properties of the CrN (111) surface considering different surface terminations. We evaluate their thermodynamic stability employing the surface formation energy formalism. According to the calculations, the N-terminated and Cr-terminated surfaces are stable under N-rich and Cr-rich environments, respectively. At intermediate conditions the octopolar, and the α-(2×2)-Cr reconstructions are stable. The ideal surfaces show metallic characteristics. In contrast, the reconstructions show half metallic behavior, as induced by the Cr vacancies in the structure. In the N-terminated and reconstructed surfaces the spin density distributions exhibit a ferromagnetic alignment in the first bilayer, and an antiferromagnetic ordering in the inner bilayers. On the other hand, the Cr-terminated surface shows a C-type antiferromagnetic behavior. In addition, a magnetic alignment switch from C-type antiferromagnetic to A-type antiferromagnetic is obtained when a tensile strain is applied to the surface. Our results show how to manipulate the surfaces properties to become suitable for spintronic applications.

[TSM-192] Study of the electronic properties of AgBi3S5 and AgBi3Se5 by first principles methods

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Electronic properties were calculated for the thermoelectric materials $AgBi_3S_5$ and $AgBi_3Se_5$ using Density Functional Theory (DFT). The aim is to determine the electronic properties of $AgBi_3S_5$ and $AgBi_3Se_5$, since these materials are promising for materials science, because they present very good thermoelectric properties. For the calculation of the density of states (DOS), the method of first principles LAPW+lo was used. The modified Becke-Johnson Tran-Blaha (TB-mBJ) potential of 2009 was used for the exchange-correlation potential. The study of the electronic properties shows that the total DOS (TDOS) of $AgBi_3S_5$ and $AgBi_3Se_5$ are similar, close to the Fermi energy, and in general they are similar only presenting some higher peaks under the Fermi energy this is due to the partial density of states (PDOS) of the Se atoms.

[TSM-213] SYNTHESIS AND OPTICAL CHARACTERIZATION OF AG-AL2O3 CERMET COATINGS

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The synthesis and characterization of Ag-Al2O3 cermet coatings is presented in this work. The coatings were synthesized by the spray pyrolysis technique from aluminum acetylacetonate, as source of aluminum, and silver nitrate, as source of silver. The coatings were characterized by scanning electron microscopy, Uv-vis spectroscopy, and spectroscopic ellipsometry. The optical properties were estimated from effective medium theory, considering silver naoparticles (Ag) embeded in a dielectric matrix (Al2O3) using the DELTAPSI2 Software Suite. A further characterization of these coatings, as possible solar absorbers, was also carried out.

Keywords: Cermets, Al2O3, Spray Pyrolysis, Spectroscopic Ellipsometry, Optical Properties
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[TSM-413] SYSTEMATIC FIRST-PRINCIPLES STUDY OF THE MAGNETIC PROPERTIES OF SILICENE, GERMANENE AND GRAPHENE SHEETS

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Magnetic materials have been an important subject for academic studies and application devices, to which low dimensionalities give new physical significance due to the strong quantum confinement effects. In particular, two-dimensional magnetic materials have attracted enormous attention since it has been revealed that it is possible to obtain 2D structures from Van der Waals crystals; this opens a huge potential to create numerous and novel devices with 2D materials. Therefore, the development of theoretical and experimental studies in this type of structures is essential to take advantage of the properties that can be obtained from them. The purpose of this work is to calculate and analyze the behavior of electronic and magnetic properties in a set of silicene and germanene structures in which the effect of doping and vacancy generation is explored. In general, a set of silicene and germanene sheets with vacancies were modeled and doped with Si, Ge, P and C. Using the Quantum Espresso code (based on the density functional theory) the optimization (through a spin polarized calculation) of the unit cell of each film was performed; exchange and correlation energy was approximated by a Perdew Burke Ernzerhof ultra-soft generalized gradient pseudopotential (GGA-PBE). Subsequently, the density of states and total magnetization were calculated for each sheet. The results show that the graphene sheet with vacancies presents a magnetic moment. A variation in the bandgap energy in the sheets is also observed, due to the effect of the vacancies and the doping with the different elements. It can be concluded that this type of materials has potential applications in different fields such as electronics and optoelectronics.

Keywords: Silicene, Germanene, Magnetic Properties, Electronic Properties, Electronic Properties.
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[TSM-62] THEORETICAL STUDY OF THE ELECTRONIC PROPERTIES OF APbI3 PEROVSKITE-TYPE MATERIALS (A = Cs+, CH3NH3+ and HC(NH2)2+)

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Metal halide (B = Ge^{2+}, Sn^{2+}, or Pb^{2+}; X = Cl^-, Br^-, or I^-) organic-inorganic (A = Cs^+, $CH_3NH_3^+$, or $HC(NH_2)^{2+}$) perovskite-type materials widely studied since its appearance in 2009, because of their outstanding performance it has had as an absorber material in a photovoltaic cell. In this context, first principles studies have acquired a leading role in studying the physical and chemical phenomena of these materials that give rise to their attributes (high mobility of holes and electrons, highly modifiable chemical composition, etc.) and to its deficiencies (instability and reactivity with external agents, etc.). However, the accuracy of the theoretical description remains in question. For this reason, in this work the perovskites $CsPbI_3$, $CH_3NH_3PbI_3$ and $HC(NH_2)_2PbI_3$ were studied based on the Density Functional Theory as implemented in the DMol^3 computational code. Making a comparison between two different bases, whose only difference between the two is the addition of p orbitals for the hydrogen atoms, it was concluded that the relative errors obtained are comparable to each other and that a good structural description can be generated with both bases. For the study of the electronic properties, the meta-GGA functionals were used: TPSS and revTPSS; as well as the functional HCTH/407 for comparison, since the latter is one of the most precise functional within GGA [1]. Although the first functional is closer to the experimental value of the gap-forbidden energy (BPE), none can describe the ultraviolet shift of the BPE that is obtained in these materials by decreasing the volume of the cation in the A site. It is hoped that the results presented here will help to improve the description of this type of compounds.

Keywords: Perovskite, Density Functional Theory, meta-GGA, forbidden energy gap.

One reference: [1] Medvedev, M. G., *et al*. (2017). *Science*, **355** (6320), 49-52.

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Sesión Oral

[TSM-101] Atomic-Scale Understanding of Li Storage Processes in the Ti4C3 and Chemically Ordered Ti2Ta2C3 Mxenes

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By first-principles calculation, we investigated the lithiation process in the Ti_4C_3 and $Ti_2Ta_2C_3$ Mxenes, also, the thermodynamic stability of the $Ti_xTa_{4-x}C_3$ Mxenes is studied. According to the calculations, five MXenes are stable, where the most stable 50% Ta/Ti ratio structure ($Ti_2Ta_2C_3$) presents a chemically ordered composition. The Li intercalation process for Ti_4C_3 and $Ti_2Ta_2C_3$ Mxenes is carried out as adatoms on the surface, with the T4 site being the most favorable. The chemically ordered MXenes provide better OCV values and can store more Li atoms than the Ti_4C_3 Mxene. Also, the Li difusion process demonstrates that $Ti_2Ta_2C_3$ is a more éficient material to be employed as an anode in batteries since it provides the lowest energy barriers. Our results demonstrate the capability of the $Ti_2Ta_2C_3$ alloy to be employed in energy storage applications thanks to the high stability and capacity to store Li ions in comparison with pristine Ti_4C_3 Mxene.

Acknowledgments
The authors thank DGAPA-UNAM projects IA100822, IN110820, and IG200320 for partial financial support. Calculations were performed in the DGCTIC-UNAM Super-computing Center, project nos. LANCAD-UNAM-DGTIC-368 and LANCAD-UNAM-DGTIC-150.

[TSM-41] CHARACTERIZATION OF MORPHOLOGICAL AND MAGNETIC PROPERTIES OF Mn SURFACES

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Abstract body: The α-Manganese phase has one of the most complex and unique crystal structures among all metals in the periodic table with a 58 atom basis and a non-collinear antiferromagnetic bulk spin-structure (Hobbs et al., 2003). Manganese is a cornerstone magnetic material for a variety of applications for example, in dilute magnetic semiconductors, as a rare-earth free magnet, and in magnetic topological insulators to name a few. Despite its prevalence in applied materials as an alloy, little real-space investigations of α-Mn surfaces have been performed. We performed a thorough analysis of the surface structures of α-Mn via first principles and scanning tunneling microscopy (STM). We present the most stable surface reconstructions and a description of the atomic arrangements at the surface as showcased by both theoretical and experimental STM images. Analysis of real-space and Fourier transformed STM images help match candidate Terrsoff-Hamann simulation surfaces with experimental STM images. Analysis of magnetic spin-structures reveals a non-collinear spin structure. Finally, a discussion of the mechanisms that lead to the difference in bulk and surface properties is presented.

Keywords: Density Functional Theory, surface reconstructions, magnetic anisotropy, non-collinear antiferromagnetism.

Reference: Hobbs, D., Hafner, J., and Spisak, D. (2003). Understanding the complex metallic element mn. i. crystalline and noncollinear magnetic structure of α-mn. Physical Review B, 68(1):014407.

This work was supported by: the DGAPA-UNAM projects IN105722 and IA100822, as well as CONACYT grant A1-S-9070. Calculations were performed in the supercomputing center DGCTIC-UNAM, through the projects LANCAD-UNAM-DGTIC-051 and LANCAD-UNAM-DGTIC-368. We thank “Laboratorio Nacional de Supercómputo del Sureste de México”, CONACYT, member of the national web of laboratories for providing computational resources and technical support. We would also like to thank the computing center THUBAT KAAL IPICYT for providing its computational resources. Finally, we thank Eduardo Murillo and Aldo Rodríguez Guerrero for their technical support.

[TSM-131] COMPUTATIONAL STUDY OF MECHANICAL AND ELECTROCHEMICAL BEHAVIOR OF Zr-BASED CERAMIC THIN FILMS IN PHYSIOLOGICALLY SIMULATED ENVIRONMENTS

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ABSTRACT: To determine the possibility of using new thin films architectures as biocompatible materials, a computational study was performed to evaluate the mechanical and corrosion properties in simulated physiological media (saliva and blood plasma) of Zr, and ZrN, coatings. The obtained results for Density Functional Theory Methods showed that electron transfer associated with the wear mechanism is kinetically impeded as a consequence of the large energy barriers for this process, associated with the adsorption of the molecular species on the ZrN surface. Additionally, calculated adsorption energies indicated that urea (from the simulated saliva solution) interacts strongly with the surface. This interaction was associated to the formation of passivating protective layers, which is a key mechanism to protect against corrosion.

Keywords: *Corrosion, Adsorption Energies, Electrochemical Process,, DFT.*
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Reference: J.M. González-Carmona, J.D. Triviño, Á. Gómez-Ovalle, C. Ortega, J.M. Alvarado-Orozco, H. Sánchez-Sthepa, A. Avila, Wear mechanisms identification using Kelvin probe force microscopy in TiN, ZrN and TiN/ZrN hard ceramic multilayers coatings, Ceramics International. 46 (2020) 24592–24604. https://doi.org/10.1016/j.ceramint.2020.06.248

[TSM-232] Electronic correlation in quasiperiodic systems

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Quasiperiodic systems changed the view that crystalline materials had, presenting fold symmetries that were considered forbidden, like fivefold symmetry. Since the discovery of these materials, their properties have been in constant research, like phonon and electronic ones, always with the goal to find an application equal in importance and strangeness as their symmetry. However, until now the interest of those materials is the non-stick surface property. In 2018 the existence of conventional superconductivity in quasicrystals was reported, in an Al-Zn-Mg alloy, which broadens the possibilities for the study of correlated systems. In this work, we study the electronic correlation using the Hubbard Hamiltonian for two coupled quasiperiodic linear chains.

[TSM-248] EXPERIMENTAL AND THEORETICAL STUDIES ON A CYLINDRICAL CONCENTRIC ELECTRODE PLASMA SYSTEM

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A plasma produced in a coaxial electrode arrangement was analyzed. Experimentally, the partially ionized gas produced in Argon was studied, the electronic temperature and plasma density of the excited species were obtained by means of Langmuir probe measurements, at different positions along the radial coordinate. The applied voltage ranged from 180 to 258 V on the stainless-steel coaxial electrodes. The background pressure used was 0.01 mbar from a mechanical pump, and measurements were performed in the pressure range from 0.1 to 2 mbar. A continuum plasma model was solved one-dimensionally with a high precision numerical algorithm, obtaining the electronic temperature, plasma density, potential and electric field. We will show the agreement between the experimental observations and the theoretical calculations.

Keywords: *Glow discharge, Electronic temperature, Hollow cathode, Numerical simulations*
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[TSM-404] Mechanical properties of porous silicon carbide passivated with hydrogen and halogens: A DFT approach.

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Silicon carbide (SiC) has been studied theoretically and experimentally in recently year, due to its attractive properties as a high point melting, hardness, etc. Particularly, on the theoretical area different studios has been carried out mainly about SiC nano structuring. In this work, we focus on the nano porous SiC, specifically on the effects of the surface pore and the type of passivation on the mechanical properties of porous silicon carbide, this through the density functional theory and the supercell scheme. To build the model, first we grow up a 3C-SiC in the [1 1 0] direction, then a column of atoms was removed on the [0 0 1] direction to create four kinds of surfaces, two with a silicon-full and carbon-full surface and other two with a silicon-rich and a carbon-rich surface, the dangling bonds were passivated with hydrogen (H). After optimization, some atoms of H from the nanopores were replaced for atoms of fluorine and chlorine to simulate a mixed passivation. The results show that properties as the young's modulus have been affected by the type of pore and the passivation, for example the carbon-full pore with a H + F passivation have the lowest young's modulus. Additionally, the Bulk modulus was calculated, this could be used for energy storage applications.

This work was supported by CONACyT and IPN through the SIP proyect 20220587.

[TSM-108] Modeling the nickel and cobalt deposit on the AlN (111)-(2í—2) surface: A DFT study

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Structural, electronic, and magnetic properties of the transition metals (nickel and cobalt) deposited on the AlN (111)-(2 × 2) surface have been investigated. Calculations have been done within the spin polarized periodic density functional theory as developed in the VASP code. The exchange–correlation energies are treated within the generalized gradient approximation (GGA). The electron-ion interaction is treated by using pseudopotentials. To perform an adequate description of the transition metals magnetic properties, we have considered the Hubbard correction (GGA + U) to treat the highly correlated electrons in the d-orbitals. This work explores the adsorption, incorporation, and substitution of the magnetic metals (Ni and Co), considering different coverage, namely: ¼, ½, ¾, and 1 monolayer (ML). Furthermore, three magnetic alignments (non-magnetic, ferromagnetic and antiferromagnetic) were taken into account. According to the results, Ni atoms needed no Hubbard correction. In contrast, Co atoms used a Hubbard correction (U=1 eV) to reproduce experimental values such as the lattice parameters, magnetic moment and cohesive energy. We employed the surface formation energy formalism to determine the thermodynamic stability of the different surfaces. In both cases, the substitutions of Ni and Co atoms are the most stable structures. Nevertheless, Co structures present a higher magnetic behavior than Ni structures. For both metals, the total density of states (DOS) and projected DOS (PDOS) show that the uppermost bilayer (BL) of the surfaces is metallic and the lower BLs are semiconductors. The valence and conduction bands are mainly formed by the N-p and Al-p orbitals, respectively. Finally, in this work AlN (111) surfaces doped with Ni and/or Co have been proposed to develop diluted magnetic semiconductors (DMS) for applications in spintronics.

Keywords: Surface structure, Magnetic materials, DFT

Reference:

A.C. Martínez-Olguín, R. Ponce-Pérez, C.A. Corona-García, D.M. Hoat, Leonardo Morales de la Garza, María G. Moreno-Armenta, Gregorio H. Cocoletzi, “Theoretical investigation of the AlN (0 0 0 1)-(2 2) surface doped with nickel : Structural, electronic and magnetic properties”, J. Cryst. Growth, 551 (2020) 125907. https://doi.org/10.1016/j.jcrysgro.2020.125907.

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[TSM-158] Strain effect on Cr2C MXene: insight from First-Principles Calculations

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Structural, electronic and magnetic properties of two-dimensional Cr2C MXene under strain were studied. Uniaxial and biaxial strain was considered from -5% to 5 % to represent compressive and tensile strain. The phonon dispersion was calculated to determine the dynamic stability, under compressive strain Cr_2C MXene remained stable, however changed to unstable when tensile strain was applied under biaxial and uniaxial strain from 1% and 2%, respectively. Concerning with the phonon density of states, the main contribution of the acoustic and optical branches are from C and Cr atoms vibrational bands. The electronic properties of the dynamically stable systems were investigated by calculating the total density of states (DOS) and projected DOS. As expected, the unstrained MXene displays a half-metal with ferromagnetic behavior and is preserved under biaxial and uniaxial tensile strain, nevertheless, the MXene under compressive strain changes to metallic behavior. These properties extend the potential applications in the spintronics area due to the electronic properties could be tunable under compressive or tensile strain.

Keywords: DFT, Cr2N MXene, strain effect, half-metal
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[TSM-298] Stretching bond force constants on carbon nanostructures: A DFT study

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In the last 30 years, carbon 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. Carbon nanostructures such as fullerenes (0D), nanotubes (1D), graphene (2D) and diamond (3D), are just a few examples that demonstrate the structural versatility of carbon, which can form a wide variety of nanostructures based on their hybridizations. Knowing and comparing the mechanical properties between carbon nanostructures, such as the stretching bond force constant (*Kr*), contributes to its early technological implementation as specific nanosensors. *Kr* value 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, *Kr* values calculated with Density Functional Theory for different carbon nanostructures are analysed. The results suggest a range of allowable *Kr* values for carbon nanomaterials, delimited by the 3D and 1D structures.

[TSM-55] Theoretical studies on the monolithic integration of GaAs on (111), (110) and (100) Silicon surfaces

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The direct fabrication of GaAs on silicon (Si) substrates has been of great interest for a long time due to its technological and economic advantages in the fabrication of devices such as photonic integrated circuits and high electronic mobility transistors. From this perspective, the grow of high-quality GaAs semiconductors films on Si is very imperative [1]. However, the thermal expansion coefficient difference and large lattice mismatch between GaAs and Si make it challenging to obtain high quality GaAs thin films. Experimentally, it was found that the morphologies and internal crystal structure quality of GaAs films grown on Si(111) was better than those grown on Si(001) [2]. Also experimentally, was found a large density of crystal defects for the case of GaAs films growth on Si(110), even for small film thickness as 8 monolayers [3]. Therefore, we can infer that the direction of growth impact directly in the epitaxial quality growth of GaAs on Si substrates, classifying Si(111), Si(001) and Si(110) from best to worst for the monolithic growth of GaAs films. In this work, we present an ab initio study of the possible origin of the internal crystal quality differences in the growth of GaAs on Si(111), Si(001) and Si(110). The structural changes, energy density differences and interfacial energy were calculated by using density functional theory. Our preliminary calculations show that dissipation of the stress energy through the relaxation of the distortion of the GaAs lattice is fundamental to obtain the best epitaxial integration of GaAs on Si substrates.

Keywords: DFT, MBE, Epitaxy
This work was supported by: CONACyT México – Estancias postdoctorales por México 2021 of J. Alanis Pérez CVU 557499.

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[TSM-118] Transport properties of blue phosphorene nanoribbons saturated with hydrogen atoms interacting with pollutant molecules

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In the last decade the theoretical and experimental studies of two-dimensional (2D) materials have grown exponentially, because of the unique optical, mechanical, electronic and transport properties of such systems. These facts make the 2D materials good candidates for new nanoelectronics devices, specially, in the post-silicon era, where new alternatives have been invoked to replace the silicon in electronic devices. Monolayers based on silicon, germanium and carbon have been explored as potential materials to build electronic devices, unfortunately, the absence of an intrinsic band gap is not a desirable property for electronic applications. On the other hand, the blue phosphorene displays an indirect band gap of 2 eV, which make it suitable for its applications in electronic devices [1]. For this reason, the transport properties of blue phosphorene nanoribbons (BPNR) with hydrogen saturated edges in the presence of pollutant molecules are investigated. Studies are done using the density functional theory (DFT) and the non-equilibrium Green´s Function (NEGF) approach. Ozone (O_3), sulfur trioxide (SO_3) and acetylene (C_2H_2) molecules are adsorbed on the NR to induce current modifications as a function of the applied bias voltage. Results of the current ratio and sensitivity of the BPNR help visualizing the change in the current when the molecules interact with the BPNR, showing that the three molecules induce increase/decrease of the I-V curves, for positive/negative bias voltage, and how sensible the I-V curve of the BPNR is in the presence of pollutant molecules. The local density of states (LDOS) shows impurity levels in the band gap of the pristine BPNR as induced by the interaction with O_3 and C_2H_2 molecules. Moreover, when the C_2H_2 molecule interacts with the BPNR, the current as a function of the bias voltage increases significantly. In contrast, electronic and transport properties results when the SO_3 is adsorbed seem quite similar to those of the pristine BPNR.

Keywords: Blue phosphorene nanoribbons, DFT, Non-equilibrium Green´s function, Transport properties.
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[1] F. Safari, M. Moradinasab, U. Schwalke, L. Filipovic, Superior Sensitivity and Optical Response of Blue Phosphorene and Its Doped Systems for Gas Sensing Applications, ACS Omega, 6 (2021) 18770−18781. https://doi.org/10.1021/acsomega.1c01898.
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THIN FILMS

CHAIRMEN

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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.

[THF-185] "Synthesis of thin films of TiO2 deposited by Sputtering thecniche and afficent for photocatalytic redution of pollutants present in water."

Fernanda Arantxa Hernandez Rodriguez (fernanda.arantxa@gmail.com) [1] *, Maria Rocio Alfaro Cruz (malfroc@uanl.edu.mx)* [1] *, Leticia Myriam Torres Guerra* [1]
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TiO_2 is the most promising photocatalyst for degrading pollutants in water, as it, has demonstrated high photocatalytic activity which makes TiO_2 a semiconductor. Structurally we can find TiO_2 in three different crystalline phases: Anatase, Rutile, and Brookite. Both Anatase and rutile phase have been reported efficient for photocatalytic processes (dye degradation), while the brookite phase has been used for CO_2 photoreduction. Obtaining thin films of TiO_2 has been reported by different methods such as the Sputtering technique, which, allows us to modify the structural properties by changing the deposit conditions as the working pressure since this condition defines the energy with the involved particles collide with the substrate. In this work, the deposition of thin films of TiO_2 is presented by the sputtering method varying the working pressure. Different phases of TiO_2 (anatase, rutile, and brookite) were obtained depending on the working pressure used. The contribution of these phases changes the physicochemical properties of TiO_2, which influence the photocatalytic reduction of heavy metals present in water.

[THF-71] (Fe2O3)x(ZnO)1-x Thick Films obtained by Ultrasonic Spray Pyrolysis

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$(Fe_2O_3)_x(ZnO)_{1-x}$ composite thick films were prepared by Ultrasonic Spray Pyrolysis on a glass substrate. at 450°C. using 0.1 M aqueous solutions of $FeCl_3$ $6H_2O$ and $ZnCl_2$ anhydride compounds. To obtain different elemental concentration of Fe and Zn, we varied the volume of each aqueous solutions. The samples were characterized by X-ray photoelectron spectroscopy (XPS), The X-ray diffraction, Raman spectroscopy and optical transmission. The XPS results shown that tha x values were varied from 1 to 0.87. The X-rays diffraction caractherization revealed that the films were composed of different phases corresponding with common stable iron oxides ($ZnFe_2O_4$ - α, -Fe_2O_3) and zinc oxide (ZnO). Results from raman spectroscopy indicate that Fe_2O_3 vibrational modes are accompanied with new modes due to the presence of additional phases ZnO compounds. The band gaps were evaluated with the help of the experimental transmittance datas using the Tauc model, the results shown a modulation of the band gap values with the incorporation of ZnO. Theorical transmittance curves were obtained using the effective medium theory, using the Bruggeman model, the results showed a good agreenment with the experimental transmittance curves.

[THF-334] AIR-ANNEALING SELENIZATION OF SILVER ANTIMONY SULFIDE THIN-FILMS DEPOSITED ON STAINLESS STEEL SUBSTRATES BY CBD

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Selenization is an important stage for the fabrication of thin-film solar cells. This work presents the methodology to achieve air-annealing selenization of silver antimony sulfide ($AgSbS_2$) films deposited by chemical bath deposition (CBD) on stainless steel substrates. Selenium incorporation was carried out by heating 100 mg of selenium powder (Se, Sigma-Aldrich, 100 mesh) at 400 ºC. The optimal distance of $AgSbS_2$ films from the selenium source was kept at 5 cm to produce homogeneous selenization without elemental Se traces. X-ray diffraction (XRD) results showed polycrystalline silver antimony sulfide selenide ($AgSb(S,Se)_2$) thin-films with a face-centered cubic structure (a = 5.6721 Å) and metal oxides, elemental selenium or compounds related to the stainless steel substrate were not observed. The selenization process promotes a shift on the optical band gap (E_g) from 1.71 eV to 1.50 eV associated with $AgSbS_2$ and $AgSb(S,Se)_2$, respectively. The air-annealing selenization demonstrates that it is not necessary the use of special atmospheres such as Nitrogen or Argon. The use of stainless steel substrates opens the opportunity to develop flexible solar cells.

Keywords: air-annealing, selenization, silver antimony sulfide selenide, thin film, stainless steel
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[THF-274] Analysis of process parameters in sputtering of TiO2 with pulsed DC.

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In the sputtering thin film deposition technique, the power source plays a vital role in the intensity of ion bombardment. Usually, in sputtering, direct current (DC) or radio frequency (RF) sources are used to generate the ions. However, not all metal oxide materials can be sputtered efficiently using these power sources. Therefore, in recent years, pulsed direct current (DC pulse) sources have been chosen to increase the ion ratio compared to DC and RF sputtering. So, it is of importance to analyze the deposition of titanium oxide thin films by DC pulse sputtering to observe the relationship of on pulse width (ton), off pulse width (toff), and cycle time (tc) with ion formation.
In this work, we present an analysis of the influence of pressure (Pt), average current (Im), ton, toff, and tc on the formation of titanium, oxygen, and argon ions during the process of thin-film deposition by DC pulse sputtering. For this purpose, the emission spectrum (OES) and the average voltage (Vm) have been taken as state variables. The study is carried out for three pressures (5.0 10 and 15 mTorr), four pulse frequencies (75, 100, 125 and 150 kHz) and four average currents (0.20, 0.25, 0.30 and 0.35 mA). These parameters are considered input variables of the system. Multivariate analysis shows that, in the ultraviolet range, in the 398.18, 399.86, and 399.98 nm lines, titanium ion emission can be observed as a function of the input variables. Under maximum titanium ion emission conditions, oxygen flux sweeps were performed using linear step functions. With positive slopes, it was passed from the metallic mode to the reactive mode and negative slopes from the reactive mode to the metallic mode. With these sweeps, it is observed that the poisoning of the target can be analyzed through the lines 777.19 and 777.42 nm, which present a relationship of the oxygen ion emission with the reactive gas flux in both the metal deposition mode and the reactive mode the instantaneous voltage profile and the instantaneous current profile present relevant information of the bench poisoning process. This study aims to find the parameters that most influence the properties of thin films prepared by DC pulse sputtering.

[THF-239] Characterization and analysis of CsPbBr3 thin films by thermal evaporation

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All-organic perovskite devices have gained considerable attention due to their higher stability under ambient conditions. Among this class of materials, CsPbBr3 is very interesting not only for its stability, but also for its good optoelectronic properties, such as high optical absorption coefficient 105 cm-1, ~2.2 eV band gap, low exciton binding energy, long carrier diffusion length, etc. characteristics such as these make it an ideal material for various applications such as photodetectors, radiation sensors, solar cells, etc. In this work, we present the material studies of thermally evaporated $CsPbBr_3$ films and a prototype solar cell. The deposited films maintained the chemical composition and structural features of the source material, which was home-synthesized $CsPbBr_3$ crystals grown using anti-solvent vapor-assisted crystallization method. The as-deposited $CsPbBr_3$ films show an intense emission centered at 525 nm that can be attributed to free excitons. The films are photosensitive with photosensitivity value ~78.0. The role of post-deposition thermal processing in grain growth and the modification of recombination channels will be discussed.

Keywords: perovskite, photodetectors, radiation sensors, solar cells, anti-solvent vapor assisted.
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[THF-210] Characterization of porous VO2 thin films deposited by simple and sustainable spray technique.

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The transition process of VO2 (M) is well known as method energy efficient in thin film on glass to regulate solar energy in response to low heat. However, the application of methods for large scale film production has not yet been extensively studied. This paper describes the facile deposition of VO2 (M) particles on the silica glass substrate to evaluate their thermochromic effect. For this, its dispersion in 2 different aqueous media such as 2-propanol and ethylene glycol was evaluated. The results show an average particles size of 100nm with 2-propanol and 110nm. Subsequently this dispersion was sprayed on glass substrate for its characterization by X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), Scanning electron microscope (SEM, Energy Dispersive Spectroscopy (EDS), Atomic force microscopy (AFM), and Cary 5000 UV-VIS-NIR Spectrophotometer. It was obtained a homogeneous and porous thin film with particles size of 150nm regarding its optical properties, it was obtained a low modulation of ΔTSol = 3.9% at 5 layers this due to the high porosity of the thin film.

Keywords: Thermochromic; Energy efficient; Thin film; Glass substrate; Simple technique

[THF-433] COMPARATIVE STUDY OF AlTiCrN COATINGS DEPOSITED BY HIPIMS AND PULSED DC-RF COSPUTERING

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This work reports the results of a study of AlTiCrN coatings deposited using HIPIMS in comparison to films deposited using a combination pulsed DC-RF magnetron sputtering deposition. Samples of AlTiCrN were deposited under identical deposition conditions, that is the same substrate temperature, pressure, substrate to target distance and Ar/N2 ratio flow rate. The film microstructure and composition were analysed by X-ray diffraction (XRD), scanning electron microscopy (SEM), optical interferometry and energy dispersive X-ray spectroscopy (EDS). The sample porosity and corrosion resistance were studied by electrochemical methods such as electrochemical impedance spectroscopy and potentiodynamic polarization while the wear corrosion was carried out bole on disk. The pulse power and current between the deposition systems affect significantly the film's properties. The relationship between growth conditions, microstructure, corrosion and wear resistance is presented and discussed in this work

Keywords: HiPIMS, hard Coatings, EIS, Corrosion, sputtering.
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[THF-22] Comparison of superconducting films of SmFeAsO1-xFx grown by MOCVD on substrates of LaAlO3 and CaF2

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In the following work we report the formation of superconducting thin films of $SmFeAsO_{1-x}F_x$ on two different substrates: $LaAlO_3$ and CaF_2. The thin films where fabricated by a process that can be broken down in two parts. First, we grow thin films by a process of metal organic chemical vapor deposition (MOCVD) employing metal organic precursors of Sm and Fe. Second, we did a diffusion process of Fluor and Arsenic towards the thin films utilizing a pellet made of $SmFeAsO_{0.4}F_{0.2}$. This last process is made by a thermic treatment at various temperature plateau and different times for each one. We do this and with the help of EDS spectroscopy we obtain the chemical stoichiometry of each thin film and with X-ray diffraction we evaluate the different crystalline phase formations for the different conditions in the diffusion process. We notice that there are mayor differences in the phase formation of crystallites if the deposition is made on $LaAlO_3$ or on CaF_2; giving place to different superconducting properties. By utilizing a scanning electron microscope (SEM) we can observe the morphology of the films and with the resistances vs temperature measurements (RT) we can see the superconducting properties. The analysis of such data allows us to indicate which are the optimal times and temperature to obtain the best superconducting properties in each substrate.

[THF-325] DEVELOPMENT OF Sb2(S,Se)3 THIN FILMS FOR PHOTOVOLTAIC APPLICATIONS: SYNTHESIS AND CHARACTERIZATION

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Finding new materials to manufacture low-cost, high-efficiency photovoltaic devices has become a significant challenge. In recent years, compounds such as $Sb_2(S,Se)_3$ have emerged as an important alternative for efficient energy conversion in the future, since they have favorable characteristics such as being made of abundant and non-toxic elements, band gap tunable between 1.1 and 1.7 eV, p-type conductivity and a high absorption coefficient (105 cm-1). Currently, the efficiency record in antimony chalcogenides corresponds to an FTO/CdS/Sb2(S,Se)3/spiro-OMeTAD/Au structure with 10.7% efficiency, reported last year. In this work, we present a study to obtain the compound Sb2(S,Se)3 synthesized by means of an innovative technique, which consists of the evaporation of elemental Sb, followed by thermal treatment at different temperatures in an atmosphere of sulfur and selenium generated at from pure powders. The films were analyzed by X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM) for structural and morphological studies, and EDS for a compositional study. Their reflectances were also analyzed to determine the band-gap values. The results were discussed regarding the feasibility of the method with which they were determined as an alternative technique to the traditional methods used so far and for the subsequent use of these thin films in the process of high-quality and low-cost solar cells.

Keywords: Sb2(S,Se)3 thin films, solar cells, thermal evaporation, thermal treatment.
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[THF-159] Effect of growth temperature and hydrogen flow in the composition and photoluminescence properties of SiCxOy films deposited by HFCVD Technique

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In this work the effect of the growth temperature and hydrogen flow (H_2) on a strong white emission (3.35 to 1.72 eV) from non-stoichiometric silicon oxycarbide (SiC_xO_y) films deposited by hot filament chemical vapor deposition technique (HFCVD) is presented. The carbon and silicon oxide compounds in gas phase were generated from ethanol vapor and the chemical reaction of atomic hydrogen (H°) with a solid fused quartz source. The SiC_xO_y films were deposited on N-type crystalline silicon (100) substrates with resistivity of 1 to 20 ohm-cm. The substrate temperature was modified between 1000 to 800° C with a fixed H2 flow (62.4 sccm), and with a fixed substrate temperature (1000° C) and varying the H2 flow from 62.4 to 187 sccm. As a results from SIMS measurements; carbon concentration decrease for both group from 11 to 5 at.%. The Fourier transform infra-red spectroscopy measurements shown that an increase in carbon content favors the formation of both: Si-C bonds located at about 816 cm^{-1} and Si-O-Si vibrations located at around 1050-1070 cm^{-1}, the last absorption peak is associates to a SiOx network. From the photoluminescence measurements the samples shown an intense PL response, associated to Si-related oxygen vacancies (Si-NOVs) and Si-related oxygen deficiency centers (Si-ODCs) due to low carbon concentration into the SiC_xO_y films. As a conclusion we argue that the intense response of PL of the SiC_xO_y films can be associated to the nature of the radiative defects as a results of the experimental growth conditions of the samples which could be associated to the growth kinetic of films.

Keywords: SiCxOy films, HFCVD, PL, SIMS, FTIR.
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[THF-377] Effect of the cap layer thickness on AlGaAs/GaAs heterostructures for optoelectronic devices

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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 [1]. In this work, the effect of surface states (Nss) on the built-in electric field and charge distribution in n-i-p GaAs-based heterostructure is investigated by the implementation of a Front Surface Field layer (FSF) placed at different distance from surface by the capping layer thickness (CLT). We grew samples by molecular beam epitaxy with 40 nm FSF of (a) GaAs and (b) AlGaAs both n-type doped with $5x10^{18}$ cm^{-3} positioned at 80 nm from surface by the GaAs n-type doped with $5x10^{18}$ cm^{-3} caping layer. $H_2O_2/HCl/H_2O$ wet etching was employed to vary the CLT from the etching time. Thus, samples with capping layer of 80, 60, 40 and 20 nm were obtained with the aim to determine the best distance to optimize the effect of the FSF. We determined the depletion region and their modification with the passivation by Raman spectroscopy by the L- and LO integrated intensity, obtaining a reduction with the CLT. Franz-Keldish oscillations (FKO) in photoreflectance spectrum were employed to evaluate the built-in electric field. We found that the total built-in electric field changes around (a) 10% and (b) 4% with the wet etching. The current-voltage behavior under AM1.5 illumination at 550 W/m^2 indicates an improvement when the surface effect is controlled.

Keywords: optoelectronic devices, surface, photoreflectance, thin films**.**
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[THF-204] Effect of thermal annealing on the structural and optical properties of SiCxOy films obtained by HFCVD technique

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In this work, we report the influence of annealing temperature under O_2, N_2 and H_2 atmospheres on the structural and optical properties of SiC_xO_y films. The SiC_xO_y films were deposited on n-type silicon substrates (100) with resistivity ρ = 1-10 Ω cm^{-1} by using Hot Filament Chemical Vapor Deposition (HFCVD) technique. For SiC_xO_y films growth a solid source quartz SiO(s) and liquid ethanol C_2H_5OH bubbled by molecular hydrogen was used. The samples were deposited at substrate temperature of 800 °C using 15.6 sccm of H_2 flow. After the deposition the samples were annealed by rapid thermal annealing in the temperature range of 300 -900 °C. The films were characterized by Photoluminescence (PL), Fourier Transform Infrared Spectroscopy (FTIR) and X-Ray Photoelectron Spectroscopy (XPS). The FTIR results of as-deposited films showed three major peaks: Si–O–Si around 450, 845 and 1080 cm^{-1} attributed to Si–O–Si rocking mode, Si–C stretching mode, and Si–O–Si antisymmetric stretching mode, respectively. Suggesting a predominant phase of SiOx structure due to presence of intense bands associated to Si–O–Si bonds and the low carbon atomic concentration as was found by XPS from 1.4 to 6.8 at.%. The PL spectrum of the as-deposited films displayed a broad band centered at approximately 418 nm. For SiC_xO_y films annealed under N_2 and H_2 atmospheres, the stretching mode associated to Si–O–Si band increased as the annealing temperature increased. The PL intensity of green and red band increases as the annealing temperature increased. For the samples annealed under a O_2 atmosphere. The intensity of the Si–O–Si bond stretching mode slightly increased as the annealing temperature was increased. In contrast the PL emission decreases and shifts towards the blue region. The PL was consistent with that observed in defect-related Si-based materials (C-NOV, Si-NOV).

Keywords: HFCVD, SiC_xO_y, PL, FTIR, XPS.
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[THF-240] Effect TiO2/VO2 bilayer for application to smart windows

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Vanadium dioxide (VO_2) is a material with great potential in applications such as smart windows, thermosensors, thermal and optical switchers, IR sensors, etc. As it presents interesting thermochromic properties through an electron-phonon interaction that serves as a driving force for the transition from the Monoclinic crystal structure at low temperature to a Rutile tetragonal phase at high temperature. This phase transition temperature is close to 67°C. This phase transition presents changes in electrical properties and changes in optical properties within the near infrared region (NIR) (from transparent to highly reflective) and no obvious changes in the visible region. However, for a good thermochromic window, the ability to modulate solar energy is needed in both the region's IR as well as in the visible region. Currently, for the improving the properties of VO_2 to be used as a thermochromic window, it has been doped with elements such as W, Mo, Nb. in the present work, VO_2 has been doped with different concentrations of TiO_2 and characterized for its structural, optical, electrical, and morphological properties using different optoelectronic techniques. VO_2 was synthesized by the chemical solution method. TiO_2 was synthesized by sol-gel and later grown as thin films on the glass substrate by the Dip-coating technique and subsequently annealing. A detailed analysis was carried out to evaluate the effect of VO_2/TiO_2 bilayer, when compared to the solar modulation in the visible and the NIR region, on its transition temperature, thermal hysteresis.

Keywords: Vanadium dioxide (VO_2), smart window, TiO_2.
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[THF-306] Electrical properties on TiO2/TiON by sputtering for UV Vis range absorbance applications

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Abstract

Several studies were carried out on TiO2 thin films.This material can produce electrons in the conduction band when it changes its structure. The anatase phase could change with thermal annealing to the rutile phase. The formed interface contributes to generating electrons attributed to nitrogen doping as TiON.The thickness of the films (less than 100 nm) were measured in the scanning electron microscope (SEM), and optical properties of the material were obtained by means of the UV-vis technique, to continue with the analysis of the electrical properties. This work was carried out with the objective of obtaining the structural contribution of each phase, which helped to estimate the electrical properties. This analysis gives us an idea about the innovation and technology for augmented reality devices by using anatase-rutile TiON phases.

Keywords: anatase, rutile, sputtering, TiO2, electrical properties

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Reference: Nowotny M.K., (2006), Electrical properties and Defect Chemistry of TiO2 Single Crystal I. Electrical conductivity, J. Phys. Chem. B, (110), 16270-16282

[THF-299] Electrodeposition of antimony sulfide selenide thin films: effect of the deposition potential.

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Keywords: $Sb_2(S_xSe_{1-x})_3$, electrodeposition, photosensitive

$Sb_2(S_xSe_{1-x})_3$ is a promising semiconductor material to be used as absorber in solar cells due to its optoelectronic properties, low cost of fabrication, abundant materials, and low toxicity. This semiconductor has been synthesized by different techniques, one of them is the electrodeposition, which allows to obtain homogenous thin films. In this work, the effect of the electrodeposition potential for the development of antimony sulfide selenide thin films was analyzed. The potential tested were -0.6, -0.66 and -0.72 V vs. SCE. The electrolyte consisted of 18 mM $Na_2S_2O_3$, 1.5 mM $SbCl_3$ and 0.8 mM H_2SeO_3. The amorphous thin films obtained were annealed at 350 °C in N_2/S atmosphere for 30 minutes to obtain the crystalline structure. The XRD, Raman and Rietveld results showed the formation of the $Sb_2(S_xSe_{1-x})_3$ with a crystallite size of 20 nm. The band gap calculated was in the range of 1.55 to 1.4 eV, and the samples were photosensitive. With these results, a simulation with SCAPS software was carried out, where it was found a theoretical efficiency of 12 %, making it attractive for solar cell applications.

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[THF-283] Electrodeposition of CuSbS2 thin films for the fabrication of a photoelectrochemical cell.

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Copper antimony sulfide ($CuSbS_2$) has been proposed as an alternative to CdTe and CIGS considering its non-toxicity, relative abundance, and excellent optoelectronic properties. $CuSbS_2$ has direct band gap in the range of 1.38-1.56 eV and high absorption coefficient of 10^{-4} cm^{-1}, which are optimal for absorber layers in solar cells. In the present work, $CuSbS_2$ thin films were developed by pulse electrodeposition technique on FTO glass substrates from a single bath. The electrodeposition bath consisted of 1.5 mM $SbCl_3$, 0.4 mM $CuCl_2$ and 18 mM $Na_2S_2O_3$. The potentials were applied in pulse form with respect to saturated calomel electrode, deposition potential (V_{on}) was fixed at -0.72 V and dissolution potential (V_{off}) was -0.1 V. Films of approximately 500 nm were obtained after 300 cycles. As deposited films were amorphous and the films were crystallized in chalcostibite phase after annealing at 300 °C in N_2/S atmosphere for 30 minutes. The estimated band gap of the films was 1.42 eV. The films were photosensitive and there was an increase in the conductivity of about one order. PEC measurements were done 0.1 M HSO using the films annealed at 300 °C which confirmed the p-type conductivity of the material. The Sb_2Se_3 photocathode exhibits a photocurrent density of almost 0.2 mA cm^{-2} at 0.4 vs saturated calomel electrode.

Acknowledgements: This work was done in IER-UNAM and was supported by the projects (PAPIIT: IN102921). Authors thank Patricia Eugenia Altuzar Coello for the XRD measurements.
Keywords: chalcostibite, electrodeposition, photocurrent.

[THF-350] High-temperature corrosion resistance of Ti-Al-Cr-N thin films prepared by reactive co-sputtering

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This work presents the methodology of the synthesis of (Cr,Al,Ti)N coatings deposited on AISI 316L by means HIPIMS, and the high-temperature corrosión behavior of the coatings was studied. The thin films were obtained using Cr and TiAl targets with 99.9% purity. The corrosion resistance was evaluated via the cyclic oxidation test at a temperature of 600°C and isothermal oxidation tests at a temperature of 700 °C. The corrosión behavior of coatings was evaluated by weight loss, following the ASTM G31-12 . The coatings and the corrosiòn products were analyzed by scanning electron microscopy (SEM), X-ray diffraction (XRD), and 3D optical microscopy. The results have shown that the coatings are polycrystalline and that the corrosion resistance of samples was improved, demonstrating that the coatings act as a protective barrier to the stainless steel. The corrosion mechanisms also will be discussed in this work.

[THF-364] INFLUENCE OF CdS THICKNESS FILM ON SnS/CdS FLEXIBLE HETEROJUNCTION DEPOSITED BY CHEMICAL BATH DEPOSITION

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The use of binary semiconductor compounds such as cadmium sulfide and tin sulfide is still attractive for the development of heterojunctions. In this work, a flexible heterojunction was obtained by chemical bath deposition on ITO-coated PET using CdS films as n-type semiconductor and SnS films as p-type semiconductor. Cadmium nitrate and thiourea were used as precursors of Cd ions and S ions respectively, by another hand, tin chloride and thioacetamide were used as precursor of Sn ions and S ions respectively. The thickness of CdS film was varied to observe its influence on the CdS/SnS heterojunction parameters, such as, lattice mismatch, built-in voltage, potential barrier, and band alignments. The bandgap energies alignment determines the characteristics of the junction. Specular transmittance and reflectance measurements were done to evaluate the absorption coefficient and band gap. The deposited CdS films shown a band gap of 2.49 eV while the SnS exhibits a band gap of 1.17 eV, this differences in band gap values promotes the formation of the heterojunction called “staggered”. X-ray diffraction (XRD) results showed polycrystalline CdS with a hexagonal structure, while SnS exhibits an orthorhombic structure, the deposition temperature for CdS was kept at 75 °C and for SnS the deposition was carried out at 35 °C. The use of ITO-coated PET substrates opens the opportunity to develop flexible semiconductor devices.

Keywords: Cadmium sulfide, tin sulfide, flexible-heterojunction, thin film, chemical bath deposition.
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This work was supported by VIEP-BUAP

[THF-186] INFLUENCE OF TEMPERATURE AND OXYGEN FLUX ON THE GROWTH OF COPPER OXIDE THIN FILMS BY REACTIVE MAGNETRON SPUTTERING

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The increasing energy demand has brought the need to use alternative energy sources for energy production. Cu_2O promises to be a good candidate as an absorbent material in energy conversion applications. It is a non-toxic compound with low cost, and it is easy to produce by different techniques. In addition, has good optical and electrical properties, such as a high absorption coefficient of $\alpha = 4 \times 10^3\ cm^{-1}$ and a band gap energy ranging from 1.9 and 2.6 eV [1]. In this work, CuO and Cu_2O thin films were obtained by deposition in a reactive magnetron sputtering system. The effect of oxygen flux (3 and 1.6 sccm) and substrate heating temperature (25 to 200 °C) on structural and optical properties was studied. The results indicated that high oxygen atmospheres (3 sccm) produce thin films with the CuO phase, while a low oxygen atmosphere (1.6 sccm) results in thin films with the Cu_2O phase. The substrate heating temperature increases the crystallite size from 15 to 21 nm for CuO samples and from 7 to 8 nm for Cu_2O samples. The evolution of the surface morphology goes from pyramidal grains to a smooth surface. However, there is the formation of cracks in the CuO samples with increasing temperature, while in the Cu_2O samples, an improvement in surface morphology was observed. The morphology evolves from a surface with cracks to a homogeneous surface with better-defined and uniform grains. The thickness of the samples increased when the heating temperature of the substrate increases. However, the band gap remains unchanged with the increase in substrate temperature. All the samples present an absorption coefficient of $10^4\ cm^{-1}$ in the 280 to 800 nm range, which favors their use as absorbent material for photovoltaic applications.

Keywords: Thin films, magnetron sputtering reactive, Cu_2O, absorbent materials, semiconductors.
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[1] A. Pérez-Tomás, A. Mingorance, D. Tanenbaum, and M. Lira-Cantú, Future of Semiconductor Oxides Next-Generation Solar Cells, Elsevier Inc. (2018) 267–356. https://doi.org/10.1016/B978-0-12-811165-9.00008-9.

[THF-287] Optical characterization of edible imitation gold sheets

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The optical behavior of edible imitation gold sheets is analyzed using diffraction patterns. Unlike iron or calcium, gold is not an essential element in the human diet; however, the consumption of this used as a visual attraction in food dates to the ancient Egyptians. Currently, due to the demand arising from the massive dissemination through social media, there is a wide catalog of edible sheets that imitate the physical properties of genuine gold sheets. Elemental gold is inert and has very low solubility, so it is eliminated by the body through simple digestion. It is extremely important to know the elements that are present in these imitations to determine in what quantities and frequency of consumption they can become harmful in human intake. The studied sheets have semi-macroscopic separations capable of diffracting wavelengths in the visible range, which provides significant information about the quality and physical characteristics that more closely resemble those of genuine edible gold.

-Keywords: Diffraction grating, Distance between gold particles. Edible gold, Fraunhofer diffraction, Fresnel – Huygens principle
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[THF-194] SnS-Bi2S3 AS A TERNARY EMERGING ABSORBER COMPOUND FOR PHOTOVOLTAIC DEVICES

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Nowadays, studies on solar cells as devices capable of producing electricity have increased; but it is also true that the limit of the materials used for their fabrication is being reached, in the configuration of these devices, the absorber materials are the most important component, so it is in search of emerging absorbers that come from abundant sources and at the same time are economical, within the multiple routes for the manufacture of such materials are the technologies based on thin films, this is because some of the manufacturing processes are low cost.
In this work, we presented the synthesis and characterization of thin films of an emerging ternary compound SnS-Bi_2S_3 that were carried out by the chemical bath deposition method, using $SnCl_2$ and $Bi(NO_3)_3$ as the source of Sn^{2+} and Bi^{3+} ions, respectively. The deposition temperature of the films was 40 °C, deposits were carried out for different times, then the films were subjected to heat treatments between 250 °C and 300 °C; the purpose of these films is the application in solar cells. The following are proposed as the first configurations for such devices: TCO/SnS-Bi_2S_3/PbS and TCO/SnS-Bi_2S_3/SnS. The obtained films were characterized by X-ray diffraction (XRD), Raman spectroscopy, spectroscopic ellipsometry, and UV-Vis spectroscopy to know their structural and optical properties. I-V curve measurements were performed, with which we obtained important parameters characteristic of the photovoltaic devices. We obtained a coincidence with the $SnBi_2S_4$ material, which is an orthorhombic system, with thicknesses between 100 and 160 nm, absorption coefficient values in the order of 10^5, and bandgap energy values between 1.5 and 1.8 eV, depending on the thickness and heat treatment.

Keywords: emerging material, thin film absorber, SnS-Bi_2S_3, CBD.
The authors would like to thank the Coordinación para la Innovación y Aplicación de la Ciencia y la Tecnología (CIACYT) for their support during the development of the project and the Laboratorio Nacional de Análisis Físicos, Químicos y Biológicos. To the announcement: support for the acquisition and maintenance of infrastructure in institutions and specialized research laboratories 2019 with project number: 299812. And to CONACYT for their support with scholarship number 755893.

[THF-317] Structural, Morphological and Electrical Characterization of Î²-Ga2O3 thin films on sapphire obtained by Sol-Gel Method.

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Thin films of β-Ga_2O_3 were obtained by synthesizing gallium oxide [Ga_2O_3] by the sol-gel method, using [Ga(NO)3 × H_2O], monoethanolamine [MEA], and 2-methoxyethanol as precursors and aging for 24 hours. The solution was deposited on (1000) c-plane sapphire substrates by spin coating with a different number of layers. An intermediate pre-annealing process at 250 °C has been carried out between each deposited layer to remove the excess solvent and the organic compounds. The resulting samples were annealed at 900 °C to obtain the beta phase. The beta gallium oxide thin films were analyzed by X-ray diffraction to obtain crystallinity information. Then, the films were analyzed by atomic force microscopy to determine the roughness. Further, I-V measurements were performed to determine the electrical properties and the influence of the film's thickness on the electrical behavior.

Keywords: Thin films, beta gallium oxide, Sol-Gel.
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Reference: Shen, Hao, et al., Growth and characterization of β-Ga2O3 thin films by sol-gel method for fast-response solar-blind ultraviolet photodetectors, Journal of Alloys Compd 766 (2018)601-608. https://doi.org/10.1016/j.jallcom.2018.06.313

[THF-245] Structural, Optical and Electronic Properties on N-doped HfO2

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HfO2 thin films doped with Nitrogen has been studied to observe their structural and optical properties. These structures were analyzed by XRD and UV-Vis spectroscopy. Typical monoclinical behavior was observed, and the optical band gap was calculated, observing the efect of nitrogen doping on the optical response. Band Structure and Density of States for m-HfO2 and doped m-HfO2 were analyzed to up to doping at 20% , to correlate DFT calculations with experimental results. In order to compare the structures, HfN doped with oxygen has been analyzed too, considering the initial crystalline structure for the nitride and the effects of the oxygen incorporation.

[THF-439] Study and evaluation of thin films synthetized by chemical deposition for the design of a window buffer layer.

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Semiconductor materials used for the build-up of thin films are one of the topics studied globally, due to the various uses that these materials can provide. The production of photovoltaic cells metallic sulfides has taken a great boom since 2011 due to the present abundance of the compounds and their low toxicity. The noticeable advantage related to the use of these materials comes the diverse methods of elaboration of a thin film. 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 said materials in a single thin film for the formation of a semitransparent window buffer layer. It is worth mentioning that the chemical deposit technique used in this project handles different cycle times that are important to establish: 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 film. A reaction mechanism is proposed for the first layer between glass and SnCl2 to explain the reaction that takes place in it. The X-ray Diffraction (XRD) and Raman spectroscopy studies showed that all the multilayer films exhibited polycrystalline nature. The absorbance data obtained 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 methods established the values are 25 Ω and 0.1 Ω respectively.

[THF-229] STUDY OF CORROSION BEHAVIOR IN SIMULATED PHYSIOLOGICAL ENVIRONMENT OF STAINLESS STEEL 17-4 PH COATED BY TiN/Ti LAYERS

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Total knee arthroplasty (RTA) is one of the most effective surgical interventions to relieve pain and restore joint function in patients with advanced degenerative arthritis or rheumatoid arthritis, where the metal implants are the most widely used in the medical industry. However, metals in contact with biological systems are corroded; thus, patients implanted with metal prostheses usually suffer sequelae due to corrosion processes. Studies have shown that implementing ceramic coatings, as single or multilayers, substantially improves the corrosion resistance of various metal materials. In this work, Arc PVD biocompatible multilayer coatings based on TiN/Ti on 17-4 PH stainless steel have undergone a simulated physiological environment to study the corrosion mechanisms.
The adhesion and surface morphology of Arc-PVD coatings were analyzed by dynamic scratching, profilometry, and scanning electron microscopy. Likewise, coatings corrosion resistance was studied by potentiodynamic polarization and electrochemical impedance spectroscopy (EIS) tests, using brine with a NaCl concentration of 3.5% w/w, as well as simulated body fluid (SBF) and Hank solution.
As is expected, a reduction in the corrosion rate of the coated specimens was found in comparison with 17-4 PH stainless steel due to the presence of a protective layer at the surface. The mechanisms involved in the corrosion phenomena are discussed. Finally, we found that coatings with TiN/Ti architectures are excellent candidates for the protection of medical devices.

Keywords: TiN/Ti, Corrosion protection, Arc-PVD, Electrochemical Impedance Spectroscopy, Physiological body fluids

[THF-354] Synthesis of ZnO-Ag/Cu nanocomposites by combining Sol-Gel and LASL.

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We seek to study the possible bactericidal and photocatalyst properties of ZnO-Ag/Cu nanocomposites and create a thin film with these properties.
Copper and silver nanoparticles have been shown to have antibacterial properties, as they have the ability to continuously release Ag ions, which are mainly reactive and toxic for microorganisms. These released ions can adhere to the bacterial cell wall and cytoplasmic membrane, due to electrostatic attraction and affinity for sulfur proteins. Once attached to the cell wall they can increase cell permeability causing the destruction of bacterial infection, and consequently the cell lysis.
The laser ablation of solid in liquids technique is a physical nanoparticle sintering method, it can work with a variety of nanomaterials in a variety of liquid solutions, with this technique we seek to produce nanoparticles in a solution of methanol and zinc acetate dihydrate which will be used to prepare thin films to make nanocomposite.
The characterization of the thin films will be carried out by uv-vis, and their photoluminescence will also be studied.

[THF-310] Temperature and Oxygen Influence on the Electrical Resistance of ITO Thin Films

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In this work ITO thin films were prepared to analyze temperature and oxygen concentration influence on electrical resistance. ITO thin films were deposited by sputtering at both, ambient temperature and 200 f; also, oxygen flow was varied from 0 to 6 ccm. For electrical resistance characterization it was used a parameter analyzer KEITHLEY 4200 SCS. Transmittance characterization was performed by Cary 5000 UV-visible-NIR. ITO thin films were deposited at 200 f and with no oxygen addition during deposition, achieving low resistance (0.134Ω) and good transparency. Highest resistance ITO thin films were obtained at ambient temperature and 6 ccm oxygen flow ($6x10^6$ Ω).

Keywords: ccm (cubic centimeters per minute), ITO, Resistance, transparency, sputtering.
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[THF-189] TiO2 thin films deposited by Sputtering technique and their performance as photocatalyst in hydrogen production

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TiO_2 is one of the most prominent materials in photocatalytic processes due to its physicochemical properties. It has shown high photocatalytic activity and good photostability and is a low-cost material. TiO_2 can be found in three different crystalline phases such as rutile, anatase, and brookite. The presence of these phases can contribute to a better performance in different photocatalytic processes, such as dye degradation, hydrogen production, and CO_2 photoreduction. In this sense, thin films of TiO_2 were deposited by the sputtering method to be used as photocatalysts in hydrogen production. The films were deposited at different working pressures to achieve the presence of the three characteristic phases of TiO_2. The structural, optical, and electrochemical properties were studied using X-ray diffraction techniques, UV-Vis spectroscopy, and electrochemical measurements. Photocatalytic efficiency in hydrogen production was evaluated using a chromatograph with a thermal conductivity detector (TCD). Results will be discussed.

Keywords: TiO2, thin films, photocatalysis, hydrogen production.
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[THF-15] Wear resistance of TiAlVCuN coatings deposited by HiPIMS and pulsed DC-RF cosputering

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This work reports the results of a study of TiAlVCuN coatings deposited using HIPIMS, with various pulse currents in comparison to films deposited using a combination HIPIMS-RF, HIPIMS-DC and conventional pulsed DC-RF magnetron sputtering deposition. Samples of TiAlVCuN were deposited under identical deposition conditions: the same substrate temperature, discharge power, pressure, substrate to target distance, and Ar/N2 ratio flow-rate. The film microstructure and composition were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), optical interferometry and energy dispersive X-ray spectroscopy (EDS). The mechanical and tribological properties were evaluated through nanoindentation, and the wear resistance was studied with the pin-on-disk technique. The pulse power and current between the deposition systems significantly affect the film properties. The relationship between growth conditions, microstructure, and wear resistance is presented and discussed in this work.

Sesión Oral

[THF-111] BISMUTH SULFIDE NANORODS DECORATED CESIUM BISMUTH IODIDE COMPOSITE THIN FILMS BY ULTRASONIC SPRAY PYROLYSIS

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The lead-free perovskite cesium bismuth iodide ($Cs_3Bi_2I_9$) has emerged as an excellent candidate for optoelectronic applications due to its stability, photosensitivity and eco-friendliness[1]. On the other hand, bismuth sulfide (Bi_2S_3) has suitable electrical and optical (Eg ~ 1.5 eV) properties for solar cell applications. Herein, we incorporate Bi_2S_3 nanorods into the $Cs_3Bi_2I_9$ thin film in a single-step ultrasonic spray deposition adding thioacetamide (TA) in the Cs-Bi-I precursor solution. The concentration of the TA in the solution was varied from 0.01 to 0.05 M, at a given substrate temperature. The films formed are investigated in detail using XRD, Raman spectroscopy, SEM and UV-Vis-NIR spectroscopy. At lower concentrations, we show that the thioacetamide can behave as a complexing agent in the spray solution which leads to controlled pyrolysis at the substrate surface resulting in high-quality polycrystalline films. The $Cs_3Bi_2I_9$ has a hexagonal structure ($P6_3/mmc$) and the films are preferentially oriented along (006) direction perpendicular to the substrate. Moreover, the thin films (thickness ~300 nm) have excellent uniformity as evident from the morphology probed by the scanning electron microscopy. The thin films demonstrate a superior absorption coefficient up to the order of ~10^5 cm^{-1} in the visible region with a calculated direct band gap of around 2 eV. The conductive Bi_2S_3 nanorods in the composite films enhance the dark current in the $Cs_3Bi_2I_9$ thin films from ~0.08 nA to ~1 nA, whereas, the lower band gap of ~1.5 eV increases photocurrent. Furthermore, we evaluate the thickness dependence of the best photosensitive thin films in photodetector as well as photovoltaic heterojunction with CdS.

Keywords: Ultrasonic spray pyrolysis; $Cs_3Bi_2I_9$ Thin films; Bi_2S_3 nanorods; Photodetectors
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Reference: Devasia, S.; Shaji, S.; Avellaneda, D. A.; Martinez, J. A. A.; Krishnan, B. In Situ Crystallization of 0D Perovskite Derivative Cs3Bi2I9 Thin Films via Ultrasonic Spray. *J. Alloys Compd.* **2022**, *893*, 162294. https://doi.org/10.1016/j.jallcom.2021.162294.
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[THF-143] Design Of Logic Gates Based On Zno-TFT On Flexible Substrates Processed At Low Temperature

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The thin film transistor Technology has been the interest of the research community in the last years because they are the key to developing novel applications. The new generation of technology required low power operation, low cost of fabrication, and high level integration of various functions. Therefore, the knowledge of these devices allow to develop the building blocks for digital gate circuits and several analog circuits in the current modern electronics [1]. However, the bottleneck for their commercialization is due to the missing understanding of these devices. Therefore, the development of 2D models for numerical simulations considering the density of states (DOS) to be incorporated into analytical models for circuit simulation programs (SPICE), in order to design logic gates or analog circuits for novel applications. In this study, we proposed analytical models of the TFTs based on oxide of zinc (ZnO-TFTs) using the experimental data obtained in our ZnO TFTs fabricated by Ultrasonic Spray Pyrolysis at a high frequency on polyethylene terephthalate plastic substrates. In addition, the simulation by SPICE provides an understanding in the design of ZnO-TFTs circuits.

Keywords: TFTs, ZnO, SPICE, the density of states, Inverter.
Acknoledgment.
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[THF-392] Effect of the filling fraction and the heat treatment temperature in the modification of the optical properties of Gold nanoislands obtained by thermal evaporation.

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The development and studies of materials with plasmonic properties is a current topic of great importance for scientific and technological reasons. It is well known that the solid state gold films shows a dewetting behavior during heat treatment. However, in this work, the evolution of the optical properties of gold nanoislands as a function of temperature, as well as the initial filling fraction of the gold deposit, is studied. The filling fraction was controlled through measuring the electrical properties of the deposited material during the evaporationthe and fitting this to percolation theory. Four differents granular gold films with different filling fractions were deposited: 0.28, 0.42, 0.49 and 0.87. The deposits obtained were isothermally treated at different temperatures between 150 and 450 degrees centigrade. The material deposited in the evaporator hood was analyzed by differential scanning calorimetry. Absorbance measurements of the heat treated deposits were analyzed with a Cary 5000 spectrophotometer. As expected, the particle size depends on the heat treatment temperature. However, it is observed that the initial filling fraction of the gold films is also important in the formation of nanoparticles on the surface. According to the theoretical adjustments of the absorption spectra to the Maxwell Garnett theory, it is inferred that while the filling fraction is lower, the particle size decreases and also the particle size distribution becomes more uniform as heat treatment temperature increases and the initial filler fraction decreases.

Keywords: granular films, percolation, thermal evaporation, dewetting, absortion
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[THF-95] EVALUATION OF SiO2@TiO2 COMPOSITE AS A HYDROPHOBIC AND ANTIFUNGAL BARRIER FOR APPLICATION AS A PACKAGE COATING.

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Package materials have wide use in the alimentary industry. Packages such as cardboard have a high moisture permeability and risk of contamination by microorganisms, offering a shorter shelf-life than other non-organic packaging material. Self-cleaning, photocatalytic, and antimicrobial properties of SiO2@TiO2 have been previously reported, which is of interest for the study of the viability as a hydrophobic and antimicrobial coating in food packaging. The following work reports the synthesis, characterization, and antifungal activity evaluation of the SiO2@TiO2 composite. The coating was synthesized by the sol-gel method coupled to sonochemistry with two different cavitation times, 30 min (S30) and 40 min (S40). The composite was obtained from the mixture of two sols of SiO2 and TiO2 under ultrasonic bath conditions. XRD analyzed the crystallinity of the material. The diffraction peak at 28.7 ° corresponds to the (110) plane of the rutile phase of TiO2, confirming its presence in the material. The surface topography analyzed by AFM revealed a rough surface with pores presence and a roughness value (Ra) of 11.31 ± 1.94 nm for S30 and 21.86 ± 7.47 nm for S40. The chemical composition of the composite was analyzed by ATR-FTIR, obtaining signals between 1044 and 934 cm-1 corresponding to the Si-O-Si bonds and at 1263 cm-1 for the -CH3 terminal groups of SiO2 and PDMS, while the signal at 934 cm-1 corresponds to the signal of the Si-O-Ti copolymerization. Contact angle measurements were performed on glass, cardboard, and aluminum substrates, obtaining contact angles c values of 93.7 °, 111.8 ° and 87.8 °, respectively. Lastly, a fungal growth inhibition effect was observed on the coated aluminum surface concerning the uncoated aluminum, which leads to the conclusion that the properties of the SiO2@TiO2 composite contribute to the impermeability of the packaging and its effect of inhibiting fungal growth.

[THF-291] FABRICATION OF ZrO2 THIN FILMS USING A SIMPLE METHOD.

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Zirconium oxide (ZrO2), commonly called zirconia, is a ceramic material with high hardness and high melting point. In its natural state, zirconia has a monoclinic crystalline structure that is preserved from room temperature up to 1150°C, known as unstabilized zirconia. At this temperature, a martensitic transformation to a tetragonal structure occurs. Above 2370°C, the oxide exhibits a stable cubic crystalline structure until melting at 2650°C. When the zirconium dioxide has a nanocrystallite size around 25 nm, the tetragonal phase can be maintained at room temperature. In the present work we show the results of ZrO_2 thin films calcined at 250 and 550 °C, created by using the sol-gel and dip-coating technique. In the XRD results we can observe a good quality of the thin films which were identified and analyzed. The particle size calculation was performed as well as the preferential orientation. In addition, a surface analysis of the thin films is presented. The crystallite sizes are in a range 15.6 to 19.6 nm. The spectrum shows a preferential orientation with the (101) peak at 30.44°. The increase of calcination temperature prove that it is necessary in order to form the crystals in the ZrO2 thin films, having a crystalline tetragonal form.

Keywords: Thin Films; ZrO_2; Nanomaterials; x-ray diffraction; sol-gel.
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This work was supported by: NanoBiotechnology and Photocatalysis Laboratory (FI-UAQ).

[THF-133] Growth & Characterization of SiC Thin Films on Glass Substrates utilizing R.F. Magnetron Sputtering

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SiC technology has been widely researched and utilized in a plethora of commonly known applications, from MOSFETs to coatings and other miscellaneous uses. Even though this material sees wide use in our modern industry, it is still ripe for testing in new applications by taking advantage of modern growth techniques & methods, as well as alloy technologies. In this study, we strived to initially obtain crystalline SiC grown on amorphous SiO_2 (glass) substrates in order to fuel further experiments with this material. Using R.F. Magnetron Sputtering, we were able to grow SiC thin films through traditional growth routes & a novel ramping method, as well as characterizing them through AFM Microscopy, Spectroscopic Ellipsometry & Raman Spectroscopy. These characterization techniques allowed us to obtain valuable information on surface morphology, band gap energy and crystalline phase. AFM measurements presented a periodic grain pattern akin to terraces with quadrilateral grains, a radically different geometry when compared to traditional semiconductor and SiC surfaces. On the other hand, band gaps were in order of traditional SiC polytypes, which we believe were confirmed through the Raman spectra obtained, revealing a mix of different phases like 3C, 2H and 6H SiC polytypes. Even though no current application is planned for this material, these studies will allow us to further develop SiC growth methods to manipulate the material properties for its wider use as a semiconductor, including control of crystal phase with growth parameters & band gap engineering through alloys.

[THF-258] Influence of Diamond Thin Films Growth Processes as Perspective for Planar Optical Waveguides Application.

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This paper describes the optical and electrical properties correlated with morphological, chemical and crystallinities characteristics of different diamond thin films from micro-crystalline diamond (MCD, 0.5–3 μm grain sizes), nano-crystalline diamond (NCD, 10–500 nm grain sizes) and ultranano-crystalline diamond (UNCD 2-10 nm grain sizes or depending on rate gas flow). The growth process is the same for MCD and NCD thin films using a high H_2 rate flow (200 scm)/CH_4 (3 sccm) and for UNCD thin films were growth modifying the H_2 flow ratios in 73.5%, 49% and 9.8% (CH_4/Ar mixture were maintained fixed during the growth) by hot filament chemical vapor deposition (HFCVD). The optical properties were correlated with thickness, grain size and chemical composition, and with this data were analyzed by computational methods obtaining refractive index, thickness, and number of modes (λ= 633 nm) for planar optical waveguide applications.

Keywords: Diamond, HFCVD, thin films, waveguide, optical properties.
Acknowledgments:
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[THF-292] Methodologies for adhesion of Au thin films on PMMA substrates

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In this work, three methodologies for adhesion of gold (Au) thin films, deposited by e-beam evaporation, to polymethylmethacrylate (PMMA) surfaces were carried out and evaluated. The considered methodologies were intermetallic deposition of titanium (Ti) film, physicochemical modification by reactive oxygen ions, and chemical functionalization of PMMA surfaces with thiol groups through cysteamine treatments. The hydrophobicity of the surfaces after the treatments was measured by the contact angle technique. Cysteamine functionalization was verified by UV-visible measurements. The feasibility of the proposals was assessed with ultrasonic vibration and detachment tests. According to UV-visible measurements, functionalization of PMMA surfaces with cysteamine is achieved by pretreatment with UV light. The results of the tests report that at higher contact angles (>110°), the greater the adherence of the Au films. Although the methodologies were tested separately, adhesion of 150-nm-thick Au film was achieved using the combination of two of these methodologies: treatment in O_2 plasma followed by deposition of a Ti film. These results can be used for fabrication of electronic devices on PMMA substrates.

Keywords: Thin film, PMMA substrate, plasma treatment, e-beam evaporation, functionalization.
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This work was supported by Consejo Nacional de Ciencia y Tecnología (CONACYT) through the *Cátedra* project No. 746 “Scientific development and prospection of microfluidic systems for the energy sector and biomedicine” and the Frontier Science 2019 No. 845132.

[THF-221] NICKEL OXIDE THIN FILMS OBTAINED BY RADIOFREQUENCY MAGNETRON SPUTTERING FOR UV-VIS PHOTODETECTORS

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An important advance on the way to new semiconductor materials for thin-film device technology is the use of metal oxides as active layer. One of the most interesting materials is nickel oxide (NiO) due to its natural p-type conductivity, high transmittance in the visible range and high chemical stability [1]. NiO is also a good candidate for optoelectronic devices and resistive memories. In this study, NiO_x thin films were deposited by r.f. magnetron sputtering of NiO target at room temperature and powers in the range of 40 – 80 W. After the deposition, part of the films were annealed at 450 ^oC for 1 h to form nanocrystals. The as-deposited and annealed films were characterized by ellipsometry, XRD, AFM and XPS. Heterojunction diodes were fabricated by deposition of thin NiO_x layers on n-type Si. The photoresponse of the diodes was studied by current-voltage measurements in dark and under UV and visible light irradiation. The obtained responsivity (R) depended on the r.f. power and was higher for the annealed diodes. The highest values of R, between ~30 and 65 A/W for light with wavelengths in the 365 -635 nm range, were found for annealed diodes with NiO_x deposited at 60 W. These values of R are among the highest ones reported for broadband photodetectors.

Keywords: nickel oxide, sputtering, NiOx/n-Si, photodetectors, high responsivity.
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Reference: X. Yu, T. J. Marks, and A. Facchetti, Metal oxides for optoelectronic applications, Nature materials, 15 (2016) 383-396.
This work was supported by E. Osorio (CVU: 1057649), gratefully acknowledges CONACYT for Master´s scholarship.

[THF-150] Onset of electronic conductivity in nanometer thick films of yttria stabilized zirconia (YSZ) at high electric fields

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Electric measurements are presented that validate equations that describe the onset of conductivity in YSZ ALD due to the application of intense electric fields at high temperatures. The YSZ decomposes into elements if the cell voltage is above the decomposition voltage. Regions near the cathode are reduced and near the anode are oxidized. A region of unreacted YSZ remained with its prominent ionic conductivity in-between regions. Thus, YSZ acts like a n/i/p junction.

1. Switching off a high electric field leads to a drastic increase to the steady-state or the initial state, respectively. This is even more pronounced if the temperature is reduced before or at the time of switching. This determines whether stored memory or the internal reaction products, respectively, become volatile or not in memristors.
2. The model used in the present study is applicable to flash sintering explaining the onset of increased electronic conductivity, which finally triggers more Joule heating in a self-accelerating way.
3. The model used in this study assumes a flat interface between the reacted and unreacted YSZ. Whether this occurs or whether finger and filament type excursions of the interface appear could be a matter of driving voltage and temperature. The agreement between experimental results and the model supports the assumption of a flat interface at least within the temperature and voltage range used in this study
4. The present analysis applies to other oxides besides YSZ as well. It could also be used to explain incubation times or lifetimes for other electric field-driven processes like the breakdown of high-k materials or the formation of memristors.

Keywords: Yttria-stabilized zirconia polycrystal; Electrical resistivity/conductivity; Atomic layer deposition (ALD); Diffusion; Single charged vacancies
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[THF-20] Optical anisotropies in Ce1-xGdxO2-x/2 / Si(001) thin films

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$Ce_{1-x}Gd_xO_{2-x/2}$ thin films were deposited by spin coating on Si (001) substrates. Reflectance Anisotropy Spectroscopy (RAS) measurements were carried out on films of different x concentration. The optical anisotropy transition near 2 eV is influenced by the incorporation of Gd in the lattice, and the CeO_2 gap transition varies from 3.2 to 2.8 eV in $0 < x < 0.4$. Two strain regimes are observed by Raman spectroscopy, for $x < 0.01$ the films induce a tensile strain on the Si substrate, meanwhile, a strain component of -71.23x cm^{-1} compensates with a 32.67x cm^{-1} bond component for $x > 0.1$. Only the films with $x > 0.1$ show a linear effect in the RAS measurements. It was possible to reconstruct the reflectivity and fit the differential reflectance (RD) measurements, using the comzplex dielectric function obtained by an ellipsometric model.

[THF-117] PYRITE (FeS2) NANOPARTICLES BY PULSED LASER ABLATION IN LIQUID AND ITS THIN FILMS FOR PHOTODIODES

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Abstract: FeS_2 is one of the earth-abundant and non-toxic semiconductors possessing a promising role in optoelectronic applications. FeS_2 has a narrow band gap, high light absorption coefficient, excellent properties in photoelectric conversion and has enormous potential as an efficient photodetector system [1]. This opens our possibility of tuning the material for various applications using its nanostructures and thin films. Pulsed laser ablation in liquid (PLAL), a cost effective, facile and chemically clean method has been adopted for successfully synthesizing pyrite (FeS_2) nanoparticles. In this study, we synthesized FeS_2 nanoparticles in different solvents (IPA, DMF) by laser ablation using Nd:YAG laser output of 532 nm wavelength. Morphology of the nanoparticles was identified by transmission electron microscopy (TEM) and the nanoparticles show different morphologies in these solvents. For thin film fabrication from nanocolloid, we present a simple and convenient method combining electrophoretic deposition (EPD) and spin-coating. FeS_2 nanoparticles in IPA were deposited on n-type silicon (Si) substrate by EPD followed by spin-coating of FeS_2 (NPs in IPA and DMF) on the surface of these films for surface morphological modification and to enhance thickness of the films. Photodiode configurations of n-Si/p-FeS_2 is achieved using the nanocolloids in IPA and DMF. Annealing of these structures is also done in vacuum at different temperatures. The optical properties of the colloids and films were evaluated using UV-Visible spectroscopy. The surface morphologies were studied using scanning electron microscopy (SEM) and Raman studies confirmed the phases. The crystalline structure of the films was characterized by X-ray diffraction (XRD) analyses. We report the photodetection properties of a p-n junction based on these FeS_2 nanoparticles on Si and the results of light sensing parameters evaluated will be presented.

Keywords : Pyrite (FeS_2) nanoparticles; Pulsed laser ablation in liquid (PLAL); Electrophoretic deposition (EPD); Spin-coating; Photodiode

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Reference : [1] M. Gong, A. Kirkeminde, Y. Xie, R. Lu, J. Liu, J.Z. Wu, S. Ren, Iron Pyrite (FeS_2) Broad Spectral and Magnetically Responsive Photodetectors, Adv. Opt. Mater. 1 (2013) 78–83. https://doi.org/10.1002/adom.201200003.

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[THF-236] Role of different atmospheres during annealing in chemical-solution-deposition NiO thin films processing

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Thermally processed nickel oxide (NiO) thin films were synthesized from Ni $(OH)_2$ films obtained by chemical bath deposition (CBD). The thin films were thermally treated at two annealing atmospheres assessing optoelectronic properties for potential applications. The NiO thin films resulted in thicknesses lying between 160 to 192 nm showing a nanowall-like morphology with the proposed synthesis methodology. The films presented an amorphous nature, an optical transmittance between 65 to 85% in the visible region, and bandgap energy around 3.7 eV. The chemical composition of the NiO films was estimated through the X-ray photoelectron spectroscopy (XPS) technique, which confirms that the films after being thermally treated are indeed NiO. The electrical properties were acquired through the Hall effect technique with a Van der Paw configuration. The NiO films exhibit a *p*-type conductivity, having a concentration of their majority carriers from 10^{14} to 10^{15} cm^{-3}. Mobility between 1 and 10 cm^2-$V^{-1}S^{-1}$ and resistivity between 10^4 and 10^2 Ω-cm. These properties are adequate for developing transparent technology in electronic devices.

[THF-349] Spatial modulation of optical microcavities by embedded metallic patterns for photonic devices

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Optical microcavities (MCs) are 1D photonic crystals formed by a periodic stacking of layers of thickness of a quarter of the target light wavelength and alternating refraction indexes with a "defect" spacer layer of thickness of half-lambda. MCs are optical resonators which confine the light of the target wavelength in the spacer layer plane. MCs are commonly used in semiconductor vertical cavity surface emitting lasers (VCSELs) devices, where quantum wells (QW) of a semiconductor such as GaAs are embedded in the spacer. The MC can be micropatterned to form mesas, waveguides or pillars to manipulate the light by means of wet or dry chemical etching combined with lithographic techniques, which are demanding in terms of infrastructure and expertise. In this work, we demonstrate that micropatterning can be achieved by embedding a thin metallic layer within the MC. We show that the metallic layer net effect is that of increasing the resonance wavelength of the MC, thereby allowing to form arbitrary planar photonic potentials by standard lithography methods, and subsequently covering it with the rest of the thin layers to complete the MC device. These novel technique offers a simpler option to existing MC patterning techniques, with the additional advantage of the possibility to use the metallic pattern as an electrical contact to locally manipulate the electrons and/or holes within the active zone of a VCSEL, for example. Besides its use in VCSELs, it can also be applied to manipulate photon-exciton quasiparticles called polaritons in MC-based devices working in the so-called strong-coupling regime. Polaritons can sustain quantum macroscopic states, or condensates, which can thus be manipulated by means of micropatterning of the MC to form, for example, periodic potentials analogue to the optical potentials used to manipulate atomic Bose-Einstein condensates.

Keywords: Optical Microcavities, Photonic Crystals
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[THF-330] STRUCTURAL, CHEMICAL, AND MIR RESPONSE OF COVELLITE CuS FILMS AS OPAQUE LOW-E COATINGS

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The increase in temperature inside buildings has led to the search for construction materials that allow a more pleasant indoor environment, considering high availability, low cost, and obtained from processes that are ecofriendly and viable for scaling. Thus, studying materials to control solar radiation is a current topic, where covellite CuS (CuS-cov) looks for an opportunity as partially opaque Low-E coating. This work explores the relationship between structural and chemical properties of SILAR deposited CuS-cov films, determining the impact on the Mid Infrared (MIR) response to evaluate their capabilities for Low-E application. Rietveld refinement, together with the compositional analysis, evidence the high control of the synthesis and stability of a nanocrystalline single phase of stoichiometric CuS-cov (from the XPS analysis an average S/Cu ratio close to 1:1 was obtained for all samples, taking in consideration the three environments for S atoms: trigonal, tetrahedral, and S-S bonds). The optical behavior in the MIR revealed the impact of the CuS-cov growth, evaluated through the thickness, crystallinity, and composition, as an increasing reflectivity, reaching 80% in the Thermal Infrared for deposition cycles ≥75 (110 nm). With these results, we demonstrate that when the reflectivity of the films is maximized in the Thermal Infrared, these opaque CuS-cov Low-E coatings have emissivities between 0.1 and 0.2 (these values were calculated and estimated applying Kirchhoff's Law and Hagen-Rubens equation for metals), among the lowest reported for commercial transparent conductive oxides. These results contribute to the current investigation to place the CuS-cov films among the Low-E coatings with high potential.

Keyword: Covellite, SILAR, Low-E, Emissivity, MIR reflectance.
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[THF-284] Theoretical characterization of the optical properties of a sensor based on Kretschmann geometry and a porous silicon photonic crystal

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The indiscriminate use of pesticides in vegetable crops has led to the contamination of soils, as well as health problems in consumers. This motivates to control the pesticides used, as well as their concentration in plants. This requires the development of technologies that are efficient and capable of being used in-situ. A promising alternative is to develop sensors based on plasmonic devices due to their high sensitivity to changes in the environment. Therefore, in this work, we present results of the theoretical characterization of the optical properties of a porous silicon photonic crystal embedded in the Kretschmann attenuated total reflection geometry. The refractive index of the porous silicon is obtained with the Bruggeman model and the materials for the metallic thin film for this study are gold and silver. The characterization is done as a function of the parameters of incident light wavelength, angle of incidence, geometrical parameters, porosity of the silicon photonic crystal, and the material contained in the pores. The results of this work are expected to serve as a basis for the experimental design of sensors for pesticides or other pollutants at low concentrations.

Keywords: Optical properties, Porous Silicon, Sensor, Surface Plasmon, Transfer Matrix Method.
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[THF-297] TiO2 THIN FILMS BY SOL GEL-DIP COATING METHOD

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Titanium dioxide (TiO2) is an important inorganic compound which is extremely significant in both the fields of experimental & theoretical research due to their attractive electronic structures and large band gap; TiO2 can be found in three different phases: rutile, anatase, and brookite. The use of titanium dioxide in nanoscale, has been of major interest in the engineering, and science community. The surface structure and it's chemical, and physical properties are studied in order to improve different materials. This compound can be used as photo catalyst, dye sensitized solar cells, gas sensor, optical fibers, antibacterial coating, et seq. Nevertheless, to synthesize the nanomaterials, the main challenge is to expose specific facets on the surface of the crystals. TiO2 thin films were deposited on glass substrates by sol gel-dip coating method and annealed to 250 °C and 550°C in air atmosphere. In the XRD results we can observe that the TiO2 thin film annealed at 550 °C presents the anatase phase. At low temperatures the thin film is amorphous. SEM micrograph revealed cracks of the films annealed at 550 °C shows a homogeneous morphology free of cracks. These results indicate that thin films could be used in photocatalysis.

Keywords: Thin Films; TiO_2; Nanomaterials; anatase; sol-gel.
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DIVULGACION DE CIENCIA Y TECNOLOGÍA

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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

[SCD-24] Ciencia de los materiales y metalurgia del aluminio

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La ciencia o ingeniería de los materiales es un campo interdisciplinario que se ocupa de desarrollar nuevos materiales y mejorar los ya existentes, mediante el desarrollo de un conocimiento mas profundo de las relaciones entre microestructura, composición, síntesis y procesamiento. Los avances en el campo de la ciencia e ingeniería de los materiales se aplican a muchos otros campos de estudio, como por ejemplo la ingeniería biomédica, ambiental, informática, farmacéutica, polimérica, minería, metalúrgica, entre muchas otras.
Es precisamente la ingeniería metalúrgica la que tiene un gran impacto económico, tecnológico y científico a nivel mundial. Actualmente existe una gran variedad de metales y aleaciones, por ejemplo, el aluminio y sus las aleaciones son ampliamente estudiados por sus propiedades muy interesantes, por ejemplo, alta resistencia a la corrosión, alta ductilidad, buena conductividad térmica-eléctrica, alta estabilidad química, etcétera. En cuanto a volumen de producción, el aluminio se sitúa en el segundo sitio a nivel mundial solo por debajo del hierro y el acero, por lo tanto, el aluminio y sus aleaciones constituyen los metales no ferrosos más importantes a nivel mundial en cuanto aplicaciones, derrama económica y producción se refiere.
Otra característica importante de las aleaciones de aluminio es la relativa facilidad para ser recuperada a través del reciclaje, siendo la chatarra de aluminio uno de los materiales que más se destinan a esta actividad. El reciclaje del aluminio presenta una oportunidad para generar nuevamente un valor agregado a un costo mucho menor, ya que el re-procesamiento requiere solo el 5% de la energía total utilizada en comparación a obtenerlo directamente del mineral.

[SCD-430] Conoce el combustible del futuro: El Hidrógeno.

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Desde hace algunos años, muchos investigadores a lo largo del mundo han investigado alternativas a los combustibles fósiles tradicionales, como el petróleo y sus derivados o el carbón, y muchos de estos estudios han encontrado que le hidrógeno es un candidato muy conveniente para sustituir en muchos aspectos a los combustibles tradicionales. Recientemente la Agencia Alemana de Cooperación Internacional indicó que México tiene un gran potencial como productor, exportador e incluso fabricante de tecnologías relacionadas con e hidrógeno. Imagina que el vehículo que utilizas a diario ya no usara gasolina, sino hidrógeno, ¿Suena irreal? Pues, a decir verdad, no lo es, actualmente hay países del mundo donde ya se comercializan vehículos con estas características. Pero el sector automotriz no es el único beneficiado con estas investigaciones acerca de el elemento mas ligero de la tabla periódica. En este trabajo, abordaremos los beneficios y retos que presenta este nuevo combustible y el por qué aún no se usa masivamente, así mismo, responderemos a preguntas como ¿Qué hace tan especial al hidrógeno? ¿Cómo se puede obtener? ¿Para qué investigar formas de obtenerlo? Finalmente, abordaremos cómo parte de nuestro trabajo diario es buscar materiales que hagan mas eficiente el proceso de obtención de hidrógeno, mediante el denominado "*water splitting*" y los beneficios que se han encontrado.

Palabras clave: Hodrógeno, Catálisis, Energías renovables, Invesigación, water splitting.
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[SCD-222] Espectros luminosos y aplicaciones de los Materiales, en beneficio de la humanidad

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Existe una gran diversidad de materiales que, al interactuar con la luz, dan pie a una amplia variedad de aplicaciones; no sólo las que sirven para nuestra comodidad, sino también algunas que nos ayudan a remediar ciertos problemas ambientales. La mayoría de estas aplicaciones, involucran el estudio de “espectros luminosos", las llamadas espectroscopías ópticas. Por ejemplo, para lograr esos bonitos colores que podemos ver en las pantallas de nuestra TV o de nuestro teléfono inteligente, fue necesario estudiar los espectros luminosos emitidos por diferentes materiales, cuando se les proporciona energía adecuadamente; y seleccionar las combinaciones más convenientes. Así mismo, para aprovechar la luz que llega desde el Sol hasta nuestro planeta, para producir energía eléctrica con celdas solares, o para eliminar contaminantes del agua, del aire o del suelo con materiales iluminados con luz solar, resulta indispensable analizar el comportamiento de nuevos materiales, cuando reciben el espectro luminoso que alcanzamos a recibir desde el Sol.
Las espectroscopías ópticas, además de ser muy vistosas, son herramientas muy importantes en el estudio de materiales, para el desarrollo de éstas y muchas otras aplicaciones. Asiste a la charla y arma tu propio artefacto para apreciar estos espectros luminosos.

[SCD-205] Estrategias para la mejora de la eficiencia de paneles solares en condiciones desafiantes

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La luz de sol, es una fuente de energía ilimitada que dota a los objetos más cercanos al sol de una considerable cantidad de irradiancia solar, la cual puede ser aprovechada mediante el uso de dispositivos relativamente simples, como lo son los paneles solares, cuya implementación ha aumentado las capacidades de la humanidad para mantener en funcionamiento por décadas satélites artificiales y robots exploradores en las inhóspitas condiciones del espacio exterior y en la superficie de diversos cuerpos celestes.La tecnología para generar energía solar fotovoltaica ha sido adapta exitosamente a diversos ambientes y en los últimos años se ha transformado en la energía renovable de mayor crecimiento. Aún con todo esto, la generación de energía solar a nivel mundial no supera el 4% de la totalidad de demanda energética, lo cual nos hace preguntarnos: ¿Qué nos impide aprovechar todo el potencial de la energía solar para satisfacer la demanda energética con fuentes renovables? Son muchos los factores a considerar cuando nos planteamos aumentar exponencialmente la cantidad de energía que se produce mediante paneles solares, entre ellas la acumulación de arena en instalaciones ubicadas en el desierto, el sobrecalentamiento de los paneles, la acumulación de nieve en la superficie de los paneles o el efecto de una alta humedad relativa en la producción fotovoltaica. Pero también son muy abundantes e ingeniosas la cantidad de propuestas y desarrollos científicos/tecnológicos que buscan aumentar la eficiencia de producción energética tanto en granjas solares como en instalaciones caseras. En esta charla se exponen algunos de los desarrollos mas representativos en los últimos años orientados a la mejora de la eficiencia de los paneles solares, en busca de instalaciones fotovoltaicas más productivas, por ende, más redituables y en ultima instancias más competentes frente a otras tecnologías de producción de energía eléctrica. Entre los mecanismos que buscan mantener y aumentar la eficiencia de los paneles solares, se encuentran sistemas de enfriamiento de los paneles o de aprovechamiento de energías residuales, el uso de métodos de limpieza para paneles solares, entre los que se encuentran el uso de robots para métodos automatizados, sistemas que se encienden al detectar cierto nivel de suciedad y muchos otros métodos preventivos como los recubrimientos autolimpiadles. Por otro lado, también se utilizan diversos sistemas de seguimiento solar que aumentan la cantidad de horas en las que un dispositivo fotovoltaico se puede acercar al máximo de producción.

Palabras clave: Eficiencia energetica, irradiancia solar, energias renovables.
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[SCD-368] Física, ciencia de materiales y su importancia en la vida cotidiana

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La ciencia de materiales se define como aquella encargada del estudio de la estructura, composición y propiedades de todos los materiales con los que convivimos cotidianamente. El estudio abarca desde los procesos de fabricación hasta los de aplicaciones de los materiales de interés, las aplicaciones son tan variadas como se pueda imaginar. Todo lo que tenemos a nuestro alrededor, está hecho de algún tipo de material que se ha sometido a estudios exhaustivos por parte de una diversidad de científicos de diferentes áreas de manera que se ha aprobado su uso para cualquiera que sea su función, por lo tanto, la ciencia de materiales ha demostrado ser la base sobre la cual se cimientan todos los avances actuales referentes al desarrollo tecnológico acelerado en años recientes. A pesar de que la ciencia de materiales, es una ciencia multidisciplinaria, la física, es la rama que al final de cuentas, soporta todos los desarrollos referentes a ella. Sabemos que la física se define como la ciencia encargada de estudiar el comportamiento del universo, estudia desde partículas subatómicas (partículas más pequeñas que los átomos) hasta cuerpos celestes, desde este punto de vista, al ser los átomos los componentes de toda la materia, su estudio y manipulación, nos permitirá entender y/o modificar las propiedades de cualquier tipo de material. En esta charla, se presentará una discusión general del avance tecnológico acelerado que nos ha permitido llevar la vida que llevamos actualmente, y como este avance ha sido posible gracias al desarrollo de la ciencia de materiales y de su pilar fundamental, la física, adicionalmente, se presentarán algunas de las líneas principales de investigación desarrolladas por el cuerpo académico de física de materiales, perteneciente al departamento de física del CUCEI en la Universidad de Guadalajara.

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[SCD-99] Hacia un mundo de ventanas con ciencia

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La producción de energía es de vital importancia para todas las actividades que realiza la humanidad, además de que el progreso y desarrollo de la sociedad siempre se han encontrado ligados al aprovechamiento de las diferentes fuentes de energía. Actualmente debido a diversos problemas como la contaminación y la sobre explotación de recursos como los combustibles fósiles se ha llevado una búsqueda extensa para aprovechar fuentes de energía renovables. Dentro de estas energías renovables, la energía que proviene del sol tiene el potencial de ser aprovechada utilizando celdas solares que convierten directamente la luz solar en electricidad. Una alternativa que ha llamado la atención, dentro de las diferentes aplicaciones de las celdas solares, es el uso de celdas solares semitransparentes como parte de ventanas de los edificios. Este tipo de celdas presenta la ventaja de ser instaladas directamente en los edificios, generando la energía directamente donde se necesita eliminando los costos y dificultades de transportar la energía, además de ser estéticamente atractivas para aplicaciones arquitectónicas. Para lograr este tipo de aplicación es necesario realizar investigación acerca de la selección y desarrollo de materiales que cumplan con las características ópticas y electrónicas para aprovechar la luz solar, mientras permiten su desempeño normal como ventana. Adicionalmente a las propiedades de los materiales, el procesamiento presenta un rol muy importante. Uno de estos métodos es el deposito por espreado, es por esta razón que actualmente existe un gran interés en esta área de investigación que podría incentivar el aprovechamiento de la energía solar, aprovechando fuentes renovables y contribuyendo a la disminución de la generación de contaminación y jugando con la estética de los edificios que nos rodean.

[SCD-212] INTEGRACIÓN DE LAS TECNOLOGÍAS FOTOVOLTAICAS A LAS SOCIEDADES MODERNAS

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Las energías renovables ya forman una parte sólida de la producción energética consumida por las sociedades de hoy. Una gran porción de estas energías es la solar fotovoltaica y, sin embargo, muchos aspectos de su generación todavía no están optimizados o están en proceso de exploración. Uno de estos aspectos es el transporte de la energía generada hasta el consumidor final. Los cálculos teóricos muestran que es suficiente cubrir tan solo el 1% de la superficie terrestre con celdas fotovoltaicas para cubrir las necesidades energéticas de todo el planeta. En la práctica resulta que las ubicaciones con mayor consumo energético se encuentran en zonas frías, con pocos días de cielo despejado al año – ubicaciones menos favorables para las instalaciones fotovoltaicas. Por otro lado, hay zonas limitadas del planeta, llamadas cinturones solares, que cuentan con las características adecuadas para una efectiva generación. Afortunadamente México se encuentra en una de estas zonas privilegiadas, lo cual le brinda un gran potencial para ser un país altamente solar-energético, siempre y cuando existan los especialistas preparados y cuenten con la infraestructura adecuada para la planeación, generación, distribución y almacenamiento de la energía fotovoltaica – lo que forma parte central de esta charla de divulgación.
Otro tema importante que se cubre en esta charla es la aplicación de la energía solar fotovoltaica en el transporte. La sociedad moderna no existiría sin las redes de transporte individual, local, estatal, nacional, internacional e inclusive espacial. La energía solar fotovoltaica ha tenido una evolución notable en estos rubros y los autores han monitoreado y contribuido en lo posible a este desarrollo durante los últimos años. En base a este monitoreo se ofrecerá un análisis de las tendencias, transformaciones, cambios estratégicos que ha sufrido la aplicación fotovoltaica en la industria del transporte en el país y en el mundo.

Palabras clave: energía solar fotovoltaica, distribución y almacenamiento de energía, sistemas de transporte
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[SCD-45] La Instrumentación Biónica en Tecnología Aeroespacial Aplicada a la Salud

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La exploración espacial se ha convertido en el impulso de inventos y de descubrimientos, tecnológicos en diferentes áreas de las ciencias, el desarrollo de estas actividades repercute en la implementación de nuevos instrumentos, tratamientos y aditamentos que propician un beneficio en la salud de los seres vivos. Parte de la tecnología desarrollada para los astronautas en el espacio se ha podido aprovechar en el sector salud, se han dado en gran parte por los avances logrados en la instrumentación Biónica y la tecnología espacial. La salud de los astronautas es prioridad en cada una de las misiones espaciales tripuladas, los que van al espacio son personas cuya preparación física y psicológica es al 100%. Se realizan estudios del comportamiento del ser humano en micro-ingravidez, cuando el cuerpo humano es sometido a estas condiciones ambientales, el funcionamiento de los órganos cambia abruptamente, el flujo sanguíneo tiende a detenerse, el ritmo cardiaco se ve afectado. Estudios que se reflejan en avances para curar enfermedades del corazón o diabetes, el sistema respiratorio sufre de estrés complicando la respiración de los astronautas, por lo que se han desarrollado sistemas de asistencia respiratoria (ventiladores mecánicos), los cuales hoy en día son ampliamente utilizados para ayudar a las personas afectadas por el SARS-COV2. La pérdida de equilibrio y orientación por la desaparición de la función vestibular, la pérdida de los receptores sensoriales, pérdida de la visión, la baja capacidad de movimiento muscular, así como la disminución de volumen muscular afectando los esfínteres que evitan realizar las necesidades fisiológicas, son condiciones que sufren las personas con paraplejia. Un fenómeno muy marcado es la separación de las articulaciones incrementando la estatura de los astronautas. Todos estos efectos se han estudiados y analizados encontrando similitudes a los padecimientos que sufren algunas personas en la tierra, lo cual han dado origen a nuevas soluciones de tratamientos y fármacos con los que pueden ser mitigados e inclusos erradicados. Otro gran avance es el monitoreo de los signos vitales de los astronautas a distancia dando origen a la telemedicina, la cual se aprovecha para las zonas muy remotas en donde es difícil contar con médicos. El comportamiento del cuerpo humano en ingravidez ha permitido el desarrollo de sistemas de asistencias a personas con discapacidad motriz, el uso de brazos robóticos con movimientos precisos en las naves espaciales, han conducido al desarrollo de los robots de cirugía, así como los equipos de ultrasonido para el diagnóstico. En la UPAEP, en la Licenciatura en ingeniería Biónica, se han aprovechado algunas de estas tecnologías para el desarrollo de prótesis y ortesis tanto para personas como para veterinaria, dando una mejor calidad de vida. Es sabido que cuando un animalito sufría de alguna fractura la mejor decisión era su sacrificio. Otro ejemplo de desarrollo es un prototipo de asistente inteligente, que permita a personas con discapacidad visual, mediante voz comandar tareas tales como leer texto impreso o digital vía reconocimiento óptico de caracteres, comunicarse con cualquier persona telefónicamente o por internet, enviar su ubicación GPS, recibir información del clima, noticias, gestionar sus notas, entre otras aplicaciones de accesibilidad. La conferencia abordará avances tecnológicos de instrumentación Biónica y Aeroespacial en el área de la salud.

Palabras Claves: Biónica, Aeroespacial, Salud, Microingravidez

[SCD-260] Las celdas solares como una alternativa limpia y amigable con el medio ambiente

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El incremento mundial de la demanda de energía, así como el impacto negativo de los combustibles fósiles en el medio ambiente ha resultado en un mayor interés por parte de la comunidad científica en el estudio y uso de fuentes de energía renovables. Entre los distintos tipos de energía renovable, la fotovoltaica resulta muy atractiva para reemplazar ya sea parcialmente o totalmente los combustibles fósiles tradicionales que contaminan el medio ambiente, ya que es capaz de transformar de manera directa la energía proveniente del Sol en electricidad. En la actualidad, el mercado de la fotovoltaica está fundamentalmente basado en el silicio, el cual es el segundo elemento más abundante de la corteza terrestre y constituye la base de la microelectrónica. Sin embargo, el silicio presenta una pobre absorción de luz y los procesos de fabricación de este tipo de celdas solares son frecuentemente costosos. A fin de resolver estos problemas, surge la segunda generación de celdas solares, en donde se emplean materiales que logren una mayor absorción de luz del Sol, así como el uso de técnicas más baratas para procesar las celdas solares. En esta conferencia de divulgación se presentarán las ventajas y retos que enfrenta la fotovoltaica para la generación futura de energía limpia y amigable con el medio ambiente. En particular, se presentará el estado del arte de las distintas generaciones de celdas solares, sus aplicaciones, los distintos materiales que están siendo estudiados que prometen un mejor aprovechamiento de la energía del Sol, así como los problemas actuales que enfrenta esta tecnología y que están siendo investigados. Se mostrará bajo qué condiciones resulta viable el uso de la fotovoltaica en los hogares.

Palabras Claves: Celdas solares, Energía limpia, Reducción del impacto ambiental
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[SCD-427] Los materiales del futuro ¿Son de bolsillo?

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Diariamente utilizamos cosas que nos facilitan la vida o mejoran nuestra calidad de vida, como los teléfonos móviles, vehículos, medicamentos, etcétera. Todas estas cosas han ido mejorando con el paso del tiempo, y los materiales de los que están fabricadas no son la excepción. Cuando hablamos de mejorar los materiales es inevitable pensar en los nanomateriales, ya que, desde mediados del siglo pasado, han cautivado a la comunidad científica por el enorme potencial que tienen. Pero ¿Qué son los nanomateriales?, ¿Por qué se llaman así?, ¿De qué me sirven? En este trabajo, responderemos a estas y a otras preguntas. Estos materiales son conocidos por el tamaño que manejan y para hacernos una idea, basta con tomar una regla, y dividir uno de los centímetros que están marcados en diez millones de partes iguales, eso es un nanómetro. Las estructuras que se modelan y sintetizan que tienen dimensiones de nanómetros son las ya mencionadas nanoestructuras, y pueden tener diferentes formas, por ejemplo, pueden ser alargadas como los nanoalambres o nanotubos, con huecos como los materiales nanoporosos o bien, ser muy delgadas como las monocapas. Las áreas de aplicación de las nanoestructuras son variadas tales como en medicina, almacenamiento y generación de energía o detección y tratamiento de gases tóxicos, además pueden servir para mejorar propiedades de los materiales como la dureza, conductividad térmica o la electroluminiscencia. En nuestro campo de investigación, estudiamos todo lo anteriormente mencionado con un enfoque teórico, empleando recursos computacionales de alto nivel, y conocimientos de física, química entre otras áreas.

Keywords: Nanomaterials, science divulgation, theoretical, nanostructure, DFT.
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[SCD-352] LOS NANOMATERIALES: IMPORTANCIA Y APLICACIONES.

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Los nanomateriales han despertado gran interés en diferentes campos de la ciencia debido a sus interesantes propiedades, diferenciadas de los materiales a granel que son los que actualmente usamos en nuestra vida cotidiana, además prometen ser el camino a seguir para la resolución de importantes problemas que nos atañen a nivel global, temas como la optimización de energías alternativas, elaboración de dispositivos de almacenamiento de energía, aplicaciones en medicina, robótica, electrónica, biología, agricultura, preservación de alimentos, remediación de aguas residuales y muchas más aplicaciones[1]. Se han desarrollado una gran variedad de técnicas de síntesis de nanomateriales, sin embargo, algunas de ellas no nos permiten la obtención de estos con la pureza deseada, lo cual es un problema al momento de realizar las evaluaciones de sus propiedades y sus potenciales aplicaciones. La técnica de fabricación de nanomateriales llamada ablación láser de sólidos en líquidos, es una técnica que utiliza la energía de un láser de alta potencia para poder generar nanomateriales dentro de un líquido, a partir de una gran variedad de materiales que podemos encontrar a nuestro al rededor, solo se necesita un láser, un material sólido y uno líquido. Es una técnica simple, rápida, amigable con el ambiente, versátil y además nos permite obtener materiales con una alta pureza, esta técnica es muy útil en ciencia básica, a pesar de que las cantidades obtenidas son bajas comparadas con otras técnicas, son suficiente para evaluar los nanomateriales obtenidos en un amplio rango de aplicaciones [2]. La versatilidad de la técnica nos permite usar una gran variedad de materiales de partida, desde materiales metálicos fundidos en forma de pastilla, hasta polvos compactados o bien suspendidos en un medio líquido, se pueden sintetizar nanopartículas de compuestos orgánicos, poliméricos, metálicos, óxidos metálicos, cerámicos, etc. Usando una gran variedad de medios líquidos como agua, alcoholes, acetona, aceites, etc. Los cuales pueden ser inertes o también soluciones reactivas, de esta forma la composición, forma, tamaño y estabilidad de los nanomateriales se puede estudiar en un amplio rango. **Trabajo apoyado por: FORDECYT-PRONACES 246648**

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Palabras clave: Nanomateriales, láser, aplicaciones.
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[SCD-165] NANOMATERIALES 2D EN ENERGÍA: PEQUEÑOS MATERIALES GRANDES OPORTUNIDADES

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La creciente evidencia nos obliga a tomar medidas para frenar y, en última instancia, revertir la tendencia actual de nuestra dependencia de los combustibles fósiles optando por direntes fuentes de energía como las renovables. Como ocurre en muchos otros campos, el desarrollo de tecnologías en energía depende de la disponibilidad de materiales adecuados.En la última década, los avances en nanotecnología se han impulsado por desarrollos significativos en la fabricación y síntesis de nanomateriales. La tecnología de nanomateriales tiene el potencial de abordar varios de los grandes desafíos científicos de la actualidad, que van desde la necesidad de tecnologías de energía alternativa más eficiente hasta electrónica más rápida y flexible. Las propiedades electrónicas, ópticas y térmicas únicas de los nanomateriales los convierte en una alternativa relevante dentro de los materiales para abordar nuestra creciente demanda de energía. La aparición de nuevos materiales, como los nanomateriales 2D, siempre inspira nuevas ideas y aplicaciones. Como ejemplo, el grafeno, una capa de grafito de un átomo, posee una estructura bidimensional (2D) única, alta conductividad y movilidad del portador de carga, gran área de superficie específica, alta transparencia y excelente fuerza mecánica. Por lo tanto, se espera que sea un material ideal para la producción, el almacenamiento y la conversión de energía.

Palabaras clave*: Nanomateriales 2D, Energía, Grafeno*
El presente trabajo recibió apoyo a través del Proyecto Interno PI-22-15, del Centro de Investigación en Materiales Avanzados, titulado: “Desarrollo de membranas basadas en materiales nanocompuestos para su aplicación como electrodos flexibles en sistemas de almacenamiento de energía"

[SCD-331] SEMICONDUCTORES DEGENERADOS: ALIADOS DE LOS SISTEMAS DE AIRE ACONDICIONADO

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En México, la mayor parte de la energía proviene de combustibles fósiles lo que contribuye al incremento de la concentración de gases de efecto invernadero resultando en un aumento de la temperatura mundial. Por tanto, durante las últimas décadas, se tiene un incremento del consumo energético de la sociedad que busca contrarrestar condiciones ambientales extremas a través del uso desmedido de sistemas de aire acondicionado (SAA) en edificaciones, principalmente. El uso de vidrio como material arquitectónico ha favorecido esta problemática, ya que permite el paso del 86% de la energía proveniente de la radiación solar fomentando el uso de los SAA. Dentro de la gran variedad de propuestas estudiadas para mitigar este problema, algunas ya han alcanzado aplicaciones reales en países extranjeros como los recubrimientos de control solar los cuales permiten el paso de radiación visible y reflejan la radiación infrarroja (principal responsable de la sensación de calor). En este sentido, el grupo interinstitucional de investigación "Diseño y Optimización de Recubrimientos Avanzados (DORA-Lab)" tiene entre sus principales intereses el desarrollo y optimización de este tipo de recubrimientos, basados en materiales con propiedades especiales y que son amigables con el ambiente, estos materiales son conocidos como "semiconductores degenerados". En esta plática se mencionarán aspectos importantes sobre este tipo de recubrimientos, resaltando la importancia de su uso y el reto que representa obtener espesores en la escala de los nanómetros. En este sentido, con el desarrollo y optimización de estos materiales resulta prometedor pensar que, en un futuro próximo, se puedan generar políticas públicas para fomentar el uso de estas tecnologías en nuestro país.

Palabras calve: Semiconductores degenerados, recubrimientos, materiales nanométricos
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[SCD-345] Sobre las telecomunicaciones: revisando la tecnología del siglo XIX hacia la era de los chips

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"Amor y atención al prójimo con Ciencia y Tecnología nacional"

El ser humano, entre sus diversas necesidades, constantemente busca las mejores condiciones para establecer las comunicaciones a distancia, cada vez más funcionales. Por ello, en esta charla se abordan los detalles principales de los inventos más significativos del siglo XIX, sobre todo el tipo de tecnología de soporte. Como referencia se abordan las limitaciones de la conectividad alámbrica del telégrafo y el teléfono en sus primeras versiones. Lo anterior como un punto de partida para entender la importancia estratégica de la tecnología de los circuitos (chips) y los beneficios actuales del microprocesador en los distintos modos de comunicación. Sí, el punto de inflexión se sitúa en el año de 1947, cuando se dio a conocer el desarrollo del primer transistor, donde los inventores presentaron la primera aplicación práctica en un circuito electrónico amplificador para teléfono. Desde entonces las telecomunicaciones y diversos desarrollos han beneficiado progresivamente a la humanidad.

Para clarificar las características y capacidades de la tecnología de los circuitos integrados, se abordan desde un punto de vista ilustrativo, las técnicas utilizadas para su desarrollo, Particularmente el concepto de vacío y su tecnología asociada, de importancia estratégica para la producción actual del microprocesador, el chip más complejo que para su funcionamiento incluye más de mil millones de transistores de tamaño nanométrico.

En la parte final, como aspecto crítico resulta importante revisar el tipo de estudios y/o desarrollos tecnológicos que soportan el desarrollo de los chips, como prospección sobre el tipo de nuevas tecnologías necesarias para que el ser humano pueda sobrevivir simultáneamente con nuestro planeta, en condiciones de la mejor longevidad posible. Siempre considerando que los seres vivos y nuestro entorno ecológico requieren de los mejores avances de todas las ciencias conocidas, que aporten en su máxima expresión y utilidad práctica para una supervivencia integral.

En otro aspecto general, considerando las capacidades tecnológicas de las telecomunicaciones en el incipiente siglo XXI, como referencia se mencionan algunos instrumentos de vanguardia en los hospitales, con la intención de identificar las posibilidades actuales de la tecnología de los chips respecto al tipo de necesidades que deben atenderse en apoyo de la tecnología biomédica.

[SCD-177] - ¡Recubrimientos desordenados!, incrementando la vida útil de las herramientas

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Desde que el ser humano tuvo uso de razón utilizó herramientas para facilitar sus actividades. Actualmente, con el avance tecnológico, los quehaceres cotidianos del hogar y de la industria se han facilitado enormemente, consiguiendo que casi cualquier actividad esté apoyada por una herramienta o máquina. Detrás de esto, la ciencia y tecnología de los materiales ha jugado un papel fundamental. Puntualizando en la industria del maquinado, las herramientas de corte y perforación han alcanzado un grado de especialización muy alto. Es precisamente este grado de especialización junto con el desarrollo y exigencia industriales lo que ha originado que se esté interesado en aumentar la vida útil de estas herramientas, mejorando sus propiedades para que puedan operar sobre superficies más duras, alcanzar mayores velocidades de uso, resistir a la corrosión y a altas temperaturas de trabajo. Estas mejoras se han dado gracias a un área interdisciplinaria de ciencia de materiales que consiste en el desarrollo de recubrimientos o películas delgadas. Un ejemplo aplica cuando recubrimos con pintura las rejas metálicas de nuestras casas, favoreciendo a que no se oxiden con facilidad, además de hacerlas lucir mejor. El caso más común en las herramientas es el nitruro de titanio, TiN, el cual es aplicado a las brocas dándoles un color dorado característico con espesores de unos cuantos micrómetros. Así como el TiN, han surgido más y mejores recubrimientos como el TiAlN, el cuál además de incrementar la dureza de la herramienta, ofrece mayor resistencia a la oxidación y corrosión gracias a la incorporación del Al. Estos sistemas son depositados principalmente por procesos físicos como sputtering, que consiste en arrancar átomos del metal a depositar mediante un proceso físico, análogo al juego de billar. En esta plática se discutirá la incorporación de más metales para el desarrollo de recubrimientos de nitruros multielementales de alto desorden, denominados de alta entropía, con el fin de mejorar aún más su rendimiento.

[SCD-386] ¿Qué tanto sabes del agua?

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Seguramente muchos se sorprenderán ante esta pregunta tan simple, de una sustancia química tan común para todos. Pero en realidad sabemos poco de este líquido con increíbles propiedades, las cuales permiten desde la existencia de nuestra propia vida hasta la del planeta tal cual lo conocemos. En esta plática se presentarán cuestiones 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 el hielo flota 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.

Palabras clave: Agua, agua pesada, cuidado del agua, agua de lluvia, agua potable.
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