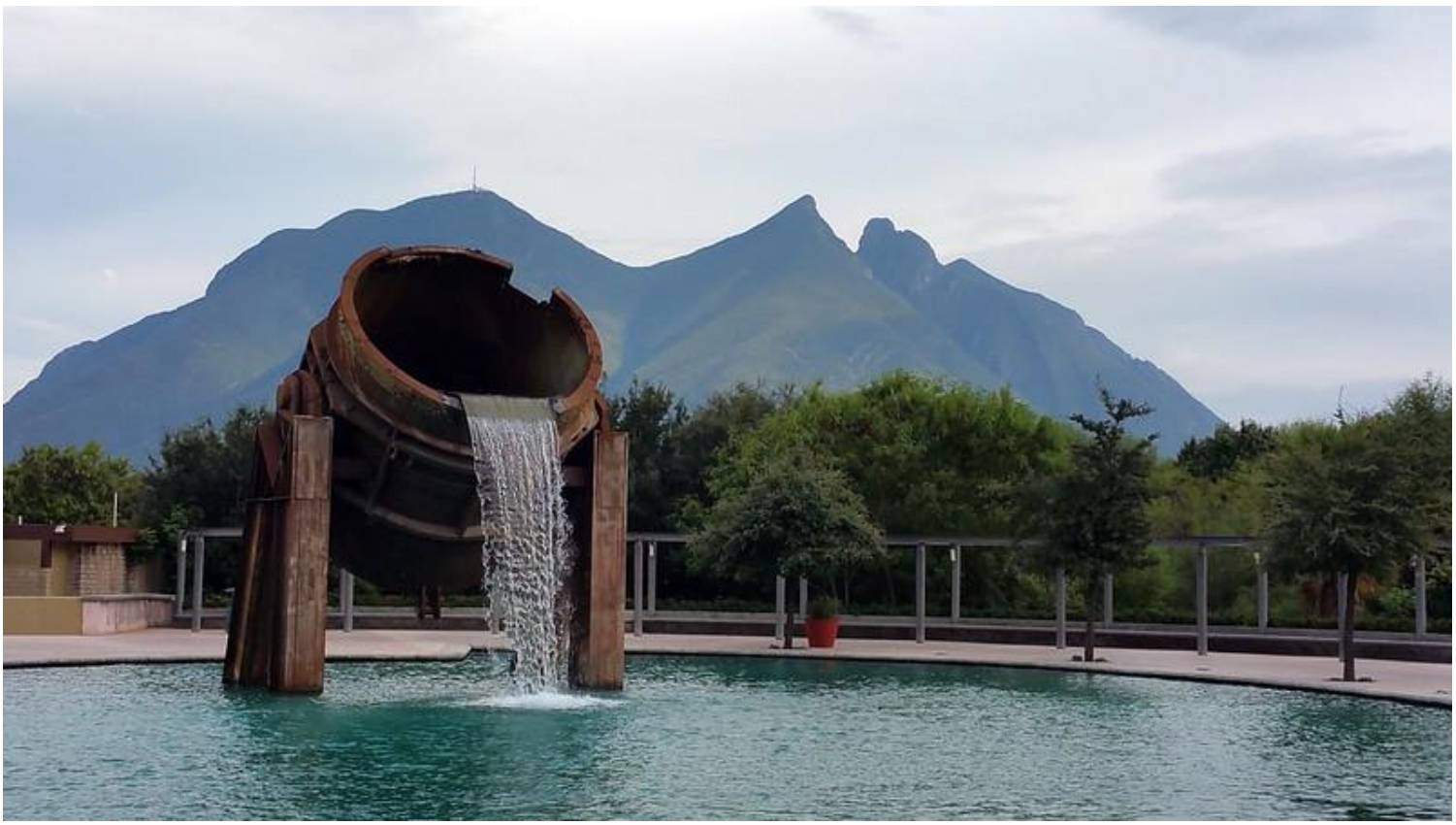
Sociedad Mexicana de Ciencias y Tecnología
de Superficies y Materiales A.C.

XIII
International Conference on
Surfaces, Materials and Vacuum



October 19-22 , 2020 Virtual Meeting. México

Book of
ABSTRACTS

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XIII INTERNATIONAL CONFERENCE IN MATERIALS SURFACES AND VACUUM

SOCIEDAD MEXICANA DE CIENCIAS SUPERFICIES Y MATERIALES AC

VIRTUAL CONFERENCE OCTOBER 19-22TH, MEXICO.

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Dear Colleagues,

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

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

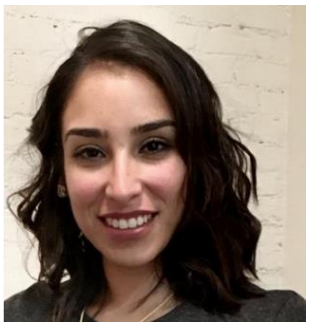
The XIII ICSMV

Organizing Committee SMCTSM

October 2020

PLENARY TALKS

HUSAM N. ALSHAREEF



ERIKA FUENTES FERNANDEZ

ERIKA FUENTES FERNÁNDEZ

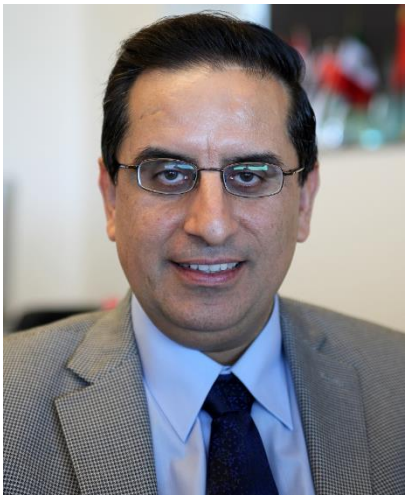
OLIVIA A. GRAEVE

DANIEL LOPEZ

ROBERTO OLAYO

ALDO ROMERO

ÁLVARO VÁZQUEZ-MAYAGOITIA



HUSAM N. ALSHAREEF

Professor, Material Science and Engineering

King Abdullah University of Science and Technology

web:
https://www.kaust.edu.sa/en/study/faculty/husam-n-alshareef

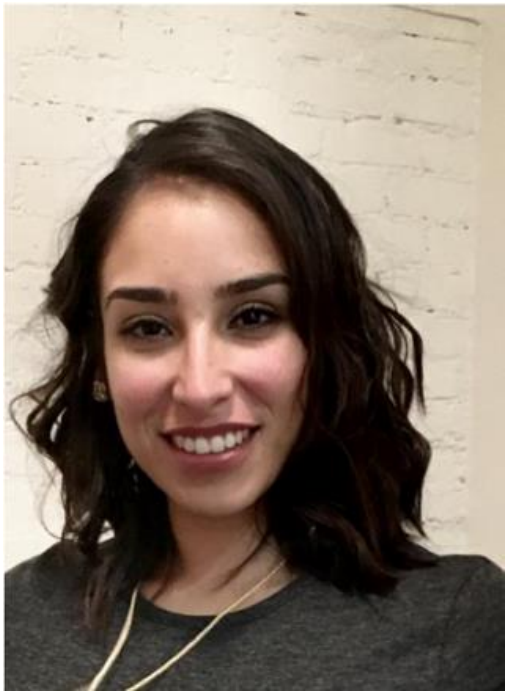
Talk: MXenes for Electronic and Sensing Applications

This talk will focus on the device applications of MXenes and MXene-derived functional materials. Our group has been developing device concepts that capitalize on the rich and promising properties of MXenes. For example, the excellent electrical conductivity of MXenes makes them good candidates as contact materials electronics (printed, wearable, and stretchable electronics) both as local and global contacts. We have demonstrated that MXenes can be used as electrical contacts in thin-film electronics, CMOS devices, quantum-dot transistors, LEDs, and solar cells. The plasmonic properties of MXenes can be used to develop broad-band plasmonic photodetectors working in the visible range. Capitalizing on the abundant surface charges of MXenes, we have developed conducting MXene-polymer hydrogels with unique (skin-like) sensing capabilities that outperform existing hydrogel sensors. These hydrogels could detect magnitude and sign of stress, speed, facial expression, touch, and sound. The hydrogel could also harvest energy from ultrasound, which can be stored or coupled to power other devices.

Further, we have developed a new direction in MXene transformations, where the 2D nature of MXenes is leveraged to make high-performance functional materials. For example, highly-textured ferroelectric crystals, piezoelectric crystals, and piezoluminescent crystals were fabricated. Besides, 2D metal-organic frameworks and their thin films were made using MXene as metal source resulting in highly-texture MOF thin films at the wafer scale. These films have several useful device applications. These and other recent developments in our group will be discussed.

BIO

Husam Alshareef is a Processor of Materials Science and Engineering at King Abdullah University of Science and Technology (KAUST). He obtained his PhD at NC State University in 1996 followed by a post-doctoral Fellowship at Sandia National Laboratory, USA. He then embarked on a 10-year career in the semiconductor industry, holding positions at Micron Technology and Texas Instruments. There he worked on developing new materials and processes for the microelectronics industry. In 2009 he joined KAUST, where he initiated an active research group focusing on energy storage and electronics. He has won the UNDP Undergraduate Fellowship, Seth Sprague Physics Award, NC State Dean's Fellowship, U.S. Department of Education Electronic Materials Fellowship, the SEMATECH Corporate Excellence Award (2006), two Dow Sustainability Awards (2011) and (2014), AH Shoman Award for Excellence in Energy Research (2016), KAUST Distinguished Teaching Award (2018), and the Kuwait Prize for Sustainable and Clean Technologies (2018). He is a Fellow of the American Physical Society, a Fellow of the Royal Society of Chemistry, IEEE Distinguished Lecturer in Nanotechnology. He is a Clarivate Analytics Highly Cited Researcher in Materials Science.



ERIKA FUENTES FERNÁNDEZ

Research and Development Engineer

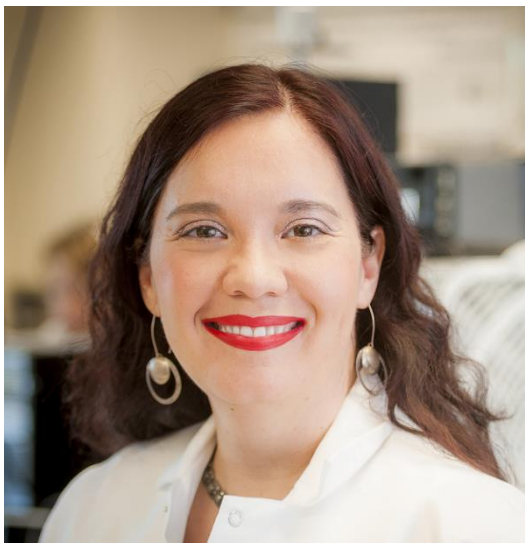
QORVO, Inc.

Talk: Materials Science in Telecommunications

BIO

Erika Fuentes-Fernandez is currently a BAW R&D Engineer at Qorvo. She obtained a Ph.D. in Materials Science and Engineering from the University of Texas at Dallas in 2013 and a B.S. in Chemistry from the Autonomous University of Coahuila, Mexico in 2008. During her Ph.D., Erika focused on the synthesis and characterization of piezoelectric materials as well as device fabrication and testing for harvesting and sensor applications. After joining R&D team in Qorvo, she centered her research in next generation radio frequency filters for telecommunication

applications. Her research interests include materials and devices for micro and nano electromechanical systems (MEMS/NEMS), energy and sensors applications, and sustainable devices. Erika is actively involved on synergistic activities and programs on science, technology, engineering, and math (STEM) fields, mainly supporting minorities and internationals students. Programs she is currently involved are, Materials Research Society (MRS)- Academic Affairs department as well as, co-Founder of Mexican Talent Network (RTM) Dallas Chapter.



OLIVIA A. GRAEVE

Professor, Departamento de Ingeniería Mecánica y Aeroespacial

University of California, San Diego

http://graeve.ucsd.edu/

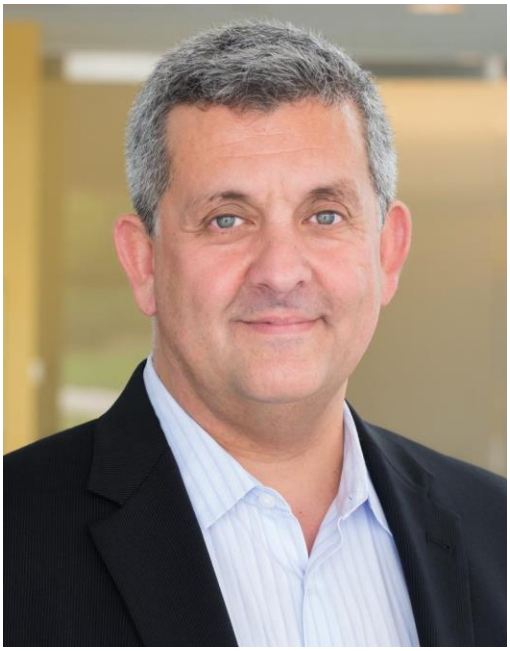
Talk: Materials for Space Environments: What will it take to colonize other planets?

The idea of living on Mars or the Moon has been a staple of science fiction since the 19th century. The justification is that we need to go there if we want to create a backup location for humanity, in the event that life on Earth becomes untenable due to issues like climate change. We could also go there to search for additional resources such as water or precious metals. However, if this sci-fi dream were to ever become reality, what would it be like to actually live there? Conditions make living on Mars extremely challenging. In particular, materials needed for such extreme environments need to be discovered and designed. In this talk, we will present an overview and current research on carbide and boride materials for potential uses at extreme environments, including ultra-high and ultra-low temperatures, impact, and radiation. High-entropy carbides and hexaborides will be a particular focus of attention.

BIO

Olivia Graeve is Professor of Engineering and Materials Science in the Department of Mechanical and Aerospace Engineering at UC San Diego, where she has been working since 2012. She received the title of Structural Engineer from the University of California San Diego, in 1995 and a PhD in Science and Materials Engineering from the University of California Davis, in 2001.

Olivia has received several prestigious awards. In 2014, she was named to the Tijuana Walk of Fame. He has also received several awards. Recently, she has been named Corresponding Member of the Academia de Ingeniería de México (2016), Corresponding Member of the Académica Mexicana de Ciencias (2019) and Fellow of the Sociedad de Cerámicos (2017). In May 2017, Forbes magazine named her one of the 100 Most Powerful Women in Mexico and in August 2020 she was recognized with the PAESMEM Presidential Award for her work in promoting engineering among Latino students. Olivia is internationally recognized for her work in the area of materials in extreme environments.



DANIEL LÓPEZ

Professor, Electrical Engineering and Materials Research Institute

Penn State University

https://www.eecs.psu.edu/departments/directory-detail-g.aspx?q=ovl5064

Talk: A perspective on the future of nanomechanical systems: embracing nonlinearity, thermal fluctuations, and kirigami-inspired manufacturing

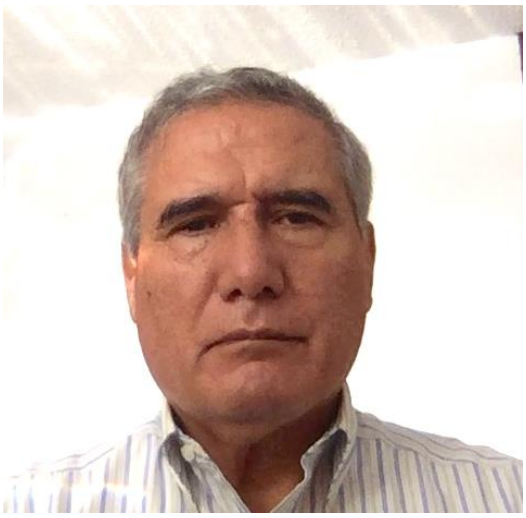
The field of micro-mechanics is now a well-established engineering domain with a demonstrated impact on science, technology, and product development. At the core of this technology are movable mechanical structures, known as Micro Electro Mechanical Systems (MEMS), with well-known fabrication processes, response time as fast as microseconds, and elastic properties well described by conventional elasticity theory (Hooke's law). The dense integration of MEMS devices has enabled the manipulation of multiple physical signals with an unprecedented level of spatial and temporal control.

Unfortunately, as the dimensions of the devices are reduced from the micro- to the nano-scale, the direct scaling of MEMS working principles and fabrication processes cease to work. When going from micro- to nanoelectromechanical systems, NEMS, the devices' linear dynamic range can be reduced to the point where the amplitudes needed for linear response are below the noise level and, as a consequence, operation in the nonlinear regime is unavoidable. Moreover, thermal fluctuations become relatively stronger, causing significant changes in the mechanical properties of the structural materials and their static and dynamic behavior. Finally, state-of-the-art nanofabrication processes produce structures with large error margins in fundamental device parameters, even when using identical fabrication processes.

In this presentation, I will propose that rather than continuing to struggle to avoid these phenomena, nonlinearity and thermal fluctuations offer unique advantages to enhance the performance of MEMS and NEMS devices and, in combination with techniques such as origami and kirigami, manufacturing of scale-invariant 3D nanostructures become closer to reality.

BIO

Daniel López is the Liang Professor of Electrical Engineering and a member of the Materials Research Institute at Penn State University. Dr. López received his Ph.D. in Physics from the Instituto Balseiro in Argentina in 1996. After obtaining his Ph. D, he worked as a Postdoctoral Fellow at IBM T. J. Watson Research Center studying high-temperature superconductors. In 1998 he joined Bell Laboratories (Murray Hill, NJ) as a full-time Research Staff member where he developed micro and nano-machines for optical communications, imaging, and quantum sensing. In 2000 he received the Bell Labs President's Gold Award, the highest recognition award at Bell Laboratories for developing disruptive technologies with a direct impact on the business. In 2008 he moved to Argonne National Laboratory to lead the Nanofabrication and Devices group. At Argonne, he received the Physical Sciences and Engineering Excellence Award, and from 2015 to 2019, he was a Fellow of the Institute for Molecular Engineering at The University of Chicago. He is presently affiliated with the Physical Measurements Lab at the National Institute for Standards and Technologies (NIST) at Gaithersburg, MD.



ROBERTO OLAYO

Professor, Departamento de Física

Universidad Autónoma Metropolitana Iztapalapa

Talk: Surface modification in biomaterials

In the case of biomaterials, both the bulk and surface properties are very important for their performance, the bulk must respond mainly to mechanical, stability and morphological properties. The surface is the main responsible of the interaction with the biological system and obtaining an optimal combination of both types of properties determines the success of the biomaterial's function. Thus, surface modification makes it possible to expand the potential for use of the biomaterial and adjust its behavior.

The talk presents different types of surface modification and their effects on the biological system, discussing in particular the work done by the groups that collaborate with the author, particularly plasma modification and polymer adsorption.

BIO

Doctor Roberto Olayo González, is a Physicist graduated from the Faculty of Sciences of the UNAM (1976), he obtained his master's degree and Ph.D. at the Metropolitan Autonomous University-Iztapalapa in Mexico, he has carried out research stays at the Universities of Minnesota USA. Guanajuato, Mexico and UNAM, Querétaro, Mexico. He has more than 100 publications, 9 patents and 1750 citations to his works. In the training of human resources directed: 14 doctoral theses, 23 masters, 13 undergraduates. He is currently a full professor at Universidad Autónoma Metropolitana and belongs to the National System of Researchers of Mexico with the level of National Researcher Level III.

His main research topics are:

PHYSICOCHEMISTRY OF POLYMERS

BIOMATERIALS

TISSUE ENGINEERING

CONTROLLED DOSCIFICATION OF SUBSTANCES

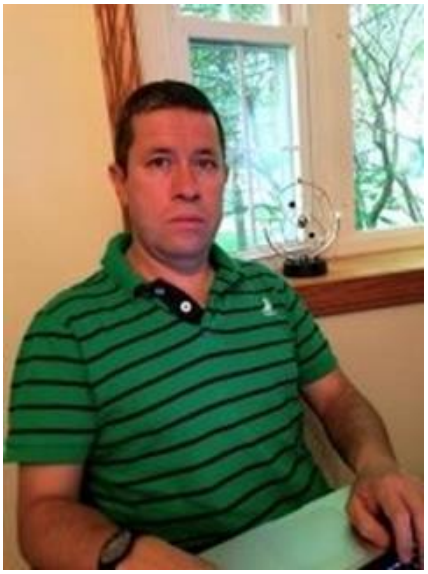
He has also served as:

Head of the Polymers Area of the Physics Department (89-94).

President of the Polymeric Society of Mexico (1995-97)

Coordinator of the Degree in Physics, Universidad Autónoma Metropolitana (1996-2000)

Head of the Physics Department, Iztapalapa Metropolitan Autonomous University (2002-2006)



ALDO ROMERO

Professor, Department of Physics and Astronomy

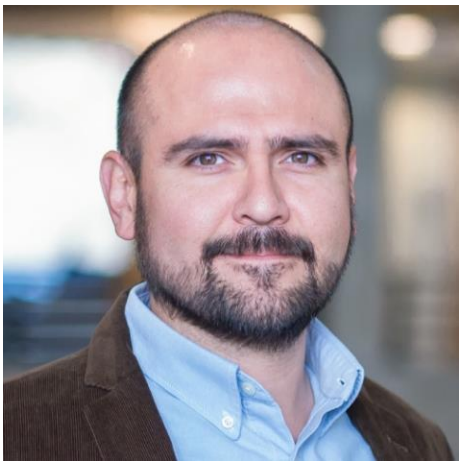
West Virginia University

https://physics.wvu.edu/faculty-and-staff/faculty/aldo-romero

Talk: New ideas for materials science old methods: From electronic structure to artificial intelligence

BIO

Aldo Romero is a full professor in the Physics and Astronomy Department at the West Virginia University in the United States. He is the author of more than 220 articles in high impact journals such as Science, Physical Review Letter, Nature, NanoACS, among others. He is also the author of the book Computational Simulation of Materials and Nanostructures in collaboration with Prof Noburu Takeuchi. Expert in calculating the electronic structure of materials, developer of different computational packages used in the study of materials at the atomic scale and in the use of artificial intelligence in the characterization and prediction of new materials.



Álvaro Vázquez-Mayagoitia
Computational Scientist - R&D Chemistry and Materials Science
Argonne National Laboratory
https://web.alcf.anl.gov/~vama/

Talk: Machine learned inter atomic potentials for large scale atomic simulations of hafnia

Atomic simulations consume almost two thirds of the computational resouces in large DOE computing facilities. Machine learning and Ariticial Intelligence is helping to accelerate atomic scale simulations reducing the computational cost of more complex methods while the accuracy of the results is preserved.

In this talk I will present some advances of my research using machine learning to predict quantum mechanical properties of bulk materials. I will present the case of Hafnium Oxide (hafnia). We use Gaussian process regression to fit a model that is able to predict the energies and forces of liquid and amorphous hafnia using many-body descriptors, such as Smooth Overlap of Atomic Positions (SOAP). With our model, we were able to perform molecular dynamic simulations with large unitary cells of hafnia with more thant 6,000 atoms, which is extremely costly to perform with accurate quantum mechanic approaches. Our results are consistent with experimental observations, and could help to understand the structure of hafina at different compositions.

BIO

Alvaro Vazquez-Mayagoitia is an expert in computational and theoretical chemistry. His experience spans both methods and applications of electronic structure theory with high-performance computing.

He joined the Argonne Leadership Computing Facility (ALCF) in 2011, as part of an Early Science Program ALCF-2. In 2013, he accepted a position as part of the ALCF Computational Science team. As a member of that team, Alvaro actively participates in the continuous enhancement of features and performance of a number of quantum chemistry codes, including NWChem, BigDFT, Quantum-Espresso, MADNESS, and FHI-aims.

With the goal of efficiently using ALCF resources and accelerating simulations, he has worked on the optimization of codes and libraries for Argonne's petascale systems, like Intrepid, Mira and Theta. At ALCF, he provides support, advice and training for scientific projects in fields related to physics and chemistry. Most recently, he has assisted in the preparation and review of proposals for grants sponsored by the U.S. Department of Energy and the National Science Foundation.

Prior to joining ALCF, Alvaro held a postdoctoral position at Oak Ridge National Laboratory and the University of Tennessee working with MADNESS and NWChem codes. He developed tools for molecular spectroscopy and evaluated weak interactions.

Research Interests: Ab inito methods; numerical basis sets; solvent models; Density Functional Theory; spectroscopy; parallel computing; machine learning approaches; workflows; and advanced materials for sustainable energy production.

https://web.alcf.anl.gov/~vama/

ATOMIC LAYER DEPOSITION SYMPOSIUM

Chairmen:

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

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

Dr. Hugo Tiznado:(CNYN-UNAM), tiznado@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-329] First-principles study of the atomic layer deposition of ZnO on carboxyl functionalized carbon nanotubes: the role of water molecules

José Israel Páez Ornelas (paez@cnyn.unam.mx)[1], Héctor Noé Fernández Escamilla[2], Hugo Alejandro Borbón Núñez[2], Hugo Tiznado[2], Noboru Takeuchi[2], Jonathan Guerrero Sánchez[2]
[1] Centro de Investigación Científica y de Educación Superior de Ensenada, Carretera Tijuana-Ensenada 3918, Apdo. Postal 22860, Ensenada B.C., México
[2] Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Carretera Tijuana-Ensenada km 107, Apdo. Postal 22860, Ensenada B.C., México

The formation of heterostructures that combine a large surface area with high surface activity has attracted the attention of the scientific community due to their unique properties and applications. In this work, we describe -at the atomic level- the full reaction mechanisms involved in the atomic layer deposition of a hybrid ZnO/CNT inorganic structure. First, the pristine CNTs are chemically activated with a carboxylic acid, a process unique to carbon materials. Diethylzinc (DEZ) and water are used as gas-phase precursors to form ZnO. Our findings show that DEZ is physically adsorbed on the CNTs during the exposure of the first precursor. The ligand-exchange to generate chemisorbed ethyl zinc on the O side of the COOH group needs to overcome an energy barrier of 0.06 eV. Very small energy if compared to the values (0.5-0.6 eV) obtained in previous works for OH functionalized surfaces. The height of the barrier is associated with the C=O side, which mediates the H proton's exchange from the OH group to the C_2H_5 ligand. Furthermore, upon exposure to the oxidant agent (H_2O), ethyl zinc exchanges his last ligand as ethane, and it accepts a hydroxyl group through a self-limiting reaction with an energy barrier of 0.88 eV. Notice that the energy barrier of the second ligand-exchange is larger than in the first. We have also analyzed the effect in the saturation of the second precursor: as the quantity of water molecules increases, the long-range interactions tends to repel them. However, the energy barrier of the second ligand-exchange decreases from 1.53 eV to 0.88 eV for one and two water molecules, showing a clear dependence with the oxidizing agent. Non-covalent interactions are used as a tool to visualize in real space the driving forces that take place during each partial reaction. Our study points out the importance of using the right functionalization agent to achieve a controlled and conformal ALD growth at the initial steps of the formation of hybrid ZnO/CNTs structures, as well as to the role played by the oxidizing agent to lower the energy barrier on the second ALD step.

[ALD-393] Depth profiling Titanium infiltrated PMMA

Pierre Giovanni Mani-González (pierre.mani@uacj.mx)[2], Caitlin McFeely[3], Matthew Snelgrove[3], Jesús Alfredo Hernandez-Márquez[2], Robert O´Connor[1]

[1] Advanced Processing Technology Centre, Dublin City University, Glasnevin, Dublin 9, Ireland

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

[3] School of Physical Sciences, Dublin City University, Glasnevin, Dublin 9, Ireland

Vapor phase infiltration (VPI) is a bottom up process that involves the infiltration of polymer brushes with atomic layer deposition (ALD) precursors. By exposing a surface to an organo-metallic precursor, area selective metal formation is achieved where the precursor reacts with regions covered by an infiltration receptive polymer brush. Combining receptive and rejecting polymers which have the capability to form complex nanopatterns could potentially allow for the creation of nanofeatures, offering a route to area selective deposition (ASD). This work is concerned with the creation and characterisation of titanium infiltrated films with a VPI process. Thin films of PMMA were infused with TTIP and subsequently analysed with ARXPS without breaking vacuum. O 1*s*, Ti 2*p* and Si 2*p* core levels revealed the successful, incorporation of titanium into the polymer. All XPS analysis and treatments were completed without breaking vacuum in our self-integrated ultra-high vacuum setup. FTIR suggests carbon bonds broken on PMMA structure due to titanium incorporation.

[ALD-412] Analysis and characterization of AlxOy obtained through homemade Thermal-ALD and Plasma enhanced-ALD

Jesús Alfredo Hernández Márquez (al194574@alumnos.uacj.mx)[2], Frank Romo García[3], Manuel Herrera Saldivar[1], Olivia Graeve[4], Pierre Giovanni Mani González (pierre.mani@uacj.mx)[2]

[1] Center of nanoscience and nanotechnology, UNAM, P.O. 356, Ensenada, BC 22800, Mexico

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

[3] Physics department University of Sonora, Hermosillo, Sonora 83000, México

[4] University of California at San Diego, La Jolla, CA 92093-0411, USA

Atomic layer deposition (ALD) technique has been recognized as one of the most useful deposition techniques, this due to its ability and flexibility for the deposition as thin films on different materials. ALD is useful in coating applications for new technologies such as solar cells and variety of optoelectronic devices fabrication. ALD has been allowing to obtain a high-quality thin film of Al_2O_3 at low temperatures which make possible to coat thermally fragile materials as polymers or biologicals materials. A two different samples deposition as thin film of Al_xO_y was obtained by using a homemade thermal ALD and Plasma assisted ALD. The deposition was done in a tubular reactor using alternating substrate exposure to trimethylaluminum [$Al(CH_3)_3$] or [TMA] and H_2O for thermal ALD using N_2 as purge gas and substrate exposure to TMA and O_2 with Ar as purge gas for the plasma enhanced deposition. Samples surface were characterized with Scanning Electron Microscopy (SEM), a first study of composition was done through Electron Dispersion Scattering (EDS). In addition, samples stoichiometry and thin films thickness were determined by X-Ray Photoelectron Spectroscopy (XPS) analysis.

[ALD-433] Impact of the thermal treatment under an oxygen atmosphere on the electrical and structural properties of Al/HfO2/Si structures

Marisol Mayorga-Garay (marisol.mayorga@cinvestav.mx)[1], Orlando Cortázar Martínez[1], Abraham Jorge Carmona Carmona[1], Joaquín Raboño Borbolla[1], Alberto Herrera Gómez[1], Andrés De Luna Bugallo[1]
[1] CINVESTAV Unidad Querétaro.

HfO_2 is one of the most promising high-k dielectrics to replace SiO_2 in MOS devices in order to improve performance and miniaturization. Usually, the MOS fabrication process involves different techniques such as substrate cleaning, ALD deposition, metallization and thermal treatments. The conditions used in each one of those techniques during the fabrication will have high influence on the structural and electrical properties of the final device.
In this work we compare the electrical and structural properties of Al/HfO_2/Si structures before and after thermal treatment under an oxygen atmosphere.
The HfO_2/Si structures were processed using standard RCA cleaning carried out on silicon n-type (100) substrates followed by the growth of HfO_2 using atomic layer deposition (ALD). We used ARXPS to determine the composition and structural properties of nominally 4 nm and 6 nm thick HfO_2 films employing the multilayer method (MLM). The thermal treatment was carried out at 400º C and 500º C for 30 min in a tube furnace after the hafnium oxide deposition under an oxygen atmosphere. The structural and electrical properties were compared before and after treatment. To perform the electrical properties, MOS structures were fabricated using thermal sublimation to deposit â�“200 nm thick layer of aluminum on top of HfO_2/Si structures as gate metal contact. The lift off technique was used for the micro capacitors pattern.
X-ray photoemission spectroscopy experimentation shows the increment of the interfacial layer thickness with a composition of $Hf_xSi_yO_2$ and the incorporation of oxygen into the dielectric and interfacial layer, specially at the higher temperature. This calculation was done fitting the spectra by means of Voigt line-shapes. Special care was given to the modeling of the background of the Hf 4f spectra, for which the Shirley component was studied in detail.
The electrical measurements of MOS capacitors shown a relationship between the treatment and the reduction of the maximum capacitance and the threshold voltage in the Al/HfO_2/Si samples. The calculation of the dielectric constant *k* was performed for each of the samples using the parallel plate model and ignoring the difference on the composition between the oxide and the interfacial layer. For the samples before heat treatment, the dielectric constant is 7.5 and 5.8 for 6 nm and 4 nm, after the thermal treatment (400º C) *k* changes to 6.3 and 5.2 and (500º C) 6.1 and 3.8 for 6 nm and 4 nm, respectively.
We conclude that the thermal treatment under an oxygen atmosphere has an important impact on thin HfO_2 films properties. This process allows the oxygen incorporation in the hafnia layer, but also increases the interfacial layer of $Hf_xSi_yO_2$, which changes considerably the dielectric constant for higher temperatures.

[ALD-441] Thermal and Plasma Enhanced Atomic Layer Deposition of TiO2 from Amide and Alkoxide Precursors: Growth Characteristics and Photoelectrochemical Performance.

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The use of atomic layer deposition in the formation of thin films to act as protective layers on photoanodes is a key step towards improving photoelectrochemical (PEC) water-splitting cells for hydrogen fuel generation. The conformality, low defect density, and tunability of ALD films allows for precise control over the film's properties, towards meeting the specific requirements for PEC cell operation.
In this work we compare two titanium precursors were employed in plasma enhanced ALD (PEALD) as well as thermal ALD (TALD) growth of TiO_2 on silicon photoanodes . The two precursors investigated in this study are titanium isopropoxide (TTIP) and Tetrakis(dimethylamido)titanium (TDMAT). The films were characterised using in-situ x-ray photoelectron spectroscopy in an integrated tool where the sample is transferred from the ALD to XPS chamber without a vacuum break by a robotic handler. This setup allows for an understanding of the growth chemistry with half-cycle resolution. XPS analysis is crucial in understanding the properties of the films grown during ALD, and for understanding the nucleation and growth chemistry. We present a comprehensive analysis of the Si *2p*, O *1s*, and Ti *2p* peaks for each ALD process. The films are also characterised by Fourier transform infrared spectroscopy, and atomic force microscopy. Finally, the photoelectrochemical performance of the resulting films under simulated sunlight is presented

[ALD-249] Photo-catalytic activity of ZnO and TiO2 nanotubes synthesized by ALD

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The direct conversion of solar energy into chemical energy, by using photo-catalytic materials, corresponds to an important alternative for environmental remediation and clean energy sources. Specifically, the removal of environmental pollutants such as dyes and recalcitrant organic compounds can be performed by photo-catalytic methods using suitable materials.

This work evaluates the photo-catalytic activity of semiconductor (ZnO or TiO2) nanotubes synthesized by the template-based ALD (Atomic Layer Deposition) method, using Carbon nanotubes as a removable template. Nitrogen-doped multiwalled carbon nanotubes (CNx-CNTs) were first coated with ZnO or TiO2 using ALD. The obtained nanotubes were annealed in a nitrogen atmosphere in order to study their crystallization degree as a function of thermal treatment temperature. The samples were systematically analyzed by X-Ray Diffraction spectroscopy (XRD), Transmission Electron Microscopy (TEM) and X-ray Photoelectron Spectroscopy (XPS). Afterward, the template removal was evaluated using two different approaches: dry air oxidation at high temperature or ozone-rich atmosphere at low temperature. After the template removal, it was analyzed the photo-catalytic activity of the obtained nanotubes using the photo-oxidation of Amaranth as probe reaction. The ZnO nanotubes obtained from the low temperature ozone treatment showed the highest photo-catalytic activity among the obtained samples.

Acknowledgements: We gratefully acknowledge financial support from the UNAM México funding through DGAPA PAPIIT IN105719 project and CONACyT funding through projects A1-S-17539 and Fordecyt 272894. The authors would like to thank F. Ruiz, J. Diaz, I. Gradilla, E. Murillo. P. Piza and E. Aparicio for technical assistance.

[ALD-341] Non-quarter-wave dielectric mirror prepared by thermal atomic layer deposition

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In this work we design and fabricate from n(λ) and k(λ) experimental data for both Al_2O_3 and TiO_2 single layer materials, an optical coating as "dielectric-mirror" following the non-quarter-wave stack formula $\mathbf{(H_xL_Y)^8H_x}$. Optical coating based on multilayer film on BK7 glass and Si(1 0 0) wafer substrates, was grown by thermal atomic layer deposition at 150 °C. Optical constants and optical properties of the TiO_2 - Al_2O_3 multilayer stack, before and after thermal treatment at 450 °C, were studied via spectroscopy ellipsometry and UV – Vis measurements in the spectral range from 200 to 1100 nm. Also, similar samples were studied by means of TEM, SEM and AFM at room temperature in order to obtain information about the morphological properties. From optical studies, we found absorption due to carbon impurities related with organometallic precursor used in ALD process; to reduce carbon related absorption, samples were submitted to an annealing process at 450 °C under air atmosphere. A reject zone or "stopband region" between 381 and 451 nm, with maximum reflection around of 99.9%, cut-off points at 371 and 455 nm after thermal treatment. This reject zone presents an acceptable bandwidth at λ_0 = 420 nm reference wavelength. Results open the possibility to fabricate dielectric-mirrors on complex geometry substrates without the restriction of direct evaporate exposed-view, due to the conformality advantage of ALD technology and its affinity with nanophotonics and integrated optics.

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

Acknowledgments

Authors would like to thank valuable technical support by Dr. Randy Dumas Quantum Design - Applications Department, Eloisa Aparicio, Eduardo Murillo, David Dominguez, Israel Gradilla, Francisco Ruíz, Jaime Mendoza, Maureen E. Cruz and Jessica I. Ortiz.

Funding: This work was partially supported 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.

[ALD-417] Effect of high carrier concentration of SnO2 as electron transport layer in perovskite solar cells efficiency

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The use of tin oxide as electron transport layer has been widely used in perovskite solar cells due to the excellent band alignment with perovskite which is the absorber material. In this work, the effect of using different oxidant agents as water, ozone in thermal ALD and oxygen and water in PEALD where evaluated at deposition temperature of 80 and 200 °C by electron spectroscopies as XPS and REELS in the thin films obtained for determining the electronic band structure. RGA analysis were performed in each synthesis to distinguish the main differences of the chemical reactions involved and finally solar cells were fabricated using these films. As a remarkably result, surface plasmon resonance with an energy of 0.5 eV was found in REELS and XPS spectra when oxygen plasma and ozone are used at 200°C being a clear evidence of a high carrier concentration of these films. This concentration can be explained in terms of substitutional hydrogen since RGA analysis show that the absence of CH_2 as byproduct, which comes from secondary reaction pathways in the oxidation step, only occur in those samples that exhibit the surface plasmon resonance. Presence of this plasmon resonance is detrimental for the power conversion efficiency of solar cells since it can promote a plasmon assisted photocatalysis that produce perovskite degradation. Efficiencies in the range of 4.38 and 7.05% are obtained when tin oxide with presence of plasmon resonance are used while the best efficiencies are in ranges between 8.12 and 12.24% for samples without plasmon resonance.

SYMPOSIUM OF BIOMATERIALS AND POLYMERS

Chairmen:

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

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

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

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-191] Cell behavior on SiO2-Hydroxyapatite coaxial composite

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In the last years an effort has been made to produce materials which aid in the recovery of damaged tissue. Hydroxyapatite (HA) is a material with lots of potential in tissue regeneration, however, its structural characteristics need to be improved for better performance. In this study SiO_2-HA non-woven electrospun membranes were prepared using HA and SiO_2 obtained through the sol-gel method. Three configurations of the membranes were obtained and tested in vitro, showing that the composite of SiO_2-HA fibers showed a high percentage of viability on a fibroblast cell line. The obtained SiO_2-HA polymeric fibers had approximately 230±20 nm in diameter and were then sintered at 800 °C average diameter decreased to 110±17 nm. The surface area of the sintered SiO_2-HA fibers was 5.77 m^2/g. After sintering the obtained composite, it was characterized by infrared spectroscopy, where the presence of bands corresponding to Si-O, Si-O-Si bonds of silica, phosphate and carbonate where found. XRD confirmed the composite composition by showing peaks corresponding to silica and hydroxyapatite. It is concluded that the fibers of SiO_2-HA set in a coaxial configuration may be helpful to develop materials for bone regeneration.

[BIO-192] Novel synthesis of hydroxyapatite-Ag composite

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Novel and better antimicrobial agents are still being developed to control associated microorganisms. Nanoparticles of metals can be toxic to bacteria, showing biocidal activities at low concentrations. Metal, oxide or compounds based on silver was applied like antimicrobial agents. The capacity of integration of metallic nanoparticles in ceramic matrices has improved the antimicrobial behavior, resulting in the search for composites with increased bactericidal properties. The aim of this study was to prepare and characterize hydroxyapatite nanopowders containing silver nanoparticles and evaluate its antimicrobial properties against various Gram-positive and negative microorganisms associated to drug-resistance infections. Hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$, HA) powders were synthesized by sol-gel and silver nanoparticles (AgNPs) were prepared by reduction in situ method of Ag+ ions with the simple addition of gallic acid. Hydroxyapatite-silver composite (HA-AgNPs) was prepared by adsorption of AgNPs at several concentrations. The results of dynamic light scattering, transmission scanning electron microscopy and UV–visible spectroscopy showed the presence of silver nanoparticles with diameters around 5.6 ± 2.9 nm. STEM and energy dispersive X-ray spectroscopy confirmed the presence of silver agglomerates distributed over the surface of hydroxiapite nanopowders. All HA-AgNPs samples showed good and specific antibacterial effect despite of low silver concentration; therefore, this activity might depend on microbiological and cell structure characteristics as well as concentration of silver. HA-AgNPs composites might have a high potential for medical applications focused to the control of drug-resistance infections.

[BIO-212] Electron spin resonance as a high sensitivity technique for CA 15-3 detection: associated with breast cancer stage.

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The diagnosis and monitoring of diseases such as cancer is of vital importance for the patient's survival. In particular cases such as breast cancer, the detection process of antigens associated with the diagnosis involves various chemical analyzes, specifically on glycoproteins derived from specific genes. Actually there are various methodologies to evaluate the molecules chemical characteristics that allow monitoring the stages of breast cancer or even know the most efficient therapy for the patient's treatment, however, most of the methodologies used present large variations in the statistical values associated with these techniques, making the early diagnosis or careful monitoring of the disease difficult. In this work, we studied the chemical structure variations of these molecules and its relationship with the cancer stages monitoring. Using the chemical analysis electron spin resonance spectroscopy (ESR) for identifying molecular chemical paramagnetic centers of antigens established associated with the stage of disease. The results show dependence on the density of these centers and direct relationship with each stage cancer.

[BIO-254] Endocytosis and exocytosis processes of gold nanoparticle with erythrocyte ghosts

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The interaction of spherical gold nanoparticles (AuNPs) of 20nm elaborated by Turkevich method with the erythrocytes ghosts (7-8 µm) cell membrane was evaluated. The AuNPs-Membrane interaction was determined using confocal microscope, UV-vis spectroscopy and SEM analysis. The result show that nanoparticles larger than 20nm are adhered to the erythrocyte ghost membrane due their size and surface modification. Smaller AuNPs enter onto the cell by simple diffusion through the plasmatic membrane voids, these data may favor the best design and application in the treatments applied in biomedicine.

[BIO-303] Spray Drying of Folic Acid within Carboxymethyl Cellulose Nanoparticles.

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Biopolymers have been used as encapsulating agents in the manufacture of nanoparticles in the food industry, to protect bioactive compounds and thereby improve the shelf life and organoleptic characteristics of the final products. A bioactive component is a folic acid (FA) or vitamin B9, the consumption of this vitamin in adequate amounts avoid coronary heart disease, megaloblastic anemia, and congenital malformations. Therefore, the FA has been added to some foods, such as cereals, baby milk, and medically formulated foods, to provide the recommended daily dose of vitamin B9 in the diet. However, FA is thermolabile and susceptible to hydrolysis, in consequence, the biological activity during food processing is minimized. Hence, in the present work, a new compound namely CMC-FA complex was synthesized by grafting carboxymethylcellulose (CMC) with FA (added in different concentrations). Finally, the nanoparticles were obtained by spray drying. The chemical structure, size, morphological and thermal characteristics of the CMC-FA complex were studied by infrared spectroscopy (FTIR), nanoparticle size analysis (NTA), scanning electron microscope (SEM), and thermogravimetric/differential scanning calorimetry (TGA/DSC). The results showed the presence of agglomerates of spherical nanoparticles with a smooth surface. The efficiency of the encapsulation of FA by the CMC-FA complex was about 90%. Finally, the thermal analysis of the nanoparticles showed high stability of FA due to the high interaction between FA and CMC.

[BIO-307] Eco-friendly composites from of sugarcane bagase ash, wood ash and metakaolin

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Wood and sugar cane bagasse ashes are waste materials that come from various industrial processes. Wood ash is the material resulting from combustion processes with semi-volatile organic compounds that can be easily captured by living beings, producing a great impact on the environment. On the other hand, cane bagasse ash is the residue of industrial boilers of sugar mills, whose ashes of a pozzolanic nature contain inorganic compounds. The use of these two wastes has recently been explored for the production of composites with lower manufacturing cost and high commercial value, to generate low density, biodegradable and recyclable products. Thus, this study evaluated the mechanical properties of composite material in relation to the ashes as well as its composition and microstructure. The composite material was produced when the two wastes were combined with metakaolin, cured at 20 °C for 24 h in their molds. They were then demoulded and cured again at room temperature up to 28 days. This study showed, the addition of wood and sugarcane bagasse ashes to metakaolin clay resulted in the formation of ceramic matrix composites, where the mechanical properties were improved as the ash content was increased from de 1.17 to 5.04 MPa.

[BIO-371] Natural Surfactants: A Non-polluting Alternative?

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Amphiphilic nature of the surfactants is responsible for exhibiting various interfacial activities like surface tension, foaming, emulsion etc. These properties make surfactants useful in a range of pharmaceutical and industrial activities. Surfactants have a wide range of applications in everyday world, for which many synthetic surfactants are in extensive use. These surfactants enter the aquatic environment and cause extensive damage. Today it is desirable to substitute synthetic surfactants by naturally obtained products.

In search of such alternatives, we investigated plant based natural surfactants extracted from Sapindus mukorossi, Albizia procera, Zephyranthes carinata, Acacia concinna and Juglans regia. Our studies report surfactant activities of Albizia procera, Zephyranthes carinata and Juglans regia for the first time. The natural surfactants exhibited good surface tension reduction and low Critical Micelle Concentration (CMC). They exhibited acid balanced characteristics and good wetting. At higher concentrations, they showed good cleaning and emulsification.

Dirt Dispersion (DD), the amount of dirt present in the foam is a vital parameter for studying the efficacy of a surfactant. We have, for the first time, quantified DD and studied it aqs a function of concentration. With increasing concentration, the amount of dirt in foam increases; reaches a maximum and then decreases. Maximum amount of dirt attaches to the foam at CMC. This gives a rapid, easy, low cost approach to measure CMC.

The natural surfactants were analysed partially using Thin Layer Chromatography (TLC), UV-Visible Spectroscopy (UV-Vis) and Fourier Transform Infrared Spectroscopy (FTIR). TLC showed the presence of saponin having a large number of polar and non-polar compounds. UV-Vis results also supported the presence of saponin. FTIR spectra showed characteristic saponin absorptions of OH, C=O, C-H, and C=C. Glycoside linkages to the sapogenins was shown by absorptions of C-O-C.

These natural surfactants are potential candidates to provide surface active properties for a wide range of domestic and industrial applications.

[BIO-152] KINETICS OF BIREFRINGENCE DURING DRYING OF DIP-COATED CELLULOSE NANOCRYSTALS FILMS

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Cellulose is considered the most abundant renewable biopolymer in nature. Because its biocompatibility, non – toxicity and other properties, cellulose-based materials have found applications in medicine, water treatment, paper and fabrics industries among other fields. Recently, optical applications of cellulose have been envisaged because the semi-crystalline nature of cellulose fibrils and the monoclinic crystalline structure of the Iβ allomorph produce birefringence. This property might be exploited in optical based technologies such as plasma screens, optical filters, waveplates, photovoltaic materials, optical sensors and iridescent materials. To fully embrace all these applications, control of birefringence must be achieved. In this work, birefringent films on glass substrates were prepared from an aqueous suspension of rod–shaped cellulose nanocrystals extracted from filter paper by acid hydrolysis. Films prepared by dip coating possess preponderant alignment of the rod-like nanocrystals due to the balance of both drag and drainage forces along the withdrawal direction. Processes occurring during the drying of films are perhaps very critical in the formation of birefringent films because the increasing concentration of nanocrystals in the film as water is evaporated leads to kinetic arrest. To characterize the birefringence, dip-coated wet films were placed between a source of linearly polarized light and a linear polarizer in the extinction configuration; while the film was drying, the time evolution of transmittance spectra was recorded and the time-dependent retardation was determined. Four different stages in the drying process were identified. The initial stage is characterized by a fast decrease of birefringence due to drainage forces from the residual suspension on the films. In the second stage, once the residual suspension was gone from the film, birefringence started to increase proving that the cellulose nanocrystals were getting aligned parallelly to the withdrawal direction. The third stage shows a further decrease of birefringence due to the drying front crosses the measurement area. Finally, when the film got dried, the birefringence remained constant. Understanding of the birefringence kinetics during drying could give a deeper explanation of the process of the alignment of the nanocrystals and thus, help to control the birefringence of the films at will.

[BIO-155] Ultrasound-Assist extrusion method for the fabrication of polymer composite based on Nylon 6 / Zeolite for anti-flame textil

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An imminent need to decrease injury or human loss in the automotive industry is to prevent and / or prevent fires. The causes that can cause this type of incident are different reasons, such as mechanical or electrical problems, since most automotive fluids are flammable and when generating an electrical charge from friction or induction processes, it can be inconvenient. In the following work, the development of polymeric compounds based on a nylon 6 polymer and micrometer-sized commercial zeolite was developed, using ultrasound-assisted extrusion for application as anti-flame materials for the textile industry. For contents of zeolite 1, 5 and 10% by weight in a 6-grade fiber Nylon polymer matrix. Compounds were evaluated by FT-IR, XPS, SEM and Cone calorimetry. The different evaluated properties suggest that the load is homogeneously dispersed throughout the matrix thanks to the ultrasonic assisted extrusion, avoiding the formation of stress concentration points, which is directly associated with the high level of dispersion of the load reached during processing by ultrasonic assisted cast extrusion. From the flammability analyzes a 20% decrease was observed in the peak HRR of sample NZ10 with respect to Ny6.

[BIO-162] PREPARATION AND CHARACTERIZATION OF BIREFRINGENT NANOCRYSTALLINE CHITIN FILMS

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Chitin is known as the second most abundant biopolymer on the planet. It is composed by linear chains of N-acetyl-D-glucosamine units linked by β(1-4) glycosidic bond. This polysaccharide is found as an arrangement of semi-crystalline microfibrils on the shells of crustaceans, insects, fungus and other microorganisms. Chitin shows biocompatibility, biodegradability, insolubility in any organic solvent, high affinity to metal ions, among other properties. These properties have led to many studies and applications of chitin in a variety of areas like biomedical, pharmaceutic, textile, cosmetic and other industries. Recently, studies for applications of chitin-based materials in the field of optics have emerged. In this work, the fabrication of nanocrystalline chitin films with birefringent properties is studied.

Chitin Nanocrystals (ChNC) were prepared by deproteinization and acid hydrolysis of practical grade chitin from crab shells. Stable aqueous suspensions of ChNC were obtained after dialysis, centrifugation, pH and solids concentration adjustments. Dispersion in a sonic bath was applied to the ChNC aqueous suspensions to provide further separation of aggregated material. The chiral nematic liquid crystal phase of the ChNC aqueous suspensions was revealed by polarization optical microscopy. ChNC films were dip-coated on glass substrates at withdrawal speeds V= 5, 15, and 30 cm/min. Just prepared wet films show birefringence as revealed when they are placed between crossed polarizers. However, the birefringence significatively decreases during drying. For a better understanding of this behavior, the time-dependent evolution of transmittance spectra T_{cp} (400 to 700 nm) of the sample between crossed polarizers during drying was determined. The spectral birefringence was determined by modeling T_{cp} as that of a rotated retarder placed between crossed polarizers. It was found that birefringence increases with wavelength. In the case of wet films, for V= 5 cm/min T_{cp} decreases with wavelength whereas the opposite dependence was found for V= 30 cm/min. The modelling shows that such opposite behavior is due to the thickness dependence with V. The effects of film shrinkage due to the loss of water during drying and kinetic arrest on the time evolution of T_{cp} are discussed.

Keywords: Nanocrystalline chitin, birefringence, dip-coating.

[BIO-286] Obtaining and characterization of nanofibers by electrospinning technique from organic waste for agroindustrial applications

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Cellulose has been the most research polymers in different fields due to its renewable and biodegradable properties. Electrospinning is an easy and potential technique for nanofiber fabrication. This method is versatile and easy to assemble, which has made it possible to process a wide variety of polymers and inorganic composites, in numerous types of applications. Industrial organic wastes are pollutants that do not have proper use and end up only in a sanitary landfill causing leaching problems poisoning the earth's deep mantle.
In this work, cellulose nanofibers were obtained from an electrospinning technique using organic wastes from orange skin and *Hibiscus Sabdariffa* whose were compared with commercial cellulose, for being used as plant protector and nutrient in agroindustrial applications. Different techniques, Scanning Electron Microscopy (SEM), X-Ray Diffraction (XRD), FTIR spectroscopy, and differential scanning calorimetry (DSC) were used to estimate the crystallinity degree and the morphology of the nanofibers compared with commercial cellulose.

[BIO-288] Polyvinyl alcohol (PVA) crosslinking methods for membranes and perspectives for ethanol dehydration.

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The crosslinking of PVA have proved being useful in providing closed pores, and less permeation flux for molecular separations. Also, this process is capable of modify the hydrophillic properties in surfaces of PVA or into composites.
The aim of this work is to show the different crosslinking pathways for processing PVA and its results over the PVA and composites for membranes. Also, to remark patterns between chemical compositions, structures and properties, and finally, propose the impact of incorporating 2D materials to modify the structures and provide efficiency on ethanol dehydration.
Beyond that, there are the novel polimeric materials known as PIMs (polymers of intrinsec microporosity) which have been studied recently since 2004, which are becoming relevant in the field of selective molecular separations. The incorporation of 2D materials into polymers, as PVA and PIMs are promising for selectivity over greener and sustainable separation methods.

[BIO-293] Microcapsules of Lemon essential oil produced by ionic gelation as wall alginate / mucilage (Opuntia ficus indica).

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Essential oils have different properties, and some, such as that from citrus fruits, are of great interest in the cosmetic and food industry. Such is the case with lemon essential oil. However, its chemical components are susceptible to being modified by environmental conditions, so they must be protected so that their properties remain unchanged. The objective of this research was to micro-encapsulate lemon essential oil by the ionic gelling method, via atomization, using as wall material a mixture of alginate / mucilage of Opuntia ficus-indica (in ratios 3:1, 2:1, 1:1, 1:2). The interaction of the polymers used as wall material was observed through infrared spectroscopy technique. The microcapsules obtained were measured particle size. The microcapsules were lyophilized to analyze their morphology using scanning electron microscopy. Subsequently, the efficiency was measured by means of UV-Vis spectroscopy. The biopolymers used in microencapsulation did not show significant interaction, observed by infrared spectroscopy. The microcapsules obtained had a particle size distribution that varied from 15-75 μ, with the particle size increasing as the mucilage content in the alginate/mucilage mixture increased. When observed by scanning electron microscopy, the microcapsules had a spherical shape and some porosity, showing a rough surface and slightly collapsed due to the loss of water when lyophilized. The determination of the amount of encapsulated oil was quantified by UV-Vis spectroscopy. The maximum encapsulation efficiency was obtained for the microcapsules made only with alginate (18.39%) followed by alginate-mucilage in a ratio 3:1 (18.06%). The atomization method using ionic gelation was a simple and effective method to microencapsulate and thus protect the essential oil of lemon.

[BIO-347] POLIMERIZATION OF EPOXIDIZED LINSEED OIL AND CARBON BLACK ON IRON-ZINC SHEETS, CATALYZED BY ALUMINUM TRIFLUOROMETHYL SULFONATE

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Metal corrosion represents a great problem, mainly at an industrial level. Therefore, application of coatings that slow down this phenomenon is essential. Cure epoxy resins have been widely used to protect metals from corrosion, such as steel. However, trend is to replace resins obtained from petroleum sources with functionalized biopolymers, specifically vegetable oils. Therefore, the main objective of the work was to study the polimerization of Epoxidized Linseed Oil (ELO) on commercial iron sheets coated with Zinc (Fe-Zn sheets). Using a Lewis acid [Aluminum Trifluoromethyl Sulfonate, $Al(OTf)_3$] as catalyst and crosslinking agents (bisphenol A, BPA; Carbon black, CB). The chemical structure of ELO polymers crosslinked with BPA and CB, were characterized by Fourier Transform Infrared Spectroscopy (FT-IR). Subsequently, to evaluate the anticorrosive performance of polymers on Fe-Zn sheets, adhesion and weathering tests were carried out (salt-fog chamber). Results obtained by FT-IR detected that using $Al(OTf)_3$ as a catalyst was effective to carry out polymerization of ELO with BPA and CB at 80 °C and 30 min. This was verified by FT-IR following the disappearance of bands corresponding to epoxy ring (821 and 798 cm^{-1}) and appearance of an absorption band that is attributed to OH groups (3550 cm^{-1}). Finally, addition of BPA and CB improved the mechanical adhesion property of polymers on Fe-Zn sheets, providing greater protection to decelerate corrosion.

[BIO-388] Obtaining resin based on unicel waste

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Expanded polystyrene (EPS), commonly known in Mexico as unicel, is a foamed plastic material obtained from polystyrene, is employed in the construction and packaging sector. It is characterized by its lightness, resistance to moisture and above all hygiene, but being one of the least environmentally friendly materials to take up to 500 years to degrade, currently looking for alternatives for recycling.

In the present work an alternative to its recycling is proposed from the manufacture of a resin based on unicel, whose production consists in the dilution of unicel residue, previously collected and washed, to dilute in an organic solvent (ethyl acetate). Different concentrations was tested until obtaining the most suitable one based on a liquid silicone consistency, in a proportion of 3:6 g/ml, after this it was allowed to dry for approximately 5 days. The material obtained was studied by scanning electron microscopy (SEM) to obtain information on the morphology and size of the samples prepared, an X-ray dispersive energy spectroscopy (EDS) analysis was performed to obtain information on the chemical composition of the samples prepared. In addition, hardness tests were carried out to measure some mechanical properties of the different samples obtained.

[BIO-395] Effect of temperature on the synthesis of Hydroxyapatite obtained sea urchin spines

Authors??

Hydroxyapatite (HA), an important crystalline material in the medical field, is composed of calcium, phosphorus and hydrogen atoms ($Ca_{10}(PO_4)_6(HO)_2$) and generally has a hexagonal crystalline structure [1]. This material is present in teeth and bones, presenting a characteristic hardness and, due to its chemical and physical properties, has the application of facilitating the regeneration of hard tissues [2].

In this work, hydroxyapatite (HA) was synthesized using sea urchin spines via a precipitation and heat treatment method at three different temperatures (500, 600 and 700 °C). Biosynthesized HA was characterized to determine the vibration of functional groups, morphology, particle size, crystalline structure and chemical composition. The XPS confirmed that the material resulting biosynthesis was HA. Hence, according to these results, the synthesis temperature of HA has a significant effect on the characteristics of the resulting material. XRD analysis presented the characteristic peaks of HA, showing a lower crystallinity when the synthesis temperature increased. EDS results showed that the Ca/P ratio increased in the samples at higher temperatures. Finally, The FTIR-ATR results reveal that the most defined characteristic HA bonds (O-H, P-O and C-O bonds) were better defined at higher synthesis temperatures. SEM also presented evidence that temperature has a significant effect on morphology.

[1] García-Garduño, M.V.; Reyes-Gasga, J. La Hidroxiapatita, Su Importancia En Los Tejidos Mineralizados Y Su Aplicación Biomédica. *TIP Rev. Espec. Cienc. Químico-Biológicas***2006**, *9*, 90–95.

[2] Erdem, U.; Dogan, M.; Metin, A.U.; Baglar, S.; Turkoz, M.B.; Turk, M.; Nezir, S. Hydroxyapatite-Based Nanoparticles as a Coating Material for the Dentine Surface: An Antibacterial and Toxicological Effect. *Int.***2020**, *46*, 270–280.

Keywords: Biomaterial, Hydroxyapatite, sea urchin

Acknowledgment:
Authors thank to CONACYT for financial support (Grant No. 295075 Infrastructure, Grant 4940 National Problems).

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[BIO-402] Encapsulation of Artemisia ludoviciana essential oil in chitosan with potential antimicrobial activity

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The results of the obtained, preliminary phytochemical characterization with GC-MS, encapsulation, characterization of particles, and evaluation of the antimicrobial activity of essential oil of *Artemisia ludoviciana* are presented. The extraction was carried out by the hydrodistillation method using the leaf of *Artemisia ludoviciana* (AlEO) with Clevenger equipment, in which 20 mL of essential oil was obtained. From the phytochemical study of essential oil, it was possible to identify with GC-MS the presence of verbenol as the major volatile compound (60%), eucalyptol (10%), alpha-pinene (5%), camphor (5%), and others minor compounds. The microencapsulation of the essential oil was very successful using the ionic gelation method and as an encapsulating polymer the chitosan (Cs). By varying the polymer concentration, it is possible to control the structural properties of the chitosan particles. The result of FT-IR shows the formation of essential oil-free (CsPs) and essential oil-loaded chitosan particles (AlEO-CsPs). The characteristic controlled release of the essential oil in the function of the structural properties of the polymeric were evaluated using UV-vis spectroscopy, optical and electronic microscopy. The antimicrobial study of the CsPs and AlEO-CsPs against *Salmonella typhi* was evaluated in vitro after 24h at 37°C. The results obtained revealed that *S. typhi* population inoculated on the control simple increased, on the contrary, both free and chitosan particles loaded with AlEO cause an immediate reduction in *S. typhi*.

[BIO-414] Modeling and printing of 3D Voronoi structures for plantar orthosis applications

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The use of additive manufacturing for biomedical applications has taken on special relevance in the last decade. [1] 3D printing of parts in nylon matrices reinforced with carbon fiber, kevlar, fiberglass, etc., used as final parts is an attractive solution due to its low-cost manufacturing compared to machining metal parts, in addition to having similar mechanical properties to metal parts. [2] On the other hand, Voronoi structures can be found in nature, such as bones, in plants, coral structures, etc. The use of Voronoi structures has shown a significant reduction in the material used during the process fabrication and the reduction of residual stresses in the material. [3]
The present work shows the modeling of Voronoi structures used as a support skeleton in the manufacture of plantar orthoses. Python and Solidworks(r) were used for modeling the Voronoi structures. The following variables were used for the design of factorial experiments: point density, thickness of the skeleton y roundness of joints. Solidworks(r) software was used to model compressive strength, used as a response variable. Based on the modeling and calculations, the best Voronoi structure found was printed on a MarkForge II equipment, in a matrix of nylon reinforced with carbon fiber.

[BIO-420] Methodologies and fractional models for measuring viscoelastic properties of cancer cells by atomic force microscopy

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We show two methodologies for measuring the viscoelastic properties of cancer cells by atomic force microscopy. The first consists of analyzing force-distance curves, and the second is through force-time curves obtained during a relaxation experiment. Both methodologies can be combined with mechanical models to characterize the viscoelastic parameters of a system. In this work we use four mechanical models with these methodologies to describe the viscoelasticity of three cancer cell lines. The cell lines that we study were MDA-MB-231, DU-145 and OSTEOSARCOMA. We made a comparison between the parameters obtained with the different models. Also, we performed an analysis of the quality of the fits achieved with each model. Finally, we observe that the fractional Zener model gives us a better way to make a physical interpretation of the results, it also provides the best fit.

[BIO-425] STUDY OF THE CONTROLLED RELEASE OF BIOHERBICIDE-STREPTOMYCES Sp., MICROENCAPSULATED.

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The results of encapsulation of a Bioherbicide formulation from *Streptomyces sp*., using the drip extrusion technique and alginate as gelling agent, are presented. Bioherbicide precursor solutions containing PVA were prepared under ambient conditions and with rigorous agitation. By varying the percentage of alginate 2.0-0.75% in the precursor solution containing calcium ions, it was possible to prepare bioherbicide capsules with sizes of 5 mm and with shell thicknesses of 957-458 µm, respectively. Characterization by light microscopy showed the formation of well-defined and homogeneous microcapsules. SEM analysis reveals the formation of different morphologies in the cross section of the shells as a function of the alginate concentration. More compact and less porous shells with increased alginate concentration. The results by UV-Vis spectroscopy revealed the presence of the bioherbicide in the capsules. The results of the release kinetics of the bioherbicide are presented using optical absorption spectroscopy in the UV-Vis range.

[BIO-430] Microspherification of Echeveria gibbiflora in a polymeric matrix of sodium alginate and controlled release properties.

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The results of the spherification of *Echeveria gibbiflora* in a polymeric matrix of alginate using the drip extrusion technique are presented. The principle of the technique relies on the gelation of alginate in the presence of calcium. Precursor solutions containing *Echevería gibbiflora* and sodium alginate were mixed and prepared under ambient conditions and with rigorous agitation. The results showed that varying the percentage of *Echeveria gibbiflora* 0.05-1.4% in the precursor solution containing alginate, it was possible to prepare microspheres with sizes of 500 – 1000 µm, respectively. Characterization by microscopy showed the formation of well-defined and homogeneous microspheres. SEM analysis reveals the formation of different morphologies in the cross section of the microspheres as a function of the concentration. More compact and less porous matrix with decreased *Echeveria gibbiflora* concentration was observed. The results by UV-Vis spectroscopy revealed the presence of the *Echeveria gibbiflora* in the microspheres. The results of the release kinetics of the *Echeveria gibbiflora* are presented using optical absorption spectroscopy in the UV-Vis range.

CHARACTERIZATION AND METROLOGY

Chairman:

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

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

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

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

[CHM-218] Automatic detection of water stress taking multispectral photography in sugarcane leaves using machine learning

Sergio Enrique Rivera Carballido (rivse120992@gmail.com)[2], Alan Hernández Rodriguez (alanhr_1224@outlook.com)[2], Edwin Alejandro Enríquez-Valdés[2], David Barrera-del-Angel[2], Sergio Osbaldo José-García[2], Noé Sierra-Romero[2], Yesenia Eleonor González Navarro[2], Francisco Hernández-Rosas[1], Juan Hernández-Rosas[2]

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In this work a system was used in the agricultural sector, capable to perform the automated determination of the water stress index in sugar cane crops at the Ingenio Central El Potrero in Veracruz, México, through the processing of images captured through a multispectral camera. Initially, the design and construction of an unmanned aerial vehicle (UAV) was carried out, later an image captured was made by using the UAV, followed by an analysis of the data applying Machine Learning tools to obtain the most suitable vegetation index (VI) choosing between Normalized difference vegetation index (NDVI), Enhanced vegetation index (EVI) and Soil-adjusted vegetation index (SAVI) , which depended on the state of the crop, the results was saved for future reference and comparison together with a database provided by the specialists in the cultivation of sugar cane showing the results in a web app.

[CHM-252] Detection of traces of Air Pollutant Particulates by Raman Spectroscopy surface reconstruction in the borderline region between Ciudad Juárez, Chih-El Paso, Tx

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Raman Spectroscopy has been established elsewhere as a suitable tool for the chemical identification of air pollutants with the primary size fraction (> 2 µm) [1, 2]. In this work, we have employed a full automated Raman system to scan 100x100 µm areas at the surface level (resolution of 1 µm) of filter collected-samples of airborne dusts. A 50x microscope objective is used to collect laser light of wavelength of 532 nm on the sample, giving a total power of nearly 6 mW. The samples are provided by Centro de Ciencias Atmosféricas y Tecnologías Verdes-Universidad Autónoma de Ciudad Juárez and have been collected from two enough separate locations in the borderline region between Ciudad Juárez, Chih. and el Paso, Tx, thus representing distinct environmental conditions and the detection of different specimens is expected. Zone one is located well inside the urban area, near downtown. Zone two is a suburban area, closer to the borderline. Besides the location variable, time as a variable also has been being studied with a period of a week; representative pairs of samples are thus studied in given time period. The reconstruction of several surfaces combined with Raman mode filtering, so far has led to the identification of Raman spectra appointing to traces of the following phases [1]: CaCO3, CaSO4 and "graphitic soot" (a form of carbon or hydrocarbon matter). Compounds based on lead (Pb) are sought [2]. The study on the dynamics of this pollutant is proposed by the identification of its population according to location and time, and on the basis of the meteorological conditions registered on representative periods of time.

[1] E. S. Etz and G. J. Rosaco, *Observation of the Raman Effect from Small, Single Particles: its use in the Chemical Identification of Airborne Particles,* In *Environmental Pollutants,* T. Y. Toriabara et al. (eds.), Plenum Press: New York 1978.

[2] R. L. Frost, W. Martens, J. T. Kloprogge, and Z. Ding, Spectrochimica Acta Part A **59**, 2705 (2003).

[CHM-291] Photoacoustic spectroscopy and application in medicine: Type 1 Diabetes

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In Mexico, there are 1 million 704 thousand diabetics who have been diagnosed with diabetes and are undergoing treatment but just over a million patients cannot control their glucose. Causing to be the second leading cause of death in addition to the cost of care estimated at 7.7 thousand million dollars. For this reason and others, in 2016 diabetes was declared an epidemiological emergency in the country.
A fundamental challenge in controlling the diabetes epidemic is the detection and use of new techniques that help to detect the disease or see the progress of this disease. And that is why we propose photoacoustic spectroscopy (PAS), which has made contributions in physics, chemistry, biology and even in medicine. PAS is a non-destructive technique and allows us to carry out studies on biological materials "in vivo" and “in vitro”. In this work, we will present one application of PAS in medicine, specifically to study blood samples of male and female rats with type 1 diabetes, as a part of the application of PAS in the study of diabetes.

[CHM-355] Automatic detection of water stress taking multispectral photography in sugarcane leaves using machine learning

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In this work a system was used in the agricultural sector, capable to perform the automated determination of the water stress index in sugar cane crops at the Ingenio Central El Potrero in Veracruz, México, through the processing of images captured through a multispectral camera. Initially, the design and construction of an unmanned aerial vehicle (UAV) was carried out, later an image captured was made by using the UAV, followed by an analysis of the data applying Machine Learning tools to obtain the most suitable vegetation index (VI) choosing between Normalized difference vegetation index (NDVI), Enhanced vegetation index (EVI) and Soil-adjusted vegetation index (SAVI) , which depended on the state of the crop, the results was saved for future reference and comparison together with a database provided by the specialists in the cultivation of sugar cane showing the results in a web app.

[CHM-415] Use of geometrical factors in XPS calibration which affect the intensity of the experiments

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X-ray photoelectron spectroscopy (XPS) is by far the most commonly used technique in areas of materials science, chemistry, and chemical engineering to assess surface chemistry, bonding structure, and composition of surfaces and interfaces. With more than 9000 papers published annually, X-ray photoelectron spectroscopy (XPS) is an indispensable technique many laboratories. This can be seen because the number of papers where XPS was employed has increased more than 15 times during last 30 years with more than 9000 papers published only in the last year.
In this work we use the geometrical factors such as the size and shape of the spectrometer analysis volume and X-ray beam and, very important, the sample height and the axis of rotation of the sample manipulator to describe the models and protocols for the correct characterization of the XPS equipment's in order to improve the intensity acquisition during experiments.
We prepared flat and thick gold films on silicon wafers through sublimation employing a tungsten filament with metallic gold (99.999% pure Sigma Aldrich). The background pressure in the processing chamber was 3×10^{-7} Torr and the pressure during sublimation was 2×10^{-6} Torr. For these experiments we use an X-ray photoelectron spectroscopy (XPS) instrument with a monochromatic X-ray aluminum source (XR5, from ThermoFisher) and a 7-channeltron hemispherical spectrometer (Alpha110, from ThermoFisher) assembled by Intercovamex. The shape of the waist of the volume of the spectrometer and the shape of the beam of the monochromatized x-ray source were determined by Knife-edge experiments. Nevertheless, the obtained parameters can be transferable to other more complex systems since they are geometrical in nature.
We use the geometric factors that affect the ARXPS measurements and the standards developed by Herrera-Gomez et. al.2010, for the calibration of XPS instruments and how this series of procedures have allowed the standards to be maintained over time. In data acquisition for XPS and ARXPS. This procedure has shown that it can be used to calibrate other XPS instruments even if they do not have the same geometry. Also, how these geometric factors have changed over time and how this method has allowed us to identify early failures in our equipment such as the wear of the channeltron.

[CHM-151] Characterization of the thermal transport mechanism in disordered and self-assembled symmetric polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) copolymer films through picosecond laser pump-probe method.

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Ultrashort optical pulses are used to excite and detect picosecond longitudinal-acoustic pulses in thin films of disordered and self-assembled symmetric polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) copolymer. The cross-plane thermal transport, generation, and propagation of coherent acoustic-phonon waves have been characterized by applying the picosecond laser pump-probe method based on the measurements obtained through the time-domain thermoreflectance (TDTR) technique. Analysis of data acquired and simulations are done for explain the principal thermal transport mechanism base on properties experimentally derived such as sound velocities, ultrasonic attenuation and photo-elastic constants. The results confirm that the interfaces between the PS and PMMA, and reorganization of the PS and PMMA chains around these interfaces, do not significantly affect the thermal transport in these PS-b-PMMA films.

[CHM-168] Photopyroelectric techniques for thermo-optical characterization of glucose solutions at wide range of concentrations

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Photopyroelectric techniques, taking the sample thickness as control variable, were used for thermal diffusivity and optical absorption coefficient measurements of glucose solutions in distilled water. Thermal diffusivities were measured for a set of 20 glucose solutions, ranging from 0 to 4 M concentration, as well as the optical absorption coefficient, at 1550 nm, for a 1 M glucose solution. Thermal diffusivities shown a monotonic decreasing behavior which was slow at small glucose concentrations and become fast at large concentrations. The glucose absorptivity in distilled water, at 1550 nm, was obtained from the measured optical absorption coefficient and resulted in 0.55 cm^{-1}/M. These results shown the feasibility of glucose quantification by the measurement of these two thermophysical properties. The optical characterization at 1550 nm results relevant since shows the feasibility of non-invasive glucose assessment in the near-infrared región, specially by using photothermal techniques.

[CHM-260] XPS and PA techniques for the study of lime used in the Talavera House of Mexico City

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To identify the structure and optical properties of compounds used in archaeology, techniques such as X-ray Photoelectron Spectroscopy (XPS) and Photoacoustic (PA) are of special interest. This study was focused in the study of samples from the restoration period 2012-2013 belonging to the archeological site of Talavera House trough spectroscopy and thermal techniques. This House is located in the historical center of Mexico City between the República del Salvador, Talavera and Roldán streets. In this work, the chemical compounds that were added to the lime used in furnaces and tanneries during the 18th and 20th century were identified. Those elements were located in the second yard and in the corridor located in the first courtyard, respectively. The samples collected were analyzed by XPS and Photoaccoustic (PA) techniques and compared to materials of other excavation sites.

[CHM-279] Intrinsic phonon-plasmon interaction in InAsSb alloys

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Keywords : Multiwavelength Raman, phonon-plasmon, antimonide, surface space-charge region.

Raman Spectroscopy is a powerful technique to analyze crystalline materials by identifying the vibrational modes that produce inelastic scattering of photons. Phononic vibrations can be coupled with plasmons in doped materials with long-range ordering. The effects of phonon-plasmon coupling has been reported in multiple III-V and II-IV binary semiconductors, but it has been difficult to observe them in ternary or quaternary alloys due to the induced disorder. In this work, we report at the first-time phonon-plasmon interaction in intrinsic InAsSb alloys observed by multiwavelength Raman spectroscopy and its relationship with its crystalline properties evaluated by HR-XRD. Raman spectra were measured with 473, 532 and 633 nm laser wavelengths, whose calculated penetration depths are 19.2, 33.4 y 61.8 nm, respectively. A main peak is observed composed of two physical signals identify as InAs-like LO phonon (227.4 cm^{-1}) and L- phonon-plasmon coupling (115 cm^{-1}) [1]. As wavelength laser increase the LO intensity of InAs-like mode falls off, nevertheless plasmon coupling intensity rise. These intensity dependencies with laser penetration length evidence the formation of intrinsic depletion region near InAsSb surface. Additionally, the ration of InAs-like LO to L- plasmon coupling intensities (indicated as dimensionless parameter) as function of Sb concentration for both $InAs_{1-x}Sb_x$ were analyzed. ratio decreases as antimonide content increases by two important reasons. In the first, crystal quality evaluated by HR-XRD of alloys decreases with antimuonium incorporation. This non-intentional crystal deterioration reduces LO phonon lifetime lowering its raman intensity. At the second, Sb variation modified the strength of phonon-plasmon interactions through a change of intrinsic carrier bulk concentration. At 500-700 cm^{-1} raman range a broad band is observed associated with L+ phonon-plasmon mode. The

broad band position depends on Sb content which agree with the hypothesis that Sb influences the intrinsic free carrier density. To corroborate this assumption, the dependence of the L+ and L- frequencies of phonon-plasmon coupled modes with carrier concentration (η_i) were calculated by an analysis of dielectric function of InAsSb alloy [2]. L+ frequency position observed in the range of 500 to 700 cm^{-1} was used to determine . Intrinsic carrier concentration change from 3.12×10^{17} to 3.88×10^{17} cm^{-3} for samples grown on p-GaSb (n-GaSb) and are originated by induced donor level at InAsSb crystal by Sb incorporation.

This work was partially supported by SIP-IPN project No. 20200459.

[1] M. Erkus and U. Serincan, "Phonon frequency variations in high quality $InAs_{1-x}Sb_x$ epilayers grown on GaAs," Applied Surface Science, vol. 318, pp. 28-31, 2014.

[2] W. Songprakob et al, "Infrared studies of hole-plasmon excitations in heavily-doped p-type MBE-grown GaAs:C," Physical Review B - Condensed Matter and Materials Physics, vol. 62, (7), pp. 4501-4510, 2000.

[CHM-294] Copper nanoparticles nonlinear refraction index vs ablation time

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In this work, the change of the non-linear refractive index vs ablation time of cooper nanoparticles is reported. This change is measured with the Z-scan technique. In this technique, the sample is exposed to different power, due to that the beam laser with a wavelength of 534 nm is focused with a lens and the sample is moved in the z-axis with a motorized stage. Then, the non-linear effect could be seen. The copper nanoparticles were obtained by laser ablation. A copper disc immersed in acetone was irradiated with a Nd:YAG laser of 1064 nm, 15 Hz, 47 mJ and pulses of 7 to 2 ns. The result showed a nonlinear refractive index increase with an ablation time increase. These non-linear refractive indices are between 6 to 37 × 10^{-8} cm^2/w. On the other hand, the samples were analyzed with UV-visible. Finally, this non-linear index increase due to the concentration increase is related to the ablation time.

[CHM-296] SYNTHESIS OF TiO2-Fe-Ni CATALYSTS VIA MICRO-WAVES FOR PHOTODEGRADATION WITH UV LIGHT AND VISIBLE LIGHT IN WASTEWATER

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Abstract
This work presents the effects of TiO_2 doping with iron (Fe) and nickel (Ni), at different concentrations of one of these doping elements, varying the other. They were synthesized by the microwave-assisted sol-gel method. These TiO_2 catalysts doped with iron and nickel change the intrinsic structure of the activation band or "band gap" of the semiconductor, improving the response of the photocatalyst in the visible light region. The photodegradation of acid blue dye 9 and Rhodamine B at 20 mg / L (or 20 ppm) is presented, the best degradation was TiO_2 (0.10% Fe) (0.25% Ni) without calcination, with 50% visible light and UV light 40%; presenting a band gap of 2.28 eV. The maximum degradation of TiO2 - Fe with visible light is 40% for Rhodamine B with a band gap of 2.2 eV. The TiO2-Ni reached 62% degradation with Visible light, having a band gap of 2.65 eV.
Keywords: Dopage, Bandgap, degradation

[CHM-299] Refractive index of carbonated drinks

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Utilizando la Ley de Snell, se determinó el índice de refracción de bebidas carbonatadas con azúcar, edulcorantes y sin azúcar. Las bebidas con azúcar tuvieron índices de refracción de valor más alto, las bebidas edulcorantes mostraron valores intermedios y las bebidas sin azúcar tienen índices de refracción de valor más bajo. Se concluye que el contenido de azúcares influye directamente en el valor del índice de refracción, aunque en apariencia son muy similares.

[CHM-310] Determination of the refractive index and thermal properties of vitis vinifera oil

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Se determinan el índice de refracción, la efusividad térmica y la difusividad del aceite de vitis vinifera. Mediante la incidencia de un rayo láser sobre la superficie plana de un refractómetro semicircular se obtiene el índice de refracción y, mediante la técnica de la foto piroeléctrica, se obtienen las propiedades térmicas mediante la relación entre la efusividad térmica y la difusividad obtenida a partir de su conductividad y capacidad térmica. de calor volumétrico.

[CHM-376] Influence of the Cantilever Stiffness in Switching Spectroscopy Piezoresponse Force Microscopy Characterizations.

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In recent years, Switching Spectroscopy Piezoresponse Force Microscopy (SS-PFM) [*Stephen Jesse, Arthur P. Baddorf, Appl. Phys. Lett., 88, 062908 (2006)*] in Dual AC Resonance Tracking (DART) mode [*Brian J Rodriguez, Clint Callahan, Nanotechnology, 18, 475504 (2007)*] has been utilized as an effective tool to study the superficial and local domain switching behavior and piezoresponse of ferroelectric materials at nanoscale level. This technique is fundamentally different from macroscopic piezoelectric properties of a sample, where piezoelectric behavior occurs due to the nucleation growth and interaction of multiple separated domains, while in PFM the piezoelectric response is taken from a local region by monitoring piezo-activity within a single domain. Phenomena related to domain activities such as nucleation, pinning, switching and time dependency, which occurs under a sharp tip by the application of a voltage, can be investigated. In SS-PFM measurements, the amplitude of the acquired signal is proportional to the effective longitudinal piezoelectric coefficient, d_{33}. However, piezoelectrical response is difficult to separate over the full electromechanical response contributions based scanning probe microscopy techniques [*A. Gomez et al., Nature Communications, 18, 113 (2017)*]. Ferroelectric samples were characterized using a scanning probe microscopy (MFP-3D Infinity, Asylum Research Inc., USA) under the SSDART-PFM mode to determine their piezoelectric behavior. Piezoresponse signals were obtained first on a PZT thin film as standard and from BCZT, and BNBT ferroelectric ceramics samples applying a triangular waveform voltage cycle and using three different cantilever´s length of a conductive tip-probe. Cantilever lengths of 125, 225 and 450 um were used in order to choice the optimal tip for better measurements with SSDART-PFM. Piezoelectric displacement-applied voltage (D-V) “butterfly” loops were obtained and converted to piezoelectric hysteresis loops according to the law of converse piezoelectric effect [*Z. Chen et al., RSC Advances, 2, 7380 (2012)*]. The dependence of local effective piezoelectric d_{33} coefficient regarding to cantilever length is discussed in this work.

[CHM-407] CHARACTERIZATION OF THE HIGH ENTROPY AL-CU-MN-NI ALLOY SYNTHESIZED BY MECHANICAL ALLOY

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High entropy alloys (HEAs) have the potential to be used in various industrial areas and these alloys are expected to replace traditional materials. On the other hand, 75% of the publications about HEAs belong to liquid metallurgy methods, and only 5% correspond to synthesis of HEAs in solid state, including mechanical alloying (MA). In this research, the high entropy alloy composed of Al-Cu-Mn-Ni was elaborated by Mechanical Alloying. The aim of this work was to study the milling times in the formation of the alloy and its effect on the microstructure.
The milling process was carried out in a planetary ball mill with a constant speed of 400 rpm, an argon atmosphere and stainless steel vials and balls with ball-to-powder weight ratio of 4: 1. Samples were obtained for different milling times (2, 4, 6, 8, 12, 16 and 20 hours) to study morphological and microstructural changes, including the size of the crystallite. The powders obtained through MA at different milling times were characterized by Scanning Electron Microscopy (SEM), X-ray energy dispersion spectrometry (EDS) and X-ray diffraction (XRD). The results show that it is possible to achieve the formation of the alloy by MA. The XRD analyzes show that, after 12 h, there are no significant changes in the diffraction peaks, likewise the crystallite size evolved 23.6 nm at 2 hours to 14.5 nm at 20 hours of milling.

LUMINESCENCE PHENOMENA: MATERIALS AND APPLICATIONS

Chairmen:

Dr. Gilberto Alarcón Flores: (CICATA-IPN), galarcon@ipn.mx
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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-301] Microwave assisted synthesis of Mn4+ doped K2MF6 (M= Si4+, Ti4+) phosphors

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Because of its optical properties, Mn^{4+} activate fluoride phosphors have drawn attention owing to its unique properties as high photoluminescent quantum yields and good thermal stability, which it makes suitable for warm light emitting diodes (WLED). In this work we report the microwave assisted synthesis of Mn^{4+}: K_2MF_6 (M= Si, Ti) phosphors in benzyl alcohol as a solvent and NH_4F as a fluorine source. These phosphors are polycrystalline and their diffraction peaks could be indexed in the hexagonal phase (ICOD 01-070-4699 card) for K_2TiF_6, and in the cubic phase for K_2SiF_6 (JCPDS 85-1382). Mn^{4+} doping was carried out by cation exchange in solution phase using K_2MnF_6 at different molar ratios and aqueous HF solutions. As synthesized Mn^{4+}: K_2MF_6 (M= Si, Ti) phosphors showed an intense red-light emission centered at 631 nm and a PLQY near to 90 %. Photoluminescence, quantum yield and kinetics measurements were carried out in order to analyze the optical properties of as synthesized materials.

[LPM-343] Some factors to improve the intensity of lanthanide-based luminescent materials

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Lanthanide-based luminescent materials have been used in multiples applications, such as biomedical imaging, disease therapy, display, solar cell and laser technology, etc. Looking for alternatives to improve lanthanide based on luminescent material intensity, here, we focus on the study of 3 factors that aid to achieve this goal: synthesis methods (hydrothermal and co-precipitation methods comparison), charge compensators in hosts doped with trivalent lanthanide ions and the use of organic ligands.

[LPM-346] CaSO4:Dy and CaSO4:Tm as long persistent phosphors: preliminary results

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Results obtained in a first stage study on the thermoluminescence (TL) and afterglow (AG) of self-agglomerating pellet-shaped $CaSO_4$:Dy and $CaSO_4$:Tm phosphors synthesized using a low cost and environmentally friendly method are reported. In order to investigate their TL and AG features, some samples were exposed to beta particle irradiation in the dose range from 0.06 to 8.0â€¯Gy. Characteristic TL glow curves for both phosphors consists of an intense TL maximum located at 120 °C, which is considered suitable for AG dosimetry, a shoulder located at 190 °C, and a maximum located at 400â€¯°C. $CaSO_4$:Dy and $CaSO_4$:Tm exhibit a highly sensitive AG response for as long as 2 hours with linear behavior from 0.06 Gy up to 1.0 Gy ($CaSO_4$:Dy) and 0.125 up to 2.0 Gy ($CaSO_4$:Tm). A remarkable reusability of the TL and AG response was observed in ten irradiation – TL/AG readout cycles with no need of any pre-irradiation annealing. The synthesized $CaSO_4$ based phosphors exhibit suitable properties to be considered promising as long persistent phosphors for real-time radiation detectors and dosimeters.

[LPM-370] Temperature dependent photoluminescence of Nd+3 doped TiO2: a suitable nanothermometer candidate.

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TiO_2 is a particularly studied semiconductor material that can be used in a vast number of applications, such as photocatalysis, gas sensors, among others. In this work, TiO_2 nanoparticles were doped with three different amounts of Nd^{+3} (0.5, 1 and 3 wt. %) and characterized as active material for temperature sensor. Nd^{+3}–TiO_2 nanoparticles were synthetized by the sol-gel method and characterized by XRD, SEM-EDX, TEM, HRTEM, XPS and NEXAFS techniques. Afterwards, the effect of the temperature in the photoluminescence intensity of the synthetized nanoparticles was investigated with an excitation wavelengths of 350 nm. The spectra were collected in the 288–348 K range. The photoluminescence spectra obtained show a broad band ranging from 380 nm to 738 nm and the well-resolved $^4F_{7/2}$—$^4I_{9/2}$, $^4F_{5/2}$—$^4I_{9/2}$ and $^4F_{3/2}$—$^4I_{9/2}$ transitions of Nd^{+3} ions centered at 758 nm, 818 nm and 884 nm, respectively. The broad band is a defect band attributed to the self-trapped excitons in TiO_2. The emission intensity of the defect band and of the Nd^{+3} bands, increase when the concentration of Nd^{+3} in TiO_2 was increased.

For increasing temperatures, the emission intensity of the $^4F_{7/2}$ —$^4I_{9/2}$ and $^4F_{5/2}$ —$^4I_{9/2}$ transitions increases, in contrast to the $^4F_{3/2}$ —$^4I_{9/2}$ transition, which intensity emission decreases with increasing temperature. These transitions occur inside the biological transparent window what allow using these nanoparticles to evaluate temperature in living organism. The fluorescence intensity ratio (FIR) between the transitions $^4F_{7/2}$—$^4I_{9/2}$ and $^4F_{3/2}$ —$^4I_{9/2}$ (I_{758}/I_{884}) and $^4F_{5/2}$—$^4I_{9/2}$ and $^4F_{3/2}$—$^4I_{9/2}$ (I_{818}/I_{884}) were used to calculate the absolute temperature and the relative sensitivity of the sensors. The relative sensitivity was near 3% K^{-1} for I_{758}/I_{884} and near 1% K^{-1} for I_{818}/I_{884}.

[LPM-374] Enhanced Photoluminescence Quantum Yield of Terbium Nano-MOFs Synthesized by Microwave Assisted Solvothermal Method

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In the present work luminescent metal-organic frameworks consisting of terbium ions as the metallic center and 1,4 benzene-dicarboxylic acid (BDC), benzene-tricarboxylic (BTC) acid and 1,3 thiophane-dicarboxylic acid (TDC), as the organic ligands, are synthesized by the microwave assisted solvothermal method at a relatively short time. The samples are studied before and after a thermal annealing process at 400 °C. The structural and chemical analysis indicate the formation of nanocrystals of about 8.8 nm, 5.0 nm and 127 nm for BDC, BTC and TDC samples, respectively. All the samples show carbon and oxygen in excess attributed probably to remnants of the N,N-Dimetilformamide used as solvent during the synthesis or to diffused particles from the atmosphere. The luminescent analysis shows a high quantum yield value for the BDC framework, 99.6%, after the annealing process, attributed to an antenna effect; whereas both the BTC and TDC samples show a higher quantum yield before annealing; 64.1% and 13.3%, respectively. The luminescence decay time is also computed in the samples resulting between 1 and 1.5 ms for both BDC and BTC samples, whereas for the TDC sample the decay time was about 0.2 ms. A noticeable daylight visible PL emission is observed in all samples.

[LPM-378] Nanometric europium-doped barium hafnate for luminescent temperature sensing in the physiological range at a sub-micrometric scale

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In the present work europium doped barium hafnate ($BaHfO_3$) is synthesized by the hydrothermal route at 473 K for 2 h. Samples with europium concentrations of 1, 3 and 5 at.% are obtained. All samples are annealed for 8 hours at 1073 K and their luminescent properties are studied as a function of temperature in the physiological range for its use in submicron luminescent thermometry. XRD indicates the presence of the $BaHfO_3$ phase mixed with traces of HfO_2, high resolution transmission electron microscopy indicates a crystallite size of 9 nm and sample doped at 3 at.% presents the highest emission intensity. The fluorescence intensity ratio technique (*FIR*) is used to study the emission of thermally coupled electronic states of europium $^5D_0$ and $^5D_1$ as a function of temperature from 289.7 K to 323.8 K. By using the $^5D_1$-$^7F_2$ transition as reference, all emission lines corresponding to $^5D_0$ - ^7F_J transitions are explored. The highest relative sensitivity of 1.8 % K^{-1}, as well as the smallest resolution value of $1.1x10^{-2}$ K, are obtained for transition $^5D_0$ à$^7F_3$ in the physiological range.

[LPM-401] Effect of Low density Polyethylene on the Luminescent Properties of Thulium Doped Yttrium Oxide Synthesized by the Polyol Method

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In the present work polyethylene is used as a support of yttrium oxide particles doped with thulium and its effect on the luminescent properties is studied. Thulium-doped yttrium oxide is prepared through the poliol method, different values of thulium are explored, as well as different calcinating temperatures, are explored in order to determine the synthesis conditions needed for the maximum emission intensity, these were 1.5 at.% of thulium and a 1000 °C. The synthesized powder is dispersed in low-density polyethylene and deposited as a thin film on glass substrates. The luminescent excitation and emission spectra present important changes attributed to the influence of the -CH_2- chain vibration; also, the presence of the polymer has an important influence on the emission decay time: while the powder presents a single emission process with a time of 9.293 µs, the film presents a two decay process with 1.156 µs and 4.086 µs, each.

[LPM-406] Effect of silica coating on the structural and luminescent properties of Sm3+/Yb3+ or Tm3+/Yb3+ co-doped TiO2 nanoparticles

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The luminescent characteristics of spherical titanium dioxide (TiO2) nanoparticles (NP's) doped with Sm^{3+}/Yb^{3+} and Tm^{3+}/Yb^{3+} with and without a silica coating were analyzed. These nanoparticles were synthesized using the spray pyrolysis technique and coated with silica through a wet chemical process. The Sm^{3+}/Tm^{3+} and Yb^{3+} doping induces a triphasic polycrystalline structure of rutile and anatase TiO_2 and a $Sm_2Ti_2O_7$/ $Tm_2Ti_2O_7$ cubic phase. A Williamson-Hall analysis was used to monitor the tensions of the NP´s crystallites at the various doping concentrations and with addition of the silica shell. The luminescent spectra presented the characteristic emission peaks for the electronic energy levels transitions of the Sm^{3+}/Tm^{3+} and Yb^{3+} ions. The Sm^{3+}/Yb^{3+} co-doped NP´s showed a maximum emission peak in the visible region at 612 nm, associated with $^4G_{5/2} \rightarrow {}^6H_{7/2}$ transitions of the Sm^{3+} ions. The IR emission peak at 973 nm ($^2F_{5/2} \rightarrow {}^2F_{7/2}$) pertaining to Yb^{3+}. For the combination of Tm^{3+}/Yb^{3+}, two emissions associated with Tm^{3+} ions were observed at 440 nm ($^1D_2 \rightarrow {}^3F_4$) and 806 nm ($^3H_4 \rightarrow {}^3H_6$). The emission at 973 nm ($^2F_{5/2} \rightarrow {}^2F_{7/2}$) is correlated to the Yb^{3+} ions. Silica coating of the NP´s resulted in luminescence emission intensity increase of about 4 times.

[LPM-153] Structural and luminescent properties of hafnium doped with different lanthanides and lithium.

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UP-conversion luminescence of lanthanum, erbium, ytterbium, and lithium multiple doped hafnium oxide powders are presented. The measured luminescent spectra were obtained using laser with wavelength of 980 nm; emission peaks were observed in the ranges of 530 to 580 nm (green emission), 630 to 680 nm (red emission). These emission peaks manifest the interactions between these ions that propitiate the phenomenon of up-conversion. The incorporation of lithium in the samples allowed an increase in the luminescent emission of visible light in red and green, with respect to the samples that were not doped with lithium. The powders, object of this study, were synthesized by means of the solvent evaporation technique using chlorides as precursors. The analysis of XRD showed a monoclinic crystalline structure of lanthanum doped hafnium oxide with the spatial group: P21/a (14); and when doping with erbium and ytterbium, the XRD diffractograms indicate that we have a cubic crystalline structure with a spatial group Fm-3m (225); hafnium oxide doped with the above lanthanides; doping with lithium, a combination of monoclinic and cubic structures is obtained; the SEM images showed a granular morphology con porosity only for samples doped with lithium with dimensions less than a micron. The chemical composition was obtained by measurements of EDS; the different luminescent emissions are also reported.

[LPM-189] Structural and optical properties of CdTe+CdTeO3 nanocomposite films with broad blueish photoluminescence

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Cadmium telluride plus cadmium-tellurite ($CdTe+CdTeO_3$) nanocomposite films were grown by radio frequency magnetron sputtering at room temperature. The $CdTe+CdTeO_3$ samples were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), Raman spectroscopy, UV-Vis absorption and room temperature photoluminescence (RTPL). XRD and TEM results indicate that films are composed of CdTe and $CdTeO_3$ nanoparticles (NP's) with 6.7 +/- 0.8 nm and 6 +/- 1 nm in size, respectively. CdTe NP's grew in hexagonal wurtzite and cubic zinc-blende crystalline phases. CdTeO 3 NP's crystalized in cubic phase. Direct band gap (Eg) (first discrete electronic transition) calculation indicates Eg = 2.6 +/- 0.2 eV for CdTe and 3.3 +/- 0.2 eV for $CdTeO_3$. RTPL spectrum evidences a wide signal in the 2.0 to 3.25 eV interval. Results reveal that the emission band maximum, which is centered in the blue region of the visible light, is related with band to band transitions in CdTe NP's

[LPM-362] Tunable blue, bluish-white and neutral-white light emission in zinc-aluminum phosphate glasses activated with Cu+ and Dy3+

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Cu^{+}/Dy^{3+} co-doped zinc-aluminum phosphate glasses were synthesized by the melt quenching technique. The amorphous (glassy) phase was confirmed by X-Ray diffraction patterns and Raman spectroscopy. The emission spectra of the Cu^{+} singly doped glass exhibited a broad blue emission band with a maximum at 470 nm upon 270 and 295 nm excitations, according to the CIE1931 chromaticity coordinates located in the (x = 0.2091-0.2147, y = 0.2467-0.2428) range. In presence of Dy^{3+}, tunable tonalities in the bluish-white, cold-white and neutral-white regions with CIE1931 chromaticity coordinates in the range (x = 0.2152-0.2586, y = 0.2508-0.3033), (x = 0.2973-0.3072, y = 0.3391-0.3659) and (x = 0.3946-0.4197, y = 0.4177-0.4636), respectively, were obtained depending the excitation wavelength. Color rendering index and photoluminescence quantum yield values up to 94 and 50 % could be respectively achieved depending on the Dy^{3+} concentration and excitation wavelength. Such fact suggests that this glass system might be suitable for W-LEDs applications. The Cu^{+} emission spectra and decay features in presence of Dy^{3+} showed the existence of radiative and non-radiative energy transfers, occurring simultaneously from Cu^{+} to Dy^{3+}. An analysis by the Dexter theory within the Reisfeld approximation and Burshtein model pointed out that an electric dipole-dipole interaction dominates the $Cu^{+} \rightarrow Dy^{3+}$ non-radiative energy transference, within Cu^{+}-Dy^{3+} ions randomly distributed.

[LPM-368] Er-doped Zn3(VO4)2 an upconversion study

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$Zn_3(VO_4)_2$ compounds doped with Er^{3+} were prepared by standard solid state reaction technique. The visible photoluminescence spectra under 350 nm excitation display a broad intrinsic emission band centered at 580 nm. As the Er^{3+} content increases, it is observed the presence of sinks at 490, 524, 554 and 660 nm, which match well with absorption bands of Er^{3+}. Such fact points out radiative energy transfer from the $Zn_3(VO_4)_2$ host to Er^{3+} ions. The NIR emission spectra under 350 nm excitation (wherein Er^{3+} is not excited) exhibit a broad emission extending from 1450 to 1600 nm, attributed to the Er^{3+}: $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transition, and where it is observed the Stark splitting due to the crystalline field of the $Zn_3(VO_4)_2$. An emission's decay analysis within the sink at 524 nm reveals a single exponential time evolution, with no variation as a function of Er^{3+} concentration, which suggests that NIR emission of Er^{3+} under 350 nm excitation is mainly reached by radiative energy transfer. Furthermore, the Er^{3+}-doped $Zn_3(VO_4)_2$ UC emission spectra, were measured under 980 nm laser excitation. The distinctive Er^{3+} ions emission bands are observed: green emission around 524 and 554 nm arises from $^2H_{11/2} \rightarrow {}^4I_{15/2}$ and $^4S_{3/2} \rightarrow {}^4I_{15/2}$ transitions; while red emission located around 660 nm is due to Er^{3+} transition from $^4F_{9/2}$ exited level to ground state. Finally, the UC emission behavior was monitored as a function of the excitation power, in order to recognize the mechanisms involved in the UC processes.

[LPM-377] Down-conversion properties of vitreous CdO-P2O5 activated with Pr3+ and Yb3+

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Pr^{3+} and Yb^{3+} co-doped cadmium-phosphate glasses were synthesized by the melt quenching technique. The amorphous (glassy) phase was confirmed by X-Ray diffraction (XRD) patterns. Their vibrational bonds were studied by FTIR spectroscopy. Optical Band Gap (*E*g) values (~3.07 eV) were calculated from the optical absorption spectra. Under 443 nm continuous excitation, emission bands appear at 528, 540, 611, 645, 708, 728, 876, 917, 1037 and 1478 nm, associated with the Pr^{3+} inter-electronic $^3P_1 + {}^1I_6 \rightarrow {}^3H_5$, $^3P_0 \rightarrow {}^3H_5$, $^3P_0 \rightarrow {}^3H_6$, $^3P_0 \rightarrow {}^3F_2$, $^1D_2 \rightarrow {}^3H_5$, $^3P_0 \rightarrow {}^3F_{3,4}$, $^1D_2 \rightarrow {}^3H_6 + {}^3F_2$, $^3P_0 \rightarrow {}^1G_4$, $^1D_2 \rightarrow {}^3F_4$ and $^1D_2 \rightarrow {}^1G_4$ transitions, respectively. An additional emission band located at 978 nm, due to the $^2F_{5/2} \rightarrow {}^2F_{7/2}$ inter electronic transition of Yb^{3+} emerges, when Yb^{3+} is incorporated. Such emission band is attained at expense of energy transfer from Pr^{3+}. The $Pr^{3+} \rightarrow Yb^{3+}$ energy transfer interaction mechanism was analyzed by means of Dexter's energy transfer expression for multipolar interaction and the Inokuti-Hirayama model, suggesting that a dipole-dipole interaction dominates the energy transfer process, within Pr-Yb clusters. A maximum theoretical quantum efficiency of 143% is achieved for glasses doped with 0.3 and 2.0 mol% of Pr^{3+} and Yb^{3+}, respectively.

[LPM-421] Analysis of optical properties in thin films ZnO:RE (Tm+3/Eu+3)_

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Rare earth doped ZnO systems are particularly attractive given potential applications in high-power lasers, visible-light-emitting phosphors on displays, and other opto-electronic devices. In particular europium, terbium, thulium and samarium show luminescence in the range of the visible spectrum. This work focuses on determining the conditions to obtain thin films of ZnO doped with RE = Eu + 3, Tm + 3, Eu + 3 / Tm + 3 looking for the concentration of impurities that favor an increase in luminescence. The films were prepared using the Ultrasonic Pyrolytic Spray technique, studying the influence on the variation of the europium and thulium concentration from 0.5 to 3% at separately. Subsequently, a co-doping was carried out (Eu + 3: Tm + 3) choosing the concentrations that presented the highest luminescent intensity.The samples were characterized by X-ray diffraction (XRD), UV/Vis and photoluminescent (PL) spectroscopies techniques. The XRD pattern showed that the ZnO:RE thin films have a hexagonal structure. The results of UV/Vis transmittance indicate a band gap close to 3.31 (Eu^{+3}) and 3.18 eV (Tm^{+3}).

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-325] Microfabricated Resistive Temperature Detector “RTD” for low scale production

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In this study, we present the methodology to design and fabricate a Resistive Temperature Detector “RTD” for low scale production. The target sensibility was corporal applications where a definition less than 1°C plays an important role. We present the RTD design considerations such as photolithography capabilities, wet etching compatibility, sensor definition, mathematical considerations, reliability and government regulations. From the Mathematical consideration a second-order model "Callendar-Van Dusen" was employed to define the RTD sensibility. An adequate " Callendar-Van Dusen" equation to Nickel was achieved, where a theoretical relation between resistivity and sensibility was obtained. The relationship between experimental and theoretical results matched, where the RTD sensibility is proportional to resistance. Once the design was ready, we analyze the low scale fabrication on four-inch wafers. The statistical analysis showed a dispersion value that can be reduced by post-treatments. In order to reduce the dispersion on the wafer, we study the thermal treatment effect on the Nickel RTD at different temperatures. The thermal effect induces two improvements in the RTD fabrication. The first one is a resistance homogenization in all the wafer, the resistance deviation between sensors is reduced from 148 ÃƒÂ¢Ã¢Â€ÂžÃ‚Â¦ to 13ÃƒÂ¢Ã¢Â€ÂžÃ‚Â¦. And the crystallinity is improvement until 300°C, for higher temperatures the metal presented oxidation.

[MEM-327] Enhancing the threshold voltage reliability in IGZO TFTs passivated with SU-8

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Decreasing the threshold voltage shift (ΔV_{th}) in IGZO-TFTs under bias stress is crucial to obtain stable and reliable devices and circuits. In order to mitigate this effect passivation layers over the semiconductor channel have demonstrated its efficacy. In this work, staggered bottom gate IGZO thin-film transistors were passivated using 450nm of SU-8 2000.5. The TFTs were fabricated by a full lithography process with a maximum processing temperature of 200°C. TFTs with W/L dimensions of 150um/40um, 150um/60um and 150um/80um were stressed under different bias conditions for 1200s. Low field (2MV/cm) and high field (4MV/cm) bias stress lead to a maximum ΔV_{th} of 0.12V and -0.38V, respectively. To explain the negative ΔV_{th}, the experimental data was fitted to conventional electron trapping mechanism combined with the mechanism of release and migration of hydrogen. The small ΔV_{th} under low field stress was found to be associated with the passivation effect of a fully cross-linked SU-8 layer.

[MEM-361] Si3N4 waveguides platform for quantum gates implementation in integrated photonic circuits

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The implementation of quantum technologies, such as quantum computation and communication, demands on the availability of efficient integrated-photonic devices and fulfills the requirements of miniaturization and scalability. Thus, the design and fabrication of waveguides with different geometries and materials have become a subject of great interest nowadays. Following this direction, we aim the development of quantum-photonic integrated circuits.

Particularly in this work, we present the objectives and methodologies for the implementation of single-qubit quantum gates. We will describe the techniques for the fabrication of Si_3N_4 waveguides as the building block to consolidate a platform for quantum circuits. Also, results regarding the synthesis and characterization of materials and waveguide fabrication will be presented.

Silicon nitride (Si_3N_4) has been highly used in the last years due to its high index of refraction (linear and nonlinear) and its transparency in the visible region of the electromagnetic spectrum. Also, its compatibility with CMOS technology makes it a good material for its use in integrated technologies.

Our proposal relies on ridge waveguides on a substrate of silicon dioxide (SiO_2) on silicon. The materials used for this purpose, the Si_3N_4 and the SiO_2, are synthesized by RF-reactive sputtering and thermal oxidation techniques. For waveguide fabrication, we perform the processes of photolithography and dry-plasma etching.

[MEM-380] Quantification of different prostate-specific antigen isoforms in human serum using a sandwich-type ELISA immunosensor based on the principle of surface plasmon resonance spectroscopy

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Gold sensor chips (GSC) functionalized with a mixed thiol (16-MHA + EG_3SH) self-assembled monolayer (SAM) were used to fabricate an optical immunosensor for the sensitive detection of prostate-specific antigen (PSA), a prostate cancer (PCa) biomarker, in human serum samples. To address and minimize the issue of non-specific protein adsorption, an organic binding matrix (Amine-PEG_3-biotin/Avidin) was assembled on the previously functionalized GSC to build up an ordered and hierarchically organized interfacial supramolecular architecture: Au/16-MHA/EG_3SH/Amine-PEG_3-biotin/Avidin. The chips were then exposed to serum controls at different concentrations of target analyte from a sandwich immunocomplex molecule ($^{Biotin}Ab\text{-}Ag_{PSA}\text{-}Ab^{Enzyme}$), and their optical response were monitored using surface plasmon resonance spectroscopy (SPRS). Calibration curves for ΔΘ vs total- and free-PSA concentration were obtained and their analytical quality parameters (viz. LOD, LOQ, dynamic signal range and linear working interval) determined and compared with a reference ELISA immunoassay. The results obtained in this work showed that the proposed immunosensor could be successfully applied to analyze serum samples of patients after radical therapy.

[MEM-387] Maximum Bending Modeling of MEMS Gyroscope under Coriolis Effect

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In this work the Coriolis effect in microgyroscopes is investigated. Since the dimensions of these microdevices are critical for their correct operation, they were optimized through maximum strain and stress calculations applying the principal maximum stress theory using COMSOL Multiphysics software. The performed simulations indicate that the beams that support the actuator and sensing mass from the gyroscope can reach a maximum displacement of 11 µm and 0.12 µm, respectively. During the design, the dimensions and parameters of the device were also optimized with the objective of not reaching the structure fracture.

[MEM-449] Development of an Electrostatic Actuation MEMS Microswitch on SOI wafer

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We present the design of a RF-MEMS switch constructed on SOI technology. The design considers electrostatic actuation using several DRIE-machined vertical plates hold to a centered shuttle section of the switch, and anchored from two sections of the shuttle by restoring springs. The electrostatic actuation on plates moves the shuttle towards a contact section of the switch and perpendicular to the (100) plane direction of the top Device layer. Previous designs were limited by the near proximity of shuttle and bottom Handle layer, and due to the lack of Handle layer under shuttle section of our new design, we expect final experiments to provide faster and cleaner response by eliminating parasitic charging and/or perpendicular attraction of the shuttle. A set of two separate springs are used as equilibrium springs to center the contact section of the switch. Metal sputter deposition on vertical contact regions on switch is deposited while rotating 45 degrees and -45 degrees the top surface of switch. We obtained a close fit between the mathematical model and the simulation results while designing the spring elements of the switch. We have developed alpha devices with handle wafer section below shuttle and will develop beta devices for final testing using a patent pending fabrication process

[MEM-169] Chemical growth and characterization of CdS and ZnS doped with Al and Cu for applications in thin-film electronic devices

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The interesting properties of semiconductor materials make them an essential part of the electronic devices we use in our daily lives. The field of application of these materials includes photovoltaic and sensor applications. Recently thin films of ZnS have been successfully used as buffer layers in polycrystalline solar cells, replacing CdS films. ZnS films are Cadmium-free and wider bandgap than CdS, by reducing the light absorption at the window layer, the density current can be boosted. However, the electrical resistivity needs to be reduced without significantly affecting the optical properties of layers, what's possible by doping with suitable impurities atoms. ZnS and CdS electrical properties can be tunned by dopping, especially those materials made solution techniques like Chemical Bath Deposition technique since the doping element can be easily incorporated by adding small amounts of salts. In this work, we present two production alternatives of a wide bandgap semiconductor by a solution method. A ZnS thin-film electrically modified by material doping, grown and doped simultaneously with Al and with Cu by CBD technique, and lastly, CdS films doped with Cu in SILAR systems. We present the methodology employed by the film electrical changes done by doping. We especially analyze the doping effect with Cu and Al, on the optical, structural, morphological, and electrical properties of ZnS and CdS films. The results show that the doping effect on the films by chemical bath deposition does slightly affect the structural and morphological properties and highly affect the electrical properties. These results indicate that our materials have high application potential for the design and manufacture of thin-film electronic devices.

[MEM-179] DEVELOPMENT OF ENERGY STORAGE SISTEM THROUGH THE USE OF NANOMATERIALS.

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Dielectric capacitors have several advantages over other energy storage devices, for instance, high-power densities (approximately 1000 times greater than batteries), extremely long-life cycles, and charge/discharge times of seconds. However, their disadvantage is a low energy density; about a thousandth of the battery's energy density. Thus, the interest of this research is to improve the dielectric capacitor energy density from the increase in its dielectric constant.

The goal of this work is to get an energy storage system of high energy density with dielectric capacitors from a nanocomposite of conductive nanoparticles embedded in a dielectric material like fluoride polyvinylidene with barium titanate nanoparticles. The conductive nanoparticles could increase the specific area (surface per unit volume) until 3 orders of magnitude in relation to micrometric conductive particles. Hence, a rise in dielectric constant will occur due to high conductive area and consequently, an increase in energy density will arise. From all compositions performed, a composition will be obtained just below the percolation threshold where the nanocomposite becomes conductive.

Initially all materials will be characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM) prior to dispersion. Subsequently, the nanocomposite will be deposited by spin coater technique on indium tin oxide substrates. These films will be characterized by SEM. After that, a metallic film will be deposited by sputtering to get parallel plates capacitors to perform electrical characterization to measure the dielectric constants in the nanocomposites. Finally, it will be made a capacitors bank with the capacitors constructed, to characterize its energy density.

[MEM-220] Synthesis of tin oxide thin films as semiconductor material by SILAR method and the effect on the deposition route

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Abstract

Metallic oxides as thin films on flexible microelectronic devices has increased during last years, it has allowed a system design and a process integration, it is specially working on the limits of material performance on the fabrication at low temperature to explore applications as sensors, detectors, solar absorbers, etc. Tin (IV) Oxide (SnO_2) is a semiconductor material, which is crystalized on a tetragonal structure. Tin oxide thin films were wet chemically synthesized over glass substrates using *Successive Ionic Layer Absorption and Reaction (SILAR)* method, which is an economical, simple and easy processing method. SnO_2 material was obtained by two different routes. The first one was by using two different precursor materials: tin sulfate as cationic source and sodium sulfate as ionic source along with two rinsing baths in deionized water after each precursor immersion. The second one comprised tin sulfate as cationic source and an empty container as drying step with two successive rinsing baths. The chemical reaction and formation of the thin films were identified thanks to the amount of deposition cycles, immersion time and bath temperature, molar concentration of precursor materials as well as final thermal treatments. The resulting thin films were characterized and studied by x-ray diffraction (XRD), ultraviolet–visible, spectroscopy (UV-Vis), x-ray energy dispersive spectrometry (EDS), and scanning electron microscopy (SEM). These analyses were conducted to identify structural, optical, morphological and chemical properties of the metallic oxide semiconductor material.

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

[MEM-381] Design and Development of a Microheater and Resistive Temperature Detector (RTD)

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Micro heaters are widely employed in microelectromechanical systems (MEMS). Most of the gas sensors work at high temperatures over 100°C. Therefore, in situ heating is one of the basic requirements for a micro gas sensor to maintain it at an elevated temperature with low power consumption. Sensor operating temperature is one of the important factors determining the gas sensitivity of materials and high control is required.
In this work is shown the comparison between microheater made with different metals. The working area or microheater size was calculated for three sizes 200 x 200 um, 300x 300 um, and 500 x 500 um for different metals; Aluminum, Nickel, Platinum, and Gold. All microheaters were calculated for 100 â„¦ resistance, with a 100 nm metal film thickness, therefore the channel width, length varies for each design. To verify heater temperature an RTD with the same metal was made next to the heater. Silicon nitride was employed to protect the metal from environmental conditions and avoid corrosion on the metals. We evaluated heating properties; heating power, heating response time, cooling time between 25 °C and 800 °C, amperage consumption, voltage-current characteristics, and resistance-temperature increment.

[MEM-384] Design of NMOS Integrated Circuits in Mexico for test/modelling purposes

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In the multi-project chip Cinvestav-Guadalajara participates with three specific projects: 3b NMOS multiplier, NMOS ring oscillator with non-overlapping phases, and planar inductors. The first two projects include digital cells (NOT, NOR, and NAND). Moderately complex circuits (ring-oscillator, non-overlapping phase-clock, flip-flop, full adder, and 1-b multiplier) are designed with these cells to achieve three objectives:

- To evaluate the electrical performance of each cell. The test will allow to quantify the delay in the propagation of the signals, and when evaluating the charge/discharge times there will be information to infer the intrinsic time constants of the cells and to know the impact of the polarization on the performance of these performance variables. It is of interest to determine the minimum bias voltage and at the same time the useful frequency ranges of operation.
- To characterize the technology. It is important to determine the effect of substrate bias on the transistor's turn-on voltage. This information is useful for developing analog design, and it is also of interest to determine the equivalent electrical circuit of the bonding PAD.
- To infer the value of parasitic capacitances and other design parameters) and improve the transistor’s spice simulation.

In the third project, the purpose of integrating inductors (square-and-octagonal) is threefold:

- To validate the advantage of a ground shielding in the performance of planar inductors.
- To build the equivalent electrical circuit (using the information obtained from the measurements of the S parameters) for applications of high frequency. The idea is to calculate the value of the elements that make up the electrical equivalent circuit of an integrated inductor on silicon, whose arrangement of elements is based on the physical structure of the inductor. This modeling is to describe the behavior of a planar inductor implemented on a silicon substrate for high frequency applications offering the designer a tool that facilitates the characterization of planar inductors.

- To implement embedding strategies to establish the limitations of the technology in terms of quantifying unwanted parasitic effects (resistive-capacitive-inductive). In this proposal Cadence-Virtuoso was used to simulate planar inductors, and ADSMomentum was our choice for electromagnetic simulation.

[MEM-386] Engineered designs of silicon nitride thin film waveguides for frequency translation of optical pulses.

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The growing interest in developing new technologies based on quantum mechanics, such as quantum computing and quantum communications, demands new schemes for generating and controlling quantum states. Motivated by such a request, our group aims to study frequency conversion processes, which allow the encoding and processing of quantum information through temporal modes of the electromagnetic field. Particularly in this work, we propose a ridge-type waveguide based on thin films of silicon nitride (Si_3N_4) on a substrate of silicon dioxide (SiO_2) and silicon, designed to achieve the spectral translation of an optical signal through the third-order nonlinear process known as difference frequency generation (DFG). The efficient implementation of the DFG process in waveguides depends mainly on the refractive index of materials and its geometry.

We synthesized the Si_3N_4 thin films using the RF reactive sputtering technique with a silicon target at room temperature, while the SiO_2 was grown by thermal oxidation on silicon wafer. The samples were characterized by spectroscopic ellipsometry in the range of 400 nm to 1700 nm, obtaining the optical constants through adjustment of optical models such as Tauc Lorentz, approximation of the effective medium, and Sellmeier. The Si_3N_4 samples exhibited a refractive index of 2.005 at 620 nm and an extinction coefficient of zero throughout the measurement range. The thickness of the samples was obtained by ellipsometry, which will define the waveguide height.

Si3N4 samples were analyzed statistically to determine the material refractive index as a function of wavelength. Besides, the chromatic dispersion properties of waveguides were calculated numerically by the finite difference method for specific geometries of the waveguides and the refractive index obtained from the synthesized samples. By implementing an optimization algorithm, we identified transverse dimensions that lead to waveguide dispersion properties engineered to efficiently demonstrate the frequency conversion of an optical signal. In accomplishing this, we imposed realistic conditions for both fabrication and optical characterization of the waveguide. The proposed design consists of a waveguide with 1.85 microns width and 0.51 microns height on 1 microns high silicon dioxide thin film.

[MEM-390] Simulation of MEMs Flexible Pressure Sensors under Large Deflection Theory

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The electromechanical analysis of a piezoresistive flexible pressure sensor with a circular-shaped diaphragm for low-pressure is presented. This analysis is developed through a finite element analysis (FEA) model. The sensor with a diaphragm of PET material with diameter of 3.8 mm and thickness of 130 mm is studied. The electric response of this sensor is obtained with a Wheatstone bridge of four piezoresistors of Nichrome located on the diaphragm surface. Two configurations of piezoresistors distributed on the diaphragm are analyzed and studied. The diaphragm exhibits a maximum deflection of 82 mm using the large deflection theory when a pressure of 30 kPa is applied. The maximum sensitivity and normal stress calculated using FEA model are 0.151 mV/ V- kPa and 25 MPa, respectively. The maximum output voltage of the flexible pressure sensor obtained from COMSOL model is 4.52 mV at 30 kPa. In addition, the COMSOL model can be easily used to predict the deflection, normal stress, electric response and sensitivity of a piezoresistive pressure sensor with a circular-shaped diaphragm under large deflections.

[MEM-397] Design and Integration of an NMOS Operational Amplifier with Resistance Temperature Detectors (RTDs)

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A two-stage gain op-amp was designed and fabricated using 5um NMOS transistors technology. Amplifiers were designed with 1,000 open loop gain, less than 5mW power consumption, and 30 MHz unity gain bandwidth with phase margin greater than 60°. Layout was designed using Electric VLSI. The integrated circuit was obtained through a 4-step mask NMOS process consisting in a p-type silicon substrate, 30 nm SiO_2 gate dielectric and heavily doped polysilicon gate. Finally, 250 nm Al thin film as top metal interconnection.
The electrical characterization of the amplifier consisted of current-voltage measurements in each of the circuit nodes, obtaining similar data to those obtained during the simulation using LTSpice. Finally, the amplifier was connected to the output of a Cr/Ni RTD to monitor water temperature with a resolution of up to 0.01 °C.

[MEM-434] Design and Fabrication of Microcavities for Membranes Application in Pressure Sensors.

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The demand for pressure sensors has recently increased as these devices are indispensable for monitoring the gases flow in medical ventilators. Piezoresistive-based sensors are mainly used to transduce deformation effects derived of pressure differentials to voltage signals. Currently, silicon-based microelectromechanical systems (MEMS) technology is used to create cavities with high precision, in which a membrane with >10 µm variation will produce negative effects. In this work, a systematic study was performed using a deep reactive ion etching (DRIE) system to evaluate etching conditions creating microcavities with a depth of 450 µm, Scanning Electron Microscope (SEM) was using to evaluate the thickness uniformity all across the membrane, scallops generated on the walls and surface quality. Results demonstrate the importance of the etching conditions regarding the membrane uniformity to fabricate pressure sensors to operate at 4.5 kPa with potential applications in medical ventilators.

MULTIFUNCTIONAL AND MAGNETIC 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-239] Magnetic composite based on MIL-101/Fe3O4 for anthracene adsorption in water samples

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Polycyclic hydrocarbons constitute an important source of very dangerous pollutants. Different materials have been used as adsorbent for their removal, but they present difficulties in the separation process. The use of a material based on metal-organic framework (MOF) with large pores and high surface area and magnetic nanoparticles with superparamagnetic properties is an interesting strategy. In this work a magnetic composite based on MOF (MIL-101) and Fe_3O_4 magnetic nanoparticles (Fe_3O_4/MIL-101) was obtained by a simple synthesis method and used as adsorbent for the removal of anthracene. The composite was characterized by transmission electron microscopy (TEM), X-ray powder diffraction (XRD) and vibrating sample magnetometer (VSM). The results showed that kinetic data followed a first-order model and equilibrium data were well fitted by the Langmuir model. The composite material was effectively separated using an external magnet, and no further centrifugation or filtration processes were needed. This composite is a great alternative to remove polycyclic hydrocarbons from water samples and has potential to extend to the removal of other contaminants.

[MUL-248] Depth profile and polarization study of the Second Harmonic Generation in LiNbO3 powders

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In the context of powdered materials (strong scattering), recently experiments have been being performed to study quantitively the second harmonic generation SHG activity of pharmaceutical materials, as a means for quality control [1]. Loss of crystallinity within organic powders, induced by mechanical grinding can also be monitored by this nonlinear second order process [2]. Thus, powder SHG (PSHG) experiments are no longer secondary as they are conceived by the Kurtz-Perry (KP) method [3], in which powders are considered as survey materials only and a PSHG study is done solely to predict the nonlinear second order capabilities of unavailable single crystals. Yet another feature that makes PSHG more attractive nowadays is the possible tuning of the SHG intensity that arises from lithium niobate ($LiNbO_3$; LN) micropowders, which can be ascribed to a proper control of the chemical composition and grain size [4].
With this work, we wish to highlight the importance of performing a combined analysis resulting from the depth profiling of the PR-PSHG, that is the characterization of polar distortion by means of rotation of the incident linear polarization (fundamental wave) and fixation of the outgoing polarization (SH) with an analyzer, as the beam focus is translated from +z to -z position, passing from the air/powder interface (z=0). On this instance, instead of thick sample (hundreds of microns) we have studied a thin layer about 50 µm thick, prepared by gently pressing LN micropowders with an average particle size of 2.6 µm and averaged crystallite size 100-300 nm and then remove surplus by gently knocking and edge of the coverslip on which is supported the adhered powder. We hereafter refer to this prepared sample the “powder-print,” in analogy to a fingerprint. This type of combined analysis, while applied to such sample preparation, would pave the way for a close and quantitative investigation of the SHG response from nonlinear optical powders, also showing the importance and use of the different scales related to the powder, as are the grain and the nanocrystal sizes.
[1] A. U. Chowdhury, S. Zhang, and G. J. Simpson, Anal. Chem. **88**, 3853 (2016).
[2] D. Wanapun, U. S. Kestur, L. S. Taylor, and G. J. Simpson, Anal. Chem. **83**, 4745 (2011).
[3] S. K. Kurtz and T. T. Perry, J. Appl. Phys **39**, 3798 (1968).
[4] O. Sánchez-Dena, E. V. García-Ramírez, C. D. Fierro-Ruíz, E. Vigueras-Santiago, R. Farías, and J. A. Reyes-Esqueda, Mater. Res. Express **4**, 035022 (2017).

[MUL-298] ZnO microparticles decorated with Au nanoparticles

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Thermal annealing in oxidizing and reduced armospheres were done on ZnO powders at a temperature of 500 °C, as means of intrinsic defect control. The powders were characterized by standard techniques X-ray Diffraction, Scanning Electron Microscopy and Raman Spectroscopy. Then the powders were decorated with Au nanoparticles of size 3 nm, with a a high-energy vibrational powder mixer. The obtained results show Raman spectra shifts of the characteristic ZnO bands, mainly that of . The blue shifts are related to the presence of oxygen vacancies. The changes are more prominent when the semiconductor is decorated with the Au nanoparticles. In the context of the fabrication of a domestic sensor, the decorated samples are expected to be more sensitive in the detection of small amounts of Ethanol. Possible applications in the industry of alcohol are envisioned, such as the distinction between agave liquor and tequila.

Acuña-Avila, P. E. *et al.* (2017) 'Identification of tequila with an array of ZnO thin films: A simple and cost-effective method', *Sensors (Switzerland)*, 17(12), pp. 1–14. doi: 10.3390/s17122943.

Fukushima, H. *et al.* (2015) 'Evaluation of oxygen vacancy in ZnO using Raman spectroscopy', *2015 Joint IEEE International Symposium on the Applications of Ferroelectric, International Symposium on Integrated Functionalities and Piezoelectric Force Microscopy Workshop, ISAF/ISIF/PFM 2015*. IEEE, pp. 28–31. doi: 10.1109/ISAF.2015.71726

[MUL-274] Spin wave localization in a magnonic crystal with defects

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A broken translational symmetry in a magnonic crystal via the introduction of tailored defects can beneficially enhance or modify its properties leading to scenarios with outstanding capabilities to connect fundamental physics with applications at microwave frequencies. Their characteristics have inspired multiple studies where detailed results on the behavior of the frequency-amplitude characteristic as a function of different structural parameters have been demonstrated. However, up to now, all the scientific reports deal exclusively with the resulting spin wave spectrum for the complete structure and little has been said about the behavior of the spin wave inside the defects. Here, we present a detailed study of the propagation of surface spin waves (MSSW) through a MC with broken translational symmetry, the influence of the defect in the spin wave propagation, the evolution of frequency bandgaps inside the MC, and the spatial energy distribution as a function of frequency and position. A time and space resolved magneto inductive probing system has been used to map the spin wave propagation in a magnonic crystal with tailored defects. The results show that the spin wave modes get trapped by the defect and the energy is localized in the space for specific frequencies.

This work has been supported by UNAM-DGAPA grant 1N107318.

[MUL-285] Structural analysis of carbon objects derived from cocos nucifera

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Nucifera coconut bagasse was subjected to a thermal process and carbonaceous fibers were obtained from it. This calcination was carried out at 100ºC, starting at T =100ºC and ending at T = 700ºC, for periods of two hours for initial temperatures and three-hour periods for temperatures above 400ºC. For the microstructural characterization of the aliquots, an X-ray diffractometer (XRD) was used and a scanning electron microscope equipped with an X-ray energy dispersion probe for the determination of the elemental composition of the processed organic product. In the results it was possible to appreciate the presence of Carbon, among other expected characteristic agents, as well as the morphology of said structures, which had variations depending on the temperature. Carbon fibers and other coconut minerals are obtained.

[MUL-313] Synthesis of thin films Gd3Fe5O12 and SrFe12O19 by laser ablation

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Materials such as $Gd_3Fe_5O_{12}$ and $SrFe_{12}O_{19}$ have been studied mainly for their magnetic and optical properties, among others, which allows them to be considered in a wide range of technical applications. A handy synthesis technique for preparing thin films of these materials is sol-gel. [1]. In the present work, the deposit of thin films of $Gd_3Fe_5O_{12}$ and $SrFe_{12}O_{19}$ by means of the laser ablation technique is presented. $Gd_3Fe_5O_{12}$ and $SrFe_{12}O_{19}$ targets were used for the deposition using fluences of 1.5 to 2 J / cm^2, with a repetition time of 10 Hz in an oxygen atmosphere of 100mT. During deposition the substrate was heated to 700 ° C. Derived from previous studies, it was noted that the structural, electrical and magnetic characteristics are susceptible to different external variables such as pressure, temperature and creep. Accordingly, this work will present the structural characterization of the films using X-rays, scanning electron microscopy and photoacoustic spectroscopic at different temperature ranges[3].

Keywords: thin films, laser ablation.

References

[1]. Fredrik Söderlind, Linnéa Selegard, et. al, Sol–gel synthesis and characterization of polycrystalline $GdFeO_3$ and $Gd_3Fe_5O_{12}$ thin films, J Sol-Gel Sci Technol (2009) 49:253–259.

[2] V.G. Kostishyn, L.V. Panina, L.V. Kozhitov, A.V. Timofeev, A.N. Kovalev, Synthesis and multiferroic properties of M-type SrFe12O19 hexaferrite ceramics, Journal of Alloys and Compounds 645 (2015) 297–300.[3] R. Castañeda-Guzmán, M. Villagrán-Muñiz, J. M. Saniger-Blesa, S. J. Pérez-Ruiz and O. Pérez-Martínez, "Photoacoustic analysis of the ferroelectric ceramics specific heat," *Appl. Phys. Lett.,* vol. 77, no. 19, pp. 3087-3089, 2000.

[MUL-330] Synthesis and structural analysis of lead-free Ba0.85Ca0.15Ti0.9Zr0.1O3 (BCTZ) thin-films prepared by pulsed laser deposition (PLD)

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Concerned by environmental and human health associated with electronic lead-based components, alternatives materials has become one of the most widely scientific topics over the past decades. To this perovskite elements are commonly used to develop new lead-free piezo/ferroelectric materials. From the parent $BaTiO_3$ structure, $(Ba,Ca)(Zr,Ti)O_3$ (BCZT) solid solution exhibits a high piezoelectric coefficient arising from a morphotropic phase boundary (MPB). ?The stabilization of the MPB near room temperature is favored by three factors: the first-order nature of the phase transitions, the increased coexistence range due to random elastic strain associated with substitutions, and the shift of transition temperatures toward room temperature with Zr and Ca substitutions. Therefore, the doping with Ca and Zr over A and B sites of the perovskite structure allows to obtain various compositions with different properties.
?The systematical studies about the growth and characterization of BCZT thin films still remain at an initial stage. The lack of progress in BCZT thin films is attributed to the challenges associated with growth of high-quality thin films. This work shows the synthesis and structural analysis of BCTZ thin-films prepared by PLD. The room temperature composition MPB, situated at x=0.15, was chosen in this work due to its large bulk piezoelectric response. The development of these thin films are expected to provide a wide variety range of applications: energy harvesting, high frequency ultrasound imaging and microfluidic control.

[MUL-340] 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

Authors would like to thank valuable technical support by Dr. Randy Dumas Quantum Design - Applications Department, Eloisa Aparicio, Eduardo Murillo, David Dominguez, Israel Gradilla, Francisco Ruíz, Jaime Mendoza, Maureen E. Cruz and Jessica I. Ortiz.

Funding: This work was partially supported 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.

NANOSTRUCTURES AND NANOSCIENCE

Chairmen:

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

The conference will be an excellent platform to exchange ideas and discover opportunities to develop novel researches, enjoying the landscape of Nuevo Leon.

We look forward to welcoming you.

[NSN-204] Optical Properties of Lithium Tetraborate Glass Using Rare Earth Elements and Silver Nanoparticles

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Lithium borate glass matrices doped with Dy^{3+} and Yb^{3+}, containing silver nanoparticles in different concentrations are synthesized and characterized in this work. The Scanning Transmission ElectronMicroscopy confirms formation of silver nanoparticles in the samples. Absorption spectra of the samples show the presence of a broadband spectrum associated due to the surface plasmon effect of the silver nanoparticles. A strong surface plasmon band bellow 400 nm appears after the annealing process, due to the formation of silver nanoparticles with radius of 5–15 nm. The transition peaks of Dy^{3+} are also observed at 386, 446, 798, 917, 1088, 1265 and 1669 nm. Additionally, a large peak at 976 nm belonging to the absorption band corresponding to the Yb3+ is observed. Emission spectra under 406 nm pumping show two prominent bands at 506 and 590 nm belonging to the Dy^{3+} transitions 4F9/2→6H15/2 and 4F9/2→6H13/2, respectively. The fluorescence in the 480 nm and 525 nm spectral ranges enhanced with the silver nanoparticles contained in the samples. Is the first time, the luminescence studies of the lithium borate matrix doped with Dy^{3+} and Yb^{3+} containing silver nanoparticles is done. The basic parameters defining the lasing-amplifying potential of the glass matrices as a function of silver nanoparticles concentration are calculated. The Thermoluminescence response to UV irradiation also exhibits significant enhancement with the increment of silver nanoparticles in the samples. Nonlinear optics field is in constant growth, particularly on the characterization and study of optical properties of glass compounds. In this sense, the plasmonic effect caused by silver nanoparticles (SNP) on the nonlinear optical (NLO) properties of different materials was studied.

[NSN-206] Irradiation of carbon nanotubes, application

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Carbon nanotubes are materials that have near-infrared absorbance. These structures by means of functionalization can bind to other molecules, in this case, to a lectin with specific recognition towards N-acetylgalactosamine, with the aim of being able to recognize cells that present this carbohydrate in their cell membrane, cancer cells. The hybrid nanocomposite was subjected to laser irradiation, which stimulated the molecules causing a localized temperature increase to a single wavelength and low power. The lectins used were noncovalently functionalized with previously oxidized multi-walled carbon nanotubes. The hybrid nanocomposite was joined with a breast cancer cell line (MCF-7) to observe the damage caused by laser irradiation specifically on the cell.

METHODS

The CNTs were placed in an acid bath for oxidation treatment. After oxidation, the CNTs were contacted with a solution of pyrenbutanoic acid succidimidilester (A1pbs) as an intermediate between the CNT and lectin. The lectin used was Sambucus nigra, SNA, at a concentration of 5 µg/ml in HEPES buffer, to which CNT was added in a 4:1 ratio. The cells used were MCF-7 in PBS were irradiated at different times. A diode laser with a wavelength of 808 nm was used, with an output power of 2.4 W/cm^2, at temperature environment using a timer-controlled through a microcontroller, the irradiation was at a distance of 8 cm. The characterization was by optical microscopy.

RESULTS AND DISCUSSION

The CNT used were acquired under the "Sunnano" brand, were characterized by SEM, before and after oxidation. Hemagglutination tests were performed before and after functionalization to observe the activity that lectin presents; SNA agglutinates with type A^+ erythrocytes. For the irradiation process, the selected times were 0, 10, 20, 30, 40 and 50 seconds. After irradiation, the cells were observed in the optical microscope.

Laser irradiation on lectin-functionalized carbon nanotubes caused damage to the breast cancer cell, MCF-7, this damage is more evident at 20 s; so, it is determined that with 20 s it is enough to achieve a break in the cancer cell.

[NSN-244] Synthesis and Characterization of WSe2 Nanosheets

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Two-dimensional (2D) layered nanostructures have received increasing interest due their unique nanoscale phenomena and their potential applications ranging from electronics and energy to catalysis. Recently in the last decade, graphene analogous materials such as transition metal dichalcogenides (TMDs), such as MoS_2, WS_2, $MoSe_2$ and WSe_2 are widely studied due to their potential applications in field effect transistors, photodetectors, solar cells, and gas sensors. In this work, we synthesize tungsten diselenide (WSe_2) nanosheets using a simple two-step additive-free growth technique by rapid selenization. The developed method is an atmospheric pressure technique that is rapid, scalable and cost-effective. The morphology and the structure, as well as the optical properties, of the so produced material have been studied using electron microscopies, X-ray photoelectron spectroscopy, photoluminescence, UV–visible and Raman spectroscopies, and X-ray diffraction. These studies confirmed the high crystallinity, quality, purity, and orientation of the WSe_2 nanosheets, in addition to the unexpected presence of mixed phases, instead of only the most thermodynamically stable 2H phase.

[NSN-262] Chitosan-based nanocoatings for the conservation of green bell pepper during storage

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Nowadays, the shelf life extension of fruit and vegetables through application of other alternatives such as chitosan an essential oils instead of pesticides as an environmentally friendly alternative is of special importance. Among the phytopathogenic bacteria responsible for the soft rot disease in bell pepper is reported *Pectobacterium carotovorum*, which causes severe loses in Mexico. In this work, nanocoatings based on chitosan and chitosan-thyme essential oil at concentrations of 15%, 30% and 45% nanoparticles were applied to inoculated and non-inoculated green bell peppers and their effectiveness on the postharvest preservation was assessed after 12 days of storage. The variables weight loss, firmness, CO_2 production, ascorbic acid content and disease incidence were evaluated. From the results, the weight loss and firmness were maintained for the bell peppers coated with the formulation containing 15% of chitosan nanoparticles and the lowest CO_2 production and disease incidence compared to other formulations. The ascorbic acid increased until day 8 and decreased at the end of the storage period. The nanocoatings based on chitosan could represent a good alternative for the conservation of this horticultural product.

[NSN-270] Encapsulation study of InAs quantum dots embedded in (Al)GaAs matrix

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The study of InAs quantum dots (QDs) has been a great topic of interest due to their unique quantum properties and great potential for optoelectronic applications [1, 2]. In this work, the effects of encapsulation of InAs QDs were investigated thru the variation in their growth surface and capping layers i.e. (Al)GaAs/QDs/(Al)GaAs. The effects in the crystal and optical properties of the heterostructures were analyzed by reflection high energy electron diffraction (RHEED), high-resolution x-ray diffraction (HRXRD), and photoreflectance (PR) spectroscopy. In situ RHEED analysis revealed information about the variation in the critical thickness (H_c) and In atoms diffusion towards their encapsulating layers. The changes in H_c are affected depending the strain fields from the GaAs or AlGaAs capping layers, the Al-containing layers reduces the In atoms mobility and therefore the In/Ga intermixing to upper layers decreases in comparison with GaAs layers. HRXRD corroborated the encapsulation periods of InAs QDs with clear differences in strain inferred from the location of the satellite's peaks. The periods between the satellites were associated to shaper interfaces, which in the case of AlGaAs encapsulating layers, the satellites peaks appeared more homogeneous, while for capping GaAs layers showed non-periodic which means that the In/Ga intermixing is more likely to happen on GaAs/InAs interfaces. Furthermore, the shape line in the PR spectra for both heterostructures revealed Franz-Keldysh oscillations (FKO), which are associated to the electric field (E_{int}) in the interfaces, the calculation exposed a difference of $1x10^{-6}$ V/m in the E_{int} from the GaAs/InAs/AlGaAs to AlGaAs/InAs/GaAs heterostructures. Therefore, it is demonstrated that the In/Ga intermixing effects involved in the QDs´ interface can be altered just by changing the type of encapsulating material chosen for the InAs QDs.

References:

[1] A. D. Yoffe. Semiconductor quantum dots and related systems: Electronic, optical, luminescence and related properties of low dimensional systems, Advances in Physics, 50:1, 1-208, (2001).

[2] Rakhlin, M.V., Belyaev, K.G., Klimko, G.V. *et al.* InAs/AlGaAs quantum dots for single-photon emission in a red spectral range. *Sci Rep* 8, 5299, (2018).

[NSN-272] Surface modification of polycrystalline titanium targets by low-energy ion irradiation

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In this work, titanium disks (10 x 3 mm) were mechanically polished and subsequently irradiated with a 1 keV Ar^+ broad ion-beam for incidence angles between 0º and 80º with respect to the surface normal. Irradiation experiments were performed for a total dose of 10^{18} ions cm^{-2} with an ion flux of 566-mA cm^{-2} at room temperature. Resulting ion-induced topographies were studied *ex-situ* by scanning electron microscopy (SEM) and stylus mechanical profilometry. Morphological changes are affected by the initial properties of the targets, including thermomechanical history and polishing procedures. A transition from randomly oriented surface ripples to sculpted pillars (facing the beam) are generally observed by increasing the incidence angle above 65º. Such behavior can be attributed to the dominance of diffusive or erosive regimes, respectively. In the first regime, the polycrystalline target nature drives the formation of confined rippled parcels (micron-size) without orientation coherence between each other. Lastly, wettability analyses were also carried out, showing an increase in hydrophobicity for treated surfaces in comparison to pristine ones. This factor has been shown in the literature to influence the initial metal-bone surface interaction for biomedical implants [J. E. Davies et al. *Biomaterials* **35** 25 (2014)]. Thus, ion beam irradiation offers a promising approach to tailor enhanced biomedical surfaces. *In-vitro* cell proliferation assays of our samples are currently under evaluation.

Acknowledgments: We acknowledge Prof. L. Vázquez for fruitful discussions, and Dr. M. Manso for support on contact angle measurements. Access to the MiNa Laboratory at IMN-CSIC for the SEM analysis is also appreciated. Additional financial support has been obtained from UNAM - PAPIIT IN-114120 and CONACyT Posdoctoral Fellowship.

[NSN-321] Interconversion energy via spin rectification with phonon and photon interactions

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The data revolution we live today is in great extent supported by decades of research in magnetism and spin phenomena. However, the ever increase of demand in data processing and storage comes with a significant increase of energy consumption and environmental concerns. In this talk we present our recent results on spin to charge conversion mechanisms mediated by light (photons) and vibrations (phonons) towards energy harvesting with spin information. Additionally, we show that beyond the energy harvesting, the interaction of phonons with thin magnetic films results in non-reciprocal phenomena with potential applications as acoustic rectifier.

[NSN-338] Structural and electronic properties of (TiO_2)_10 clusters with impurities: A simple model for bulk system

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We report the structural, energetics, and electronic properties of free-standing binary clusters $(TiO_2)_{10}$ with substitutional metallic and non-metallic impurities. The selected $(TiO_2)_{10}$ cluster has tetrahedral symmetry and is the putative low energy structure for this size. The substitutional impurity can be located at a vertex (4 sites) or at an edge (6 sites). The former has a binding energy only 0.03 eV/atom less than the latter, so they can be considered as almost degenerate. A total of 28 impurities are considered in the present report. We study the edge substitutional place since this environment is very similar to the corresponding one in the bulk, which makes these system a possible model for the bulk-like structures. Another advantage of the cluster considered here is that its energy gap is as large as the one presented in the bulk phases (anatase and rutile).

This system allows us to mimic the bulk behavior without the use of intrasite Coulomb corrections (U) which are generally applied as parameters to fit the real energy gap observed in bulk (TiO_2) systems. We show results for the formation energies, energy gaps and magnetism suggesting a way to control the band gap by means of the use of the appropriate impurity used in the substitution.

The impurity case of a vacancy in an oxygen site is also considered and compared with experiment result for bulk systems.

[NSN-382] Synthesis and characterization of ZnO/graphene composite

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Graphene is the most fascinating nanomaterial because of its unique structure of carbon atoms arranged in hexagonal honeycomb lattice, and with fascinating mechanical, thermal, optical and electrical properties. Graphene was synthesized via the liquid phase exfoliation method and ZnO solution was prepared in DI water and methanol. The graphene is mixed with ZnO solution to form of ZnO/G composite. After that, ZnO/G composite solution was put on an oven at 90°C for 2 days to get the dust.
In this work presents the characterization of ZnO/G composite powder. The powder was characterized by X-Ray Diffraction (XRD), Raman Spectroscopy, Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM), Scanning Electron Microscope (SEM), Energy dispersive spectroscopy (EDS), X-ray Photoelectron Spectroscopy (XPS). XRD results revealed that the G-ZnO that composite presents a structure polycrystalline with a hexagonal wurtzite ZnO phase had preferential orientations along (002) planes. TEM studies showed that ZnO thin film morphology was totally affected by an incorporation of graphene. In general, the results showed that graphene composited presents ZnO nanoparticles and its behavior could be used in differents applications.
Authors gratefully acknowledge: Leonardo Morales de la Garza acknowldege the sabbatical grant from DGAPA-UNAM, Gabriel Alonso Núñez and Dra. Yasmín Esqueda Barrón (Measurements Raman); Mario H. Farias Sánchez and MC. David Domínguez (XPS measurements); Francisco Ruíz Medina (TEM measurements), José Juan Gervacio Arciniega (AFM measurements); Miguel Ángel Méndez Rojas (Elemental mapping composition-SEM measurement), Mario Moreno Moreno and Netzahualcoyotl Carlos Ramírez (SEM measurements), Javier Martínez Juárez and Dra. Primavera López Salazar (XRD measurements), Also, We would like to thank the facilities given by laboratory equipment of the department of Nanocharacterization of CNyN-UNAM, laboratory equipment of department of electronic of INAOE, Laboratory equipment of CEMMATL of CIDS-ICUAP and the semiconductor laboratory of Ecocampus Valsequillo-CIDS-BUAP.

[NSN-391] Adsorption of serum protein in chitosan-coated and polyethyleneimine-coated magnetite nanoparticles

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Magnetic nanoparticles have been developed for a variety of biomedical applications including gene therapy. Magnetite nanoparticles (MNP) stands out nowadays as a non-viral vector for transfection when combining with a cationic polymeric coating. However, to ensure its performance as a non-viral transfection agent, the interaction of nanomedicine systems with biomolecules in blood plasma should be evaluated. This work aims to study the serum protein adsorption, namely opsonization, that could lead the MNP being excreted if they were exposed to in vivo systems. MNP were synthetized by coprecipitation method and further coated with chitosan (MNP-Ch), as well as coated with polyethyleneimine (MNP-PEI). Dynamic Light Scattering (DLS) reveled average diameters of 68 ± 65 nm nm for uncoated-MNP, 453 ± 332 nm nm for MNP-Ch and 817 ± 340 nm for MNP-PEI, individual MNP presented a size of 10nm. In this way, the increase in size is attributed to the formation of agglomerates. The spherical shape and size, as well as the elements in the samples were confirmed using Scanning Electron Microscopy (SEM) and Energy-dispersive X-ray spectroscopy (EDS). Likewise, Fourier-transform infrared spectroscopy (FTIR) corroborated bands at 578 cm^{-1} due to Fe-O bond, while the bands at 1468 cm^{-1} in MNP-Ch and 1380 cm^{-1} and 1620 cm^{-1} in MNO-PEI was attributed to the vibratory stretching mode of C-N, symmetrical and asymmetrical elongations of carboxylic groups, respectively. Additionally, Raman spectroscopy showed bands at 291, 598 y 1300 cm^{-1} for MNP, 584 and 1249 cm^{-1} in chitosan and MNP-Ch, as well as bands at 1065 and 1320 cm^{-1} for PEI and MNP-PEI. To measure the protein adherence, a bovine serum albumin (BSA) in PBS calibration curve was made using Nanospectrophotometer at wavelength 280 nm. Both graphics, MNP-Ch and MNP-PEI showed that coated nanoparticles have a BSA absorption greater than bare MNP.

[NSN-436] Study of point defects in semiconductor and dielectric nanostructures by cathodoluminescence technique

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We present recent results about using the cathodoluminescence (CL) technique in the scanning electron microscope (SEM) to determine the point defects present in ZnO, GaN, and hydroxyapatite nanostructures. CL measurements of single ZnO nanobelts revealed that the incorporation of N generates donor-acceptor pair (DAP) and free-electron acceptor (FA) transitions between N_O acceptor states, confirming its formation by X-ray photoelectron spectroscopy (XPS) measurements. Recently we demonstrated that the synthesis of ZnO nanowires by physical vapor deposition (PVD) in the presence of an AC electric field aligns these nanostructures, inhibiting native oxygen vacancies (V_O) and generating zinc vacancies (V_{Zn}), which exhibit CL emissions of 2.5 and 3.23 eV, respectively. CL studies of Mn-doped GaN nanowires reveal that this semiconductor exhibits emissions centered at 2.45 and 2.9 eV associated with gallium vacancies (V_{Ga}), which participate in generating ferromagnetism (FM). Moreover, Cu incorporation in GaN promotes the generation of the well-known green and blue emissions of the GaN, centered at 2.6 and 3.0 eV, respectively, attributed to V_{Ga} that participate in the generation of FM in this semiconductor. Finally, CL measurements in hydroxyapatite (Hap) nanobelts revealed the presence of calcium, oxigen, and hydroxyl vacancies as native point defects, identified as emissions of 0.81, 2.10, 2.95 eV, respectively, which were confirmed by electron paramagnetic measurements (EPR).

[NSN-150] Characterization of ZnCoFeO-Carbon nanoparticles synthesized using arc-Discharge immersed in distilled water, a simple method

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Since last two decades, the nanomaterials have been extensively studied worldwide because of their unique properties that are not exhibited by the corresponding bulk materials. Among various nanomaterials, the spinel ferrite Nanocrystals have become immensely popular magnetic materials due to some unique properties exhibited by these materials. These properties include large magnatocrystalline anisotropy, high coericivity, mechanical harness and chemical stability.

Ferrite materials have been widely used through several studies on various materials for instance Cobalt-Zinc ferrite. The magnetic properties of Zn-substituted Co-ferrites have attracted great consideration due to the importance of these materials for data storage application, among other.

Different synthesis techniques like hydrothermal treatment, microwave sintering, electrochemical synthesis, to mention some, are frequently used for the synthesis of ferrite nanomaterials. In this work, we synthesize ZnCoFeO-Carbon nanoparticles using arc-Discharge technique, which is very simple. To characterize these structures, the following techniques were used: Transmission Electron Microscopy, spectroscopy IR, spectroscopy Uv-Vis and Vibrating Force Magnetometer.

[NSN-157] Synthesis of MnTiO3 powder by coprecipitation method.

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Titanate-based perovskites ($ATiO_3$) have been studied for different applications such as heterogeneous photocatalysis, solar energy, electrodes and gas sensors, due to their light absorption capability in the ultraviolet wavelength range[1]. $MnTiO_3$ is a semiconductor material obtained through naturally abundant elements, has ferroelectric and pyroelectric properties that enhance charges separation and photocatalytic activity [2]. In general, the $MnTiO_3$ synthesis is carried out by methods such as hydrothermal, sol-gel, and solid state. However, the $MnTiO_3$ synthesis by the coprecipitation method has been scarcely studied. Coprecipitation method provides high yield, high purity in the material, does not require organic solvents and it is reproducible. Reaction parameters such as temperature, pH and ions concentration can be controlled to determine the properties of the material [3]. In this work, $MnTiO_3$ powder was prepared by the coprecipitation method. The synthesis was realized using manganese oxide (II) (MnO) and titanium isopropoxide ($C_{12}H_{28}O_4Ti$) as precursors of Mn^{2+} and $Ti^{4+,}$ respectively. Manganese ions were obtained dissolving manganese oxide (II) in hydrochloric acid and titanium ions with titanium isopropoxide in distilled water. After, the powder was dried at 150°C and calcinated at 750°C, 850°C, 950°C and 1000°C. The MnO: $C_{12}H_{28}O_4Ti$ molar ratios were varied (1:1, 1:0.8, 1:0.6 and 1:0.4) in order to assess the crystal structure according to the calcination temperature. The physicochemical properties were assessed by X-ray diffraction (XRD), field emission scanning electron spectroscopy (FESEM), UV-VIS spectroscopy and electrochemical impedance spectroscopy (IES).

[1] T. Alammar, I. Hamm, M. Wark, and A.-V. Mudring, "Low-temperature route to metal titanate perovskite nanoparticles for photocatalytic applications," *Appl. Catal. B Environ.*, vol. 178, pp. 20–28, Nov. 2015.

[2] M. Enhessari, A. Parviz, E. Karamali, and K. Ozaee, "Synthesis, characterisation and optical properties of MnTiO 3 nanopowders," *J. Exp. Nanosci.*, vol. 7, no. 3, pp. 327–335, 2012.

3] M. Nawaz *et al.*, "Magnetic and pH-responsive magnetic nanocarriers," in *Stimuli Responsive Polymeric Nanocarriers for Drug Delivery Applications*, Elsevier, 2019, pp. 37–85.

[NSN-161] ZnO QD´s embedded in matrix Methanol + MEA

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ZnO nanomaterials have attracted tremendous interest in the fields of photocatalysis, sensors, solar cells, for it´s interesting properties. The obtension of ZnO QD´s prepared succesfully by coloidal syntesis process with 6 nm on average size, have been encapsulated within a Methanol + MEA (monoethanolamine) Matrix only using part of Sol – Gel process, for the implementation on thin films by Solar Cells. The deposit is by spin coating and by CVD (chemical vapor deposition) on cristal substrate. Changing the deposit concentration of QDs to take advantage of the photoconductive properties of ZnO QDs, as well as its photoluminicence in the region of the visible (UV), and for obtension of the uniform of thin film, to seek to improve the efficiency of a solar cell.

[NSN-164] Synthesis, characterization, and comparison of reduced graphene oxide by pulsed CO2 laser and CVD

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Since the discovery of graphene in 2004, its properties have been investigated, which represent a great contribution in the applications of solid state physics. For this reason, finding techniques that simplify its synthesis or growth and that are also low cost, is a topic of interest for its technological applications.

A comparison between two reduced graphene oxides is presented, which are grown using two different techniques; the first, is by using a pulsed infrared CO_2 laser, receiving the name of laser reduced graphene oxide (LrGO); and the second, by chemical vapor deposition (CVD) where ethanol is used as a carbon source, which was simply named as reduced graphene oxide (rGO). Both materials are obtained from a commercial Graphene Oxide (ID-nano supplier, GOx-ID01) synthesized by chemical exfoliation, a dispersion (4.5g/100ml) in three-distilled water was prepared, and with this solution GO thin films were deposited on quartz substrates. In the CVD technique rGO is obtained from 800°C after 25 minutes of ethanol flow; on the other hand, LrGO is obtained by irradiating the GO film with a power of 2.7 watts from the CO_2 laser.

Four-terminal resistance measurements show that the GO has an average resistance of 4MΩ/square, after laser reduction the LrGO has a resistance of 3KΩ/square is reached, on the other hand, the rGO has a resistance of 15KΩ/square, reducing the GO resistance by three orders of magnitude in both cases. Furthermore, from Raman spectroscopy we find the D, G and 2D bands typically found in graphitic materials. From them, ratios between bands D and G of 0.495 and 1.072 are obtained for the LrGO and rGO respectively, also showing the disappearance of the 2D band in the case of rGO.

[NSN-187] Systematic characterization of the crystalline phase transformation of annealed electrospun TiO2 nanofibers for photocatalysis applications

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TiO_2 nanofibers were synthesised by the electrospinning technique, which were annealed at high temperatures to achieve the crystalline phase transformation. The chemical stoichiometry of slectrspun TiO_2 nanofibers was estimated by EDS, finding that at low annealing temperatures there is excess oxygen and at high temperatures excess titanium. By TEM corroborates the presence of TiO_2 nanofibers that are homogeneous and continuous form without the presence of crystalline defects, whose surface morphology depends strongly on the annealing temperature. The crystalline phase transformation was studied by Raman dispersion, which revealed that annealed TiO2 nanofibers showed a crystalline phase transformation from pure anatase, anatase-rutile mixed and pure rutile as the annealing temperature increased, which was corroborated by X-ray diffraction and High-resolution transmission electron microscopy. The grain size is increased with the crystalline phase transformation from 10 to 24 nm for anatase and from 30 to 47 nm for rutile, estimated by the Scherrer-Debye equation. The band gap energy, obtained from optical absorption spectra, decreases monotonically but a local minimum is observed at 700 °C, which ranged from 3.75 to 2.42 eV, caused by the crystalline phase transformation anatase→rutile. The photoluminescence shows that radiative bands redshift as the temperature increases due to the reduction of the band gap energy.

[NSN-202] ZnSe nanoparticles prepared by coprecipitation method for photocatalytic applications

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A simple coprecipitation method was used to synthetize pure zinc selenide (ZnSe) nanoparticles (NP's) and ZnSe NP's with traces of elemental selenium (ZnSe:Se). The physicochemical properties of ZnSe and ZnSe:Se NP's were analyzed and correlated with their photocatalytic activity for hydrogen production and RhB degradation under UV irradiation. The X-ray diffraction (XRD) analysis indicated the formation of a zinc blende-type ZnSe with the presence of elemental Se and a crystallite size of ~6 nm. The scanning (SEM) and transmission (TEM) electron microscopies showed ZnSe NP's with a spherical morphology. A red shift of absorption edge was observed when Se traces are present in ZnSe-NP's. The improved photocatalytic activity of ZnSe:Se NP's for hydrogen production via water splitting and RhB degradation was related to the fact that elemental Se acts as a co-catalyst to separate the photogenerated charge carriers. The energy band positions of ZnSe were estimated from the Mott-Schottky plots, allowing to evidence the degradation of RhB is due to indirect oxidation of water molecules to the hydroxyl radical by reactive oxygen species.

[NSN-209] Colloidal silicon nanoparticles synthesized by picosecond laser ablation

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Silicon nanoparticles suspended in deionized water were obtained by the laser ablation of solids in liquids technique. A silicon wafer target was ablated with a Nd:YVO4 pico-second laser emitting at 1064 nm with 10 ps pulse width at a repetition rate of 402 kHz with an energy per pulse of 106 µJ. The effect of fluence changes in nanoparticle size and optical properties was studied. The fluence was varied from 2 to 6 J/cm^2 by attenuating the beam by means of optical attenuators. Results show a strong relation between nanoparticles size and fluence values. Optical characterization gives bad gap values higher than that of bulk Si, indicating the existence of quantum confinement effects produced by size reduction of Si nanocrystals.

[NSN-214] Chemical, structural and optical properties of In0.145Ga0.855AsySb1-y alloys

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The antimonide family is compounded by binary, ternary and quaternary alloys; all of these displaying a zinc-blende structure, a lattice constant very close to each other, and a direct band gap energy that may cover a large part of the solar spectrum, the near-infrared (1.7 µm) to mid-infrared (3.5 µm) at room temperature. These properties allow us to engineer semiconductor devices with a wide range of uses, going infrared detectors to superlattices for quantum cascade lasers, considering that one of the fundamental aspects responsible of these applications is the structural and optical changes of the alloy as a function of the precursor elements content at the growth time. Using energy-dispersive spectroscopy (EDS), High-Resolution X-ray Diffraction (HR-XRD), and photoluminescence spectroscopy (PL), we analyzed the chemical, structural, and optical properties of different $In_{0.145}Ga_{0.855}As_ySb_{1-y}$ samples. The quaternary alloys were grown on GaSb (100) substrates by liquid phase epitaxy (LPE) varying the As content. We calculated the interplanar distances of the heterostructures θ-2θ scan, followed by that, the lattice constants of the quaternary alloys and of the GaSb substrate were obtained. The lattice constant of the $In_{0.145}Ga_{0.855}As_ySb_{1-y}$ decreases as the As content (y) increases, from 6.0938 to 6.0915 A. Likewise, the lattice constant of the GaSb at 6.0957 A with a full width at half maximum (FWHM) of 56.15 was found. We determined with EDS the atomic content of each element (In, Ga, and Sb) in the quaternary alloys, and the As content (*y*) for the different alloy, according to Vegard's Law was obtained. We found As content (*y*) between 0.1364 and 0.1327. The emissions of the $In_{0.145}Ga_{0.855}As_ySb_{1-y}$ alloys were also measured by PL. The alloys presented two optical transitions, the first one attributed to bound-exciton states, and the second one to donor-acceptor-pairs.

[NSN-235] Study of phase transitions in hydroxyapatite using XRD at variable temperature

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Hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$, (HAp), is almost known as an alternative as bone substitute or replacement includes complete or partial bone augmentation. Due to similarity inorganic components of bone matrix, recent studies show its ability to regenerate cells of bone tissue using scaffolds based on Hydroxyapatite and biological polymers like type I collagen.
HAp powders were obtained by coprecipitation method assisted by Ultrasonic Radiation, using Ca $(NO_{3)2}$ • $4H_2O$ and $(NH_4)_2HPO_4$ as precursors. X-ray powder diffraction was performed using the Huber Kappa Goniometer at the beamline XRD-1 at Elettra Synchrotron, Trieste, Italy. The experimental set up consisted of a bending magnet in the light source, a double crystal monochromator Si (111), a focusing mirror of Pt-coating, and a detector Dectris Pilatus 2 M (DECTRIS Ltd., Baden-Daettwil, Switzerland). A monochromatized 0.7 Å X-ray beam was utilized with the sampler rotating 180º to prevent orientation effects. For study the phase transitions Oxford Cryostrem 700 (N_2 laminar flow, temperature range 80 – 400 K) was employed like temperature control system, obtaining diffraction patterns at 25º, 250º, 450º and 850º C. By XRD patterns we observed that in all cases the hexagonal phase of HAp is maintained. In addition to appreciating that as the temperature increases, the crystallinity increases too, observing a greater definition of the peaks.

[NSN-236] Structural and compositional characterization of TiO2/Ag nanoparticles

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Titanium dioxide (TiO_2) is a wide band-gap semiconductor material widely used for many applications in photo-electrochemist and photocatalysis activity, as ultrasound sensor, pigment and in solar energy conversion. TiO_2 presents three crystalline structures: anatase, rutile, and brookite. Recently, titanium dioxide nanoparticles have gained importance as an anticancer agent in photodynamic therapy, due to their ability to kill cancer cells.

In this work, we describe the synthesis of pure and Ag-doped titanium dioxide by ultrasound-assisted sol-gel method. The silver ion dopant concentration was varied from 2 to 10% atomic weight. We use Ti $(OC_4H_9)_4$ and $AgNO_3$ as sources of titanium and silver ions, respectively. Synchrotron X-ray diffraction and Raman Spectroscopy were used for structural characterization. The compositional characterization was carried out by Wavelength-Dispersive X-ray fluorescence technique (WD-XRF).

The Synchrotron XRD confirmed the presence of anatase phase of TiO_2. The crystallite size was determinated using modified Scherrer equation that allowed us to know that there is a variation of crystallite size due to the incorporation of silver ions in the crystal lattice. The photonics modes in Raman spectroscopy correspond to the anatase phase and are in accordance with the XRD. The WDXRF characterization shows the nominal amount of Ag in the Ag-doped TiO_2 as 1.89 at. %, 3.11 at. %, 4.05 at. %, 4.33 at. %,respectively.

[NSN-243] Initial Stages of Hydrogenation of HOPG-supported Gold Nanoparticles

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Many modern catalysts are composed of nanomaterials. In particular, gold nanoparticles are used to catalyze the hydrogenation of hydrocarbons, etc. At the same time, despite the long-term studies of nanocatalytic systems based on gold nanoparticles the mechanisms of elementary acts of even model reactions remain unclear. The purpose of this work is to determine the locations of adsorbed hydrogen on the surface of gold nanoparticles deposited on the surface of highly oriented pyrolytic graphite (HOPG). The experiments were carried out at a facility consisting of a scanning tunneling microscope (STM), Auger spectrometer, quadrupole mass spectrometer and auxiliary equipment, at T = 300 K and a residual gas pressure of $P = 1 \times 10^{-10}$ mbar. Quantum chemical simulation of the interaction between atomic deuterium and gold clusters on carbon substrate – supercluster $Au_{13}C_{138}$ – was carried out within the framework of the density functional theory (DFT). Experimental investigation showed that nanoparticles have a oblate spheroidal shape. The maximum of the lateral size distribution is in the range of 4–8 nm with an average height of approximately 1.5–2 nm. As it was found previously the exposure of the sample to hydrogen resulted in a significant perturbation of the local electron density of nanoparticles. The periphery of gold nanoparticles has been found experimentally to be the preferred region for hydrogen adsorption. Quantum chemical simulation has shown hydrogen adsorption in this region to be more beneficial in energy in compare with other sites of gold-carbon system. With increasing exposure and saturation of the interface adsorption sites, hydrogen interacts with the rest of gold nanoparticle surface, gradually covering it from periphery to the center.

[NSN-246] Ferroelectric properties and phase transitions of high performance vertically aligned potassium-sodium niobate (KNN) nanowire-arrays

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Pulsed laser deposition (PLD) was used to synthesize piezoelectric nanowire-arrays of $K_{0.5}Na_{0.5}NbO_3$ (KNN) on $Pt/TiO_2/SiO_2/Si$ substrates. These arrays were successfully prepared by using two different deposition conditions than the previously reported for KNN. KNN with orthorhombic structure and minority secondary phases were identified by XRD. Ferroelectric and Piezoelectric properties were confirmed by piezoresponse force microscopy, and showed that nanowire-arrays have an improvement in their effective piezoelectric coefficient of d33eff = 94.6 pm/V and 133.6 pm/V, higher than previously reported coefficients. Pulsed laser photoacoustic technique was used to analyze the phase transition temperatures and they showed a phase transition (O-T) at ∼170â—¦C and a phase transition (T-C) at ∼360â—¦C, lower temperatures than those found for bulk ceramics. Furthermore, it was identified the presence of minor amount of secondary ferroelectric phase (K4Nb6O17).

[NSN-250] Study of the surface passivation of GaSb semiconductor alloy for applications in infrared devices

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Antimonide alloys have become one of the most promising III-V semiconductor families for developing infrared (IR) optoelectronic devices, such as LEDs, light-emitting diodes, thermo-photovoltaic cells, and detectors. To this family belong GaSb alloy, which has a direct bandgap in the near IR wavelength of 1.7-um. This alloy is highly reactive with oxygen; therefore, an oxide surface layer is easily formed, which negatively impacts the performance of the devices. Surface passivation techniques based on sulfides are used to remove the oxides. This work presents the surface passivation of the GaSb binary alloy with Ammonium Sulfide, Sodium Sulfide, Dodecanethiol and a biodegradable alkaline detergent. Taking as experimental variables the immersion time of the alloy and the temperature of the chemical solution. The effect of passivation on the optical and thermal properties of the binary alloy are analyzed by mean of photoluminescence and photoacoustic techniques. We find that radiative recombination and recombination surface velocity increases in passivated GaSb samples.

[NSN-251] SYNTHESIS OF 2D NANOMATERIALS (h-BN, Bi2Te3, MoS2) BY TOP-DOWN TECHNIQUES

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The 2D materials are stacked on layers attracted each other by Van der Waals forces, there are a large range of materials in this category with properties and possible applications which haven´t been researched deeper yet. An example of these materials are: Boron nitride (BN) with a graphene alike hexagonal configuration, Bismuth telluride (Bi_2Te_3), whose single layer composition is a five layer stack of alternating Bismuth and Tellurium, Molybdenum disulfide (MoS_2), whose monolayer is a sandwich-type arrangement with a thickness of 3 atoms. BN and Bi_2Te_3 possess a high heat conductivity, but different electric properties, BN is an insulator (Bhimanapati, Glavin, & Robinson, 2016), Bi_2Te_3 has a low voltage activation semi-conductor properties (Li, Ren, & Luo, 2011), while MoS_2 has interesting electronic applications as a semi-conductor (Xiao Li & Zhu, 2015). In this work are analyzed two Top-Down obtention methods for 2D materials. The 2D material synthesis is developeded by a liquid phase exfoliation and Wet-Jet Milling processes, (Del Río et al; 2018). Morphology is compared of the resulting materials by Transmission Electron Microscopy. The bandgap of the materials of each method was obtained of the UV-Vis spectroscopy results applying Tauc plot approaches. The obtained 2D materials can be objects of other studies with a view to different possible applications.

Bhimanapati, G. R., Glavin, N. R., & Robinson, J. A. (2016). 2D Boron Nitride: Synthesis and Applications. Semiconductors and Semimetals, 95(1). 101–147 (ed. Francesca Iacopi, John J. Boeckland Chennupati Jagadish) in 2D materials semiconductors and semimetals, Elsevier Science, https://doi.org/10.1016/bs.semsem.2016.04.004

Del Rio Castillo, A., et al; 2018. High-yield production of 2D crystals by wet-jet milling. Materials Horizons, 5(5), 890–904. https://doi.org/10.1039/c8mh00487k

Li, Xiao, & Zhu, H. (2015). Two-dimensional MoS2: Properties, preparation, and applications. Journal of Materiomics, 1(1), 33–44.https://doi.org/10.1016/j.jmat.2015.03.003

Li, X., Ren, H., & Luo, Y. (2011). Electronic structure of bismuth telluride quasi-two-dimensional crystal: A first principles study. Applied Physics Letters, 98(8), 2011–2014. https://doi.org/10.1063/1.3556654

[NSN-256] Zr-aminoacid-graphite oxide compounds with possible applications in water defluoridation

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The region Altos Norte of Jalisco is characterized by having groundwater with fluoride levels higher than the permissible limit in drinking water. It has been reported that the ingestion of this pollutant at a concentration higher than 1.5 ppm and for a long time can cause negative health effects, such as dental and skeletal fluorosis, among others. Various methods have been used for the elimination of this pollutant, including filtration, adsorption, ion exchange, etc. Of these methods, the adsorption has been of great interest since it presents high efficiencies and facile application. A wide variety of adsorbents have been developed, including polymers composites and metallic nanoparticles. Among these zirconium-based compounds have been studied, due to their high affinity and stability with the fluoride ion, but as a disadvantage the pH ranges of action are acidic, and the contact times are relatively high.

Therefore, this research presents the synthesis of Zr-aminoacid-graphite oxide compounds (Zr-aa-OG), as an alternative for the removal of the fluoride ion from drinking water.

These compounds were synthesized using amino acids (aspartic acid and glutamic acid) and different percentages of graphite oxide (5% y 30%). The characterization of the compounds by infrared spectroscopy (FTIR) was performed to determine the functional groups present in the material. Preliminary tests were performed to identify the compounds with the best fluoride removal percentages. Among the synthesized compounds, the group synthesized with 5% graphite oxide presented the highest removal percentage of fluoride removal.

[NSN-257] Thermal Diffusivity measurement of Graphene-Water based Nanofluids by thermal lens technique

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Graphene nanoparticles were synthesized using the microwave assisted hydrothermal method. The thermal diffusivity of graphene nanoparticles suspended in water were measured by mode-mismatched dual-beam thermal lens technique. Different concentrations were prepared to measure the changes in the thermal diffusivity due to the presence of graphene nanoparticles in the nanofluid. The thermal parameter characteristic time constant of the transient thermal lens was calculated by fitting the experimental data to the theoretical expression. The thermal diffusivity of the nanofluids was strongly dependent on nanoparticles concentration. There was higher enrichment of this thermal property compared to the water base fluid. Higher diffusivity was found for nanofluids with higher nanoparticle concentration. The morphology and structure of graphene nanoparticles was characterized by UV-Vis spectroscopy, transmission electron microscopy (TEM) and X-ray spectroscopy. This novel nanofluids have applications in advanced heat transfer fluids, electronic circuits and motor cooling systems.

[NSN-259] Modulation of confined states by interface corrugation control on AlGaAs/GaAs (631) MQW and SL heterostructures

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Within the framework of wave function engineering the one-dimensional (1D) nanostructures have particular relevance due to the unique set of phenomena arising from them [1]. MBE self-assembly growth processes have been used throughout the last decades to obtain quantum dots (QDs) and quantum wires (QWRs) nanostructures. Owing to the complexity of their nucleation and self-organization requirement conditions the QWRs are harder to accomplish. In the last few years, our aim has been to achieve the synthesis of nanostructures of quantum wire superlattices grown over the anisotropic high index (631) plane. The intrinsic anisotropic and kinetic properties of this template are ideal to achieve nanocorrugation and 1D QWRs, whose geometry essentially depends on the growth temperature and III/V BEP ratio, Π. Therefore, as a first step to reach this objective we have manufactured a series of multi-quantum well (MQW) samples by varying Π along both extreme- and optimized values in order to allow for the analysis and effects of the different corrugation order inserted in-between the MQW interfaces. With this methodology we were able to characterize the modulation inflicted on the conduction and valence subbands via surface finishing and optical properties. Photoreflectance characterization as a function of temperature was done to the series of samples in order to get the energy of the confined state transitions. It is observed, that an interface corrugation that is not balanced in terms of lateral and vertical periodicity, red shifts the energy of the optical transitions between subbands. In other words, the interface corrugation downgrades the oscillator strength of the optical matrix element for the confined states. On the contrary, an optimized interface corrugation strengthens the oscillator of n>1 subbands allowing for additional transitions that in principle would be prohibited and blue shifts their energy. These results are in agreement with atomic force microscopy (AFM) measurements taken from the capping layer surface of the samples.

REFERENCES

[1]S. Tomonaga, Prog. Theor. Phys. 5,544 (1950).

ACKNOWLEDGMENTS: The authors acknowledge the financial support from CEMIE-SOL 22, FRC-UASLP and CONACYT-Mexico through grants: CB 2015- 257358 and PNCPN2014-01-248071.

[NSN-263] 3D printing Acrylic Nanocomposites for Skin Regeneration

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Many human activities make us risk of having an accident, such event might require organ replacement or regeneration. Even though there are some instances for organ donation, the requirement is always faster than the donation. Due to that situation recently has been intended to make human organs from human cells, growing them up and printing with them the required organ in a 3D printer. The cells are printed on a biocompatible structure that sometimes is also biodegradable. Although researchers have advanced greatly, they don't know yet what is the better way to build a functional organ. In this research a 3D printer will be used to print cellular scaffolds; flat structures that will be dip into epithelial cells and the assembly is expected to work as replacement of scarred or burned skin. The scaffolds will be printed using nanocomposites of acrylic resin with rounded silver nanoparticles, and with silver nanowires; In this paper present results of physical properties, e. g. curing time, hardness, heat diffusivity and microstructure of these 3D-printed scaffolds and propose a theory that could explain the differences between them.

[NSN-265] Assembly of Gold Nanoparticle-Decorated Buckypapers for Plasmonic-enhanced Electrochemistry

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Localized surface plasmon resonance (LSPR) on plasmonic nanoparticles (NPs) can decay through non-radiative transfer of energy to conduction band electrons, producing highly energetic (‘‘hot’’) charge carriers. Generated hot-holes can participate in the oxidation of adsorbed molecules and enhance chemical conversion rates. In order to increase the lifetime of plasmon-induced excited carriers, carbon nanotubes (CNTs) have been proposed as possible charge transfer mediators due to their excellent electrical conductivity. By promoting an intimate contact between both nanostructures, charge injection from plasmonic NPs to CNTs can inhibit the recombination of hot-holes, enabling their participation in the transfer of electrons from an adsorbate to the plasmonic NPs. Moreover, CNTs can be assembled into high-surface area membranes (known as ‘‘buckypapers’’) with great potential for electrocatalytic applications **[1]**.

The work herein presented aimed to assemble plasmonic buckypapers from colloidal dispersions of gold nanoparticles (AuNPs) and multi-walled carbon nanotubes (MWCNTs), which were prepared as follow: AuNPs (~15 nm) were synthesized by reducing $HAuCl_4$ with sodium citrate and then coated with poly(allylamine hydrochloride); CNTs were synthesized via CVD spray-pyrolisis, hydrothermically treated for their dispersion in water and then coated with poly(sodium 4-styrenesulfonate). After mixing both solutions together, TEM micrographs confirmed anchoring of AuNPs over the CNTs surface. The composite solution was then subjected to a vacuum-assisted filtration through a PTFE membrane, resulting in the assembly of an AuNPs-decorated buckypaper. Thermal annealing under an air atmosphere was performed to increase the electrical and thermal contact of AuNPs with

CNTs. Electrical conductivity was measured at different stages. Finally, electrocatalytic performance for alcohol oxidation reactions (AOR) was studied with cyclic voltammetry under white light and darkness conditions.

[1] Contreras, E. et al. ACS Applied Energy Materials (2020). DOI: 10.1021/acsaem.0c01293

Acknowledgements: We gratefully acknowledge financial support from the UNAM México funding through DGAPA PAPIIT IN105719 and DGAPA PAPIME PE108319 projects and CONACyT funding through projects A1-S-17539 and Fordecyt 272894. The authors would like to thank F. Ruiz, J. Diaz, I. Gradilla, E. Murillo, E. Aparicio and J. Mendoza for technical assistance.

[NSN-268] Synthesis and Growth of ZnO nano/nanostructured particles via a simple-polyol method

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In this work, we informed with the processing of PVP-capped ZnO nanoparticles employing a simple-polyol method, varying only the molar concentration (0.01 and 0.1 M) of Zn(CH3COO)2•2H2O as zinc precursor using ethylene glycol (EG) as solvent and polyvinylpyrrolidone (PVP) as a capping agent. Physical-chemical characteristics of as-synthetized ZnO particles were studied by X-ray diffraction (XRD), scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). SEM micrographs reveleted monodisperzed quasi-spherical particles, so-called secondary, formed by aggregation of primary nanosized subunits obtained for a precursor concentration of 0.01 M. At higher concentration, no aggregation occurs and only tiny primary particles in the nanosized range are obtained. XRD patterns revealed that the ZnO nanoparticles had a hexagonal wurtzite-type structure with average crystallite sizes in the nanorange. Result of EDS characterization shows that the above route produced ZnO nanoparticles has good purity. Based on the results it is suggested a high dependence between morphology and molar concentration of the (zinc acetate dihydrate) precursor. Results are discussed and interpreted.

[NSN-269] Simulation and experimental study of strain distribution in multi-stacked layers InAs/GaAs quantum dots.

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Self-assembled of InAs/GaAs quantum dots (QDs) has acquired great importance in the last decade due to the great potential in the development of next generation nanodevices, for such application, it has been demonstrated that vertically stacked QDs plays an important role for an effective active region in QDs devices [1]. However, geometry control and structural parameters implemented in vertically stacked InAs QDs get more challenging during the growth, with each grown layer since other effects are involved such as: diffusion, segregation, intermixing alloying, strain fields among others. In this work, numerical simulations are performed to analyze the strain distribution of multi-stacked layer of QDs (MLQD) in function of the geometry of the QDs, wetting layer (WL) and spacer layer (S) thickness. Pyramidal shape was considered for the QDs in the heterostructures, and the εxx strain tensor was chosen to analyze the average strain distribution in the QDs´ apex and base, under the variation of parameters such as: number stacked layers, QDs´ base area, wetting layer and spacer layer thickness. First, similar behaviors in strain were obtained independent of the number of stacked layers and with the other parameters remaining constant. Nevertheless, it was noticed that the main changes occurred for the first periods of the MLQDs, until the numerical value of εxx seems to reach quasi equilibrium conditions. Furthermore, it has been reported that as the number of stacked layers increase, the critical thickness (Hc) decreases due to accumulated strain and the QDs´ area increase for the first periods of MLQD. Therefore, through these experimental observations another set of simulations were performed considering morphological variations, the QDs´ heights decreased from 2 - 1 nm and added to their base for the first to the fourth MLQD periods. Then, it was found that the strain decreases significantly in comparison with heterostructures´ with constant areas for all the MLQDs periods. Furthermore, εxx results more affected were when the variation of S changed, these simulations showed that average εxx decrease half its value when S increases from 12 - 20 nm due to the compensation of strain.

References:

[1] J. Wu, P. Jin, Self-assembly of InAs quantum dots on GaAs(001) by molecular beam epitaxy. Front. Phys. 10 (2015) 7–58.

[NSN-276] The TWRC technique to measure the thermo-optical properties of graphene nanofluid in water for application in biomarkers

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Graphene oxide (GO) is an oxidized form of graphene, synthesized through the oxidation and exfoliation of graphite. Because its higher conductivity, it is used in many applications such as sensor energy converters accessories and catalysis. The GO is fluorescent, so it can be used to create fluorescent biosensors. GO films have shown to be antibacterial with multiple applications in the field of medicine or the food industry, among others. In this work, the TWRC (Thermal Wave Resonant cavity) technique was used to determine the thermal diffusivity of this colloid, depending on the concentration of GO found in the water. With the modification of this technique, the thermal effusivity can be determined. Knowing these two parameters, the thermal conductivity is calculated. The absorbance of these samples was also determined and the range of light that it can absorb and emit, with possible applications as a thermosensitive biomarker.

[NSN-278] Synthesis of SiO2 Nanoparticles for Drug Delivery

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This work presents the synthesis of mesoporous silicon nanoparticles (SiO_2) used for drug transport prepared by the modified Stöber method. From the synthesis, it was possible to obtain monodisperse SiO_2 mesoporous nanoparticles in water. The absorption range was from 90 to 620 nm. The nanospheres were obtained with a diameter of 120 nm and a pore diameter of 3 nm, varying their physical and chemical parameters of the process. It was also observed that by varying the pH of the reaction and the reaction temperature at 80 ºC, different sizes of nanoparticles and mesopores can be obtained. For the analysis of the size, structural and morphological properties, as well as the measurement of their thermo-optical properties, the obtained samples were characterized using UV visible spectroscopy, TEM microscopy, SEM, EDS and resonant cavity, respectively. In this work, the first results of the thermal properties of the SiO_2 mesopores obtained by means of the TWRC (Thermal-wave resonant cavity) technique will be presented. These investigations are aimed at the use of mesoporous silicate nanoparticles for applications in medicine for drug transport.

[NSN-283] Nitrogen-doped CNTs and their electrocatalytic activity for DSSCs

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The development of high-efficiency, low-cost and clean solar energy technologies is of great current priority. Dye Sensitized Solar Cells (DSSCs) are becoming an important alternative for converting solar energy into electricity. A typical DSSC device is composed of interconnected TiO2nanoparticles coated by a dye sensitizer as the photo-anode, iodine / iodide electrolytes and a counter-electrode. The photo-anode generates electrons under solar irradiation and the counter electrode collects them from the external circuit, while the redox couple in the electrolyte transport the charge from the counter electrode to the photo-anode closing the device circuit. One of the key elements is the counter-electrode, as an electro-catalytic interface between the redox couple in the electrolyte and the external circuit. Its main role corresponds to the exchange of electrons with the electrolyte by the tri-iodide reduction reaction (IRR). The tri-iodide molecules are reduced into three iodide molecules which transport the charge from the counter electrode to the photo-anode.

Recent studies have confirmed that carbon materials doped with nitrogen posses favorable electrocatalytic activity. When carbon materials are nitrogen doped, several species are included such as: pyridinic nitrogen, pyrrolic nitrogen and graphitic nitrogen. However, little is known regarding the specific role of the different nitrogen species on the IRR. In the present work [1], nitrogen-doped carbon nanotubes (CNx-CNTs) were synthesized and their electrocatalytic activity for the IRR was evaluated. The CNx-CNTs synthesis was performed exploring two different nitrogen precursors (Triphenylamine 0.5 wt% in benzylamine and Prussian blue 1.0 wt% in benzylamine) in order to modify the proportion of nitrogen species present in the obtained carbon nanotubes. The obtained CNx-CNTs samples were heat treated for further tuning of the nitrogen species content in the samples. The samples were analyzed by SEM, TEM and XPS. Moreover, we performed cyclic voltammetry to check the efficiency of the different CNx-CNTs samples for the IRR. Finally, the CNx-CNTs were incorporated into a water-based ink using chitosan as the binder and the CNx-CNTs based ink electrocatalytic activity was analyzed for the IRR.

[1] J.M. Ruiz-Marizcal et al. Carbon 167: 209 (2020).

Acknowledgements: We gratefully acknowledge financial support from the UNAM México funding through DGAPA PAPIIT IN105719 project and CONACyT funding through projects A1-S-17539 and Fordecyt 272894. The authors would like to thank F. Ruiz, J. Diaz, I. Gradilla, E. Murillo, E. Aparicio and J. Mendoza for technical assistance.

[NSN-295] Immobilized glucose oxidase bioreceptor based on a TiO2-Ni nanocomposite by sol gel

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The objetive of this work presents the development of an amperometric bioreceptor for glucose oxidase immobilized in a TiO_2-Ni nanocomposite obtained by sol-gel. The nanocomposite was characterized morphologically and structurally by X-ray diffraction (DR-X), Fourier transform infrared spectroscopy (FTIR), RAMAN spectroscopy, diffuse reflectance (DRS), scanning electron microscopy (SEM) and crystal size. The results indicate the presence of anatase phase and $NiTiO_3$ in the sample. Electrochemical tests of impedance spectroscopy (EIS) and cyclic voltimetry (CV) were carried out to know the electrochemical behavior of the nanocomposite and the bioreceptor, the results indicate that the nanostructure has low resistance to the passage of electric charge and that both the nanostructure and the bioreceptor do they exhibit electrochemical activity. Finally, the biosensor was able to detect glucose and showed a sensitivity of 0.625225 mA/mMol.

[NSN-309] Morphological characterization of amphiphilic peptide nanoparticles

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Las características morfológicas de las nanopartículas de péptidos anfifílicos (APnPs) las hacen buenas candidatas para ser utilizadas como recubrimientos para implantes metálicos, ya que son vectores de carga genética no viral que pueden autoensamblarse en micelas esféricas o estructuras fibrosas con recubrimientos hidrofílicos y centros hidrofóbicos con acuosos. soluciones y se utilizan comúnmente como transporte de drogas. Los APnPs contienen el péptido ácido arginilglicilaspártico (RGD), que no solo promueve la adherencia celular sino también otras funciones celulares como la proliferación celular.

[NSN-311] Photocatalytic degradation of 2, 4-chlorophenoxyacetic acid (2,4-D) using the TiO2-ZrO2 metal mixed oxide

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2,4-Dichlorophenoxyacetic acid, more commonly known as 2,4-D, is a commonly used herbicide worldwide. It has been used in the agricultural field for more than 50 years [1] and its excessive use has caused environmental deterioration. The numerous applications of chlorophenols favour a rapid and widespread introduction of these into the environment, which constitutes a serious risk to human health and ecosystems due to their high toxicity and persistence [2]. In this study was evaluated the photocatalytic activity of TiO_2-ZrO_2 metal mixed oxides over the degradation of 2,4-D. The crystalline structure of TiO_2-ZrO_2 catalysts was confirmed by X-ray diffraction analysis and the morphologies of samples were observed by SEM. Furthermore, chemical properties of photocatalysts were characterized via FTIR, XPS and UV–Vis spectrophotometry analysis. The photocatalytic degradations showed that TiO_2-ZrO_2 exhibited higher photocatalytic activity than TiO_2 nanoparticles. Moreover, differences in photocatalytic activities were found in TiO_2-ZrO_2 nanocomposites in the organic degradation of 2,4-D, those differences were attributed to the light absorption region, smaller crystal sizes and more surface OH groups, which resulted in a lower band gap energy.

[NSN-315] Effective zero refractive index in layered aperiodic systems with metamaterials

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Multilayer systems with effective zero refractive index [1] are proposed considering an infinite stack of nanometric bilayers constructed with a rigth handed slab whose refractive index and width are constant and a metamaterial slab with negative refractive index $Nb = -(e_b\ m_b)^{1/2}$ and a variable width modulated by Fibonacci, Thue-Morse, Cantor and Pascal's Triangle aperiodic sequences [2]. The optical respone is calculated using the transfer matrix method [3] and the rational aproximation [4]. These systems present new modes not observed in periodic right handed multilayers. Also, the band diagrams and the dispersion relations present autosimilar properties similar to the the sequences modulating the width of the metamaterial slab.

[1] D. Bria, B. Diajari-Rouhani, A. Akjouj, L. Dobrzynski, J. P. Vigneron, E. H. El Boudouti and A. Nougaui, Phys. Rev. E, 69 (2004) p. 066613.
[2] D. A. Contreras-Solorio, C. Ortíz, X. Saldaña and E. López-Cruz, Phys. Stat. Sol. (C), 2 (2005) p. 3622.
[3] P. Yeh, Optical Waves in Layered Media; John Wiley and Sons, (1988).
[4] P. Hawryilak, G. Eliasson and J. Quinn, Phys. Rev. B, 36, (1987) p. 6501

[NSN-318] Theoretical Study of the mechanism to the formation of Y junction semiconductor GaAs Quantum Wires

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Nowadays, technology bring us a variety of techniques to fabricate more complex nanostructures to innovate some devices/ components used in nanoelectronics such as the junction of one-dimensional (1D) nanostructures to form structures of bifurcated quantum wires (Y-Junction QWrs), which have showed great and unique potential to be used as a new type of logical device in nano-electronic.

The current problem is that the synthesis of the Y-Junction QWrs nanostructures, in a controlled and reproducible way, is a complex task that the scientific community continues to investigate

We have reported the controlled formation of the Y-Junction semiconductor QWrs without crystalline defects and with the possibility of varying its dimensions and its degree of electrical resistivity by using self-assembly on high index (H-I) substrates by molecular beam epitaxy (MBE).

On the other hand, due to the H-I substrates usually provide energetically unstable surfaces that tend to break up into low free-energy facets and naturally form a periodic corrugation array, the theoretical models to study these processes are based in the study of coarsening. For MBE, the model that better describe this mechanism is given by the Kuramoto-Sivashinsky equation.

In this work we present a theoretical study about the mechanism to the formation of Y-junctions by using a modification that we have proposed at the Kuramoto-Sivashinksy equation to add more realistic parameters involved at the growth conditions to be used in the experimental part. The results of our simulations are directly compared with the experimental results obtained from AFM results.

[NSN-322] H2 and H adsorption over organometallic Ni3(HITP)2

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Recently, shortage and increase in the price of fossil fuels and the environmental problems has promoted research to find new sources of energy. Hydrogen is one of the most attractive due to its energy density of 33.3 kWh/Kg, besides, is the most abundant chemical element in the universe and has a clean burning. Despite its enormous energy density per unit mass, hydrogen as a carrier of energy presents problems as a function of low energy density per unit volume, making this element difficult to store and transport. Fortunately, hydrogen can be stored in a wide variety of solid materials under various conditions of pressure and temperature using chemical storage processes or by physisorption. Materials implemented to carry out the storage of hydrogen are usually porous materials. Carbon-based materials (fullerenes, nanotubes and graphene), zeolites, among others are porous materials which have been studied for hydrogen store. In this direction, a new class of solids known as organometallic networks with outstanding properties have emerged in recent years. Organometallic networks (MOFs) are made by inorganic bonds and organic units through strong links. In this work we present results about the adsorption of molecular and atomic hydrogen over the surface of the organometallic graphenoid material $Ni_3(HITP)_2$ and decorated with lithium. Calculations were made with DFT and VASP code with VDW correction. Physical adsorption reports a energy of 50meV over the surface. No changes in semiconductor character is observed in DOS in case of hydrohen direct adsorption with the material.

[NSN-326] Determination of human gamma globulin Raman spectrum using gold nanoparticles as SERS substrate

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Context: Immunoglobulins (Ig) are glycoprotein molecules produced by plasma cells in response to a variety of antigenic stimuli involved in various physiological and pathological conditions. Intravenous immunoglobulin (IVIG) is a concentrate whose composition corresponds to the concentrations of Ig in human plasma, especially IgG. It is used as a replacement treatment in primary and secondary immunodeficiencies. Determination of IgG concentrations is useful in the diagnosis of these immunodeficiencies, and in the evaluation of the replace treatment. Surface-Enhanced Raman Spectroscopy (SERS) is a technique that allows protein quantification in a reproducible and straightforward way.

Objective: To determine the Raman spectrum of IgG at physiological concentrations using quasi-spherical gold nanoparticles (AuNP) as a SERS substrate.

Methods: We initially determined the Raman spectrum of IVIG at 5%. Subsequently, for the characterization by SERS, decreasing dilutions of the protein were made by adding deionized water and an equal volume of the 5 nm AuNP colloid. The Raman spectrum was determined using 532 and 785 nm lasers, in a range of 500-1800 cm^{-1}, with 5 acquisitions and an acquisition time of 30 seconds. We focus the laser spot on the surface of the sample with a 10x objective.

Results: We obtained the IVIG spectrum by SERS up to a concentration of 75 mg/dl. The Raman bands obtained correspond to aromatic amino acid side chains and the characteristic beta-sheet structure of IgG.

Conclusion: IVIG could be detected at a concentration of 75 mg/dl, ten times lower than the normal IgG concentration in plasma, using AuNP as SERS substrate.

[NSN-334] Many-electron redistribution in n-doped semiconductor quantum wires under external electric field

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In recent years, quantum wires have been of great interest due to the opportunities that are generated to explore physical phenomena that can be translated into potential applications. Specifically, for its implementation as logic gates for quantum computing [1-2], fundamental studies related to the electronic charge redistribution produced by an external voltage must be performed. In this work, we present a theoretical study of the electronic redistribution in GaAs quantum wires and experimental results about its fabrication. The synthesis of these one-dimensional nanostructures was carried out by molecular beam epitaxy (MBE) by using a 13.3 nm-thick GaAs layer sandwiched between AlGaAs barriers were grown on GaAs (631) substrate. The arrangement of the GaAs quantum wires self-assembled are described in Ref. [3]. The n-type doping of the nanostructures was carried out with Si by using two delta doping layers inside the AlGaAs barriers. The surface characterization of the sample was performed by atomic force microscopy to verify the formation of the quantum wires. A study by photoluminescence allowed to establish the Al molar fraction corresponding to the AlGaAs ternary as well as the determination of crystalline defects and impurities in the samples. A simulation was also performed by means of finite element resolution using the COMSOL MULTIPHYSICS software in order to compare with the effective potential model reported in Ref. [4] and, in the near future, to compare with experimental results. The redistribution of the electron probability density for the quantum wire's ground state is discussed in the presence of an electric field. Some remarks about the Wigner molecule formation under an external electric field are also presented [5]. [1] Achintya Singha, et al., Correlated Electrons in Optically Tunable Quantum Dots: Building an Electron Dimer Molecule, PRL 104, 246802 (2010).
[2] C. Ellenberger, et al., Excitation Spectrum of Two Correlated Electrons in a Lateral Quantum Dot with Negligible Zeeman Splitting PRL 96, 126806 (2006).
[3] E. Cruz-H, et al., Highly ordered self-assembled nanoscale periodic faceting in GaAs(631) homoepitaxial growth, APL 101, (2012).
[4] Reyna Méndez-Camacho et al., Many-electron redistribution in n-doped semiconductor nanostructures under external electric field by using a center-of-mass approach, Phys. Rev. B 102, 035403 (2020).
[5] L. H. Kristinsdóttir, et al. Signatures of Wigner localization in epitaxially grown nanowires, Phys. Rev. B 83, 041101(R) (2011).

[NSN-342] Current trends in carbon-based nanomaterials for 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. Recently, the strategies to reduce and control breast cancer have focused on its prevention, as well as its early detection and treatment, since 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. 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. In this regard, the use of nanotechnology in medicine involves the application of nanoparticles, offering new alternatives for the design and synthesis of desirable nanomaterials that can be used in the identification, diagnosis, and treatment of cancer. The nanomaterials used for targeting cancer cells should 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 nanomaterials, carbon-based nanomaterials (fullerenes, nanotubes, and graphene) are of particular interest to scientific community due to their physical properties, versatile chemical functionalization, and biocompatibility. In recent years, scientific evidence shows that carbon-based nanomaterials have potential uses as therapeutic agents, devices for selective and controlled drug release, contrast agents for the diagnosis and localization of tumors, and biosensors. 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. Here, we present the trend of the number of cancer investigations reporting the implementation of carbon-based nanomaterials for different applications to diagnose and treat cancer, as well as the corresponding reports exclusively dedicated to breast cancer. In general, all research findings presented here contribute to elucidate the future implementation of carbon-based nanomaterials for breast cancer treatment.

[NSN-345] Effect of mechanical grinding time on the formation of carbon nanostructures using recycled graphite from alkaline Zn-C batteries

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Batteries have become a source of energy for electronic devices and nowadays their use has increased at an alarming rate. Consequently, these hazardous wastes have caused environmental and health concern around the world. Therefore, recycling spent batteries is an alternative to mitigate the environmental impact. This work focused on using graphite electrodes extracted from Zn-C alkaline batteries, for the synthesis of carbon nanostructures in a dry environment through high energy mechanical ball milling. The samples were obtained at grinding times of 6, 12 and 18 h. They were analyzed by Raman spectroscopy (RS), scanning electron microscopy-energy dispersive (SEM-EDS) and transmission electron microscopy (TEM). The graphite structure, size and quality of the crystal were calculated by RS, using the relations of the relative intensities of the Raman bands D, G and 2D, and the Tuinstra-Koenig model. The particle size decreases when increasing the grinding time, which was corroborated through SEM pictures. The detailed morphology of the nanostructures, as well as their size, were determined by TEM. For the

sample obtained at 6 h of grinding time, spherical nanoparticles of around 10 nm in diameter and amorphous graphite agglomeration were obtained; while, for the samples subjected to 12 h and 18 h of grinding, the formation of nano-sheet structures was preferential. The morphology and sizes of the nanostructures are associated with the grinding medium, the type of atmosphere, the grinding time, as well as the contaminants contained in the graphite of the batteries. These conditions can promote distorted carbon and the coexistence of different morphologies.

[NSN-356] DFT Study of the electronic and mechanical properties of [001]-Ge nanowires as anodic material

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The renewable sources of energy require the development of more efficient storage energy devices in the small a great scale in order to offer technological advantages to the society. In this work, we present a theoretical study of the electronic and mechanical properties of hydrogen passivated Ge nanowires (GeNWs), grown along [001] crystallographic direction considering different diameters and concentrations of interstitial Na and Li atoms. The study is performed by the density functional theory in the local density approximation incorporated in the SIESTA code. The results indicate that the GeNWs have a metallic behavior with one interstitial Na atom and semiconductor when two or more Na atoms are in the structure. The formation energy analysis indicates that it increases as a function of the concentration of Na atoms for all studied morphologies, whose values are close to the same configuration of the GeNWs with interstitial Li atoms. The binding energy results show values almost constant for concentrations from two to eight Na atoms for the GeNW with the largest diameter, followed of an increment for 10 and 12 interstitial Na atoms. In contrast, for the Li atoms, the binding energy follow a monotone grow as a function of the concentration for all studied morphologies. By other side, the Young's modulus follows a trend to diminish as function of the concentration of Na and Li atoms with values from 40 GPa for the pure H-Ge nanowire to 25 GPa for the maximum concentration of Na and Li atoms. This results seems to indicate that the mechanical resistance of the GeNWs is enough strong to support the structural changes during the charge-discharge process in a rechargeable battery using Na and Li atoms, and open the possibility to incorporate the GeNWs as anodic material in the development of the new generation of rechargeable batteries.

Acknowledgments

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

[NSN-357] Theoretical study of [111]-Si nanowires with Li and Na at the surface for energy storage

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Nowadays the new technologies require a new generation of rechargeable batteries in order to attend the grown energy demand for portable and great scale devices. In this work, we present a density functional theory study of the mechanical and electronic properties of hydrogen (H) passivated silicon nanowires (SiNWs) with diamond structure, grown along the [111] crystallographic direction. The model considers the substitution of H atoms for sodium (Na) or lithium (Li) ones for different concentrations in three different morphologies of SiNWs. The study is performed applying the supercell method, within the Local Density Approximation incorporated in the SIESTA code. The results indicate that all studied nanowires present a semiconductor behavior, and the size of the energy band gap follows the known confinement effect as function of the diameter, and a strong effect in the band gap as a function of the concentration of surface Na and Li atoms. Likewise, the formation energy results, indicates that the SiNWs increases their energetic stability as a function of the number of Na and Li atoms. The binding energy values are close to 2.0 eV according with theoretical reports. The Young´s modulus analysis indicates that the values remains almost constant for all studied concentrations of Na atoms. These results open the possibility to incorporate the SiNWs as anodic materials in Na and Li in energy storage devices as rechargeable batteries.

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

[NSN-358] Synthesis of self-assmbled Ag nanoparticles based SERS substrates by termal evaporation on deep eutetic solvent for Surface enhanced Raman Spectroscopy sensing

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Metal nanoparticles (NPs) with controlled size, shaped and self-assembled structure have received increasing attention owing to their desirable physicochemical properties and their promising applications in catalysis, plasmonics, surface enhanced Raman scattering (SERS), biosensors, and biomedicine. Engineering the self-assembly structure of metallic NPs of Au and Ag, while simultaneously attaining size and shape-control has emerged recently for their application in SERS. In this work, a thermal evaporation of metallic nanoparticles on choline chloride: Urea (ChCl:U, molar ratio of 1:2)-derived deep eutectic solvent (DES) surface and subsequent formation of three-dimensionally self-assembled structure is demostrated. A relatively simple experimental setup was designed to controlled evaporation of bulk Ag on to the glass substrates containing DES, in which the Ag NPs size, and self-assembly nature is varied by changing the synthesis parameters such as applied potential, pressure, and distance between substrates and evaporation point. The resultant AgNPs deposited glass substrates were characterized using SEM, AFM, UV-vis, XRD techniques. The deposited AgNPs was utilized as an efficient SERS-active substrate containing abundant SERS “hotspots” for detection of crystal violet (CV) probe molecule. As-prepared self-assembled AgNPs based SERS substrate exhibits highly enhanced SERS performance with a SERS enhancement factor close to 10^5, high sensitivity (low detection limit upto 10^{-12} M), and excellent stability. The synthesis approach afforded in this present study for the preparation of self-assembled AgNPs based SERS substrates offers promising platform for preparation other metallic nanoparticles based SERS-substrates and their potential application in SERS based molecular sensing.

Keywords: Silver nanoparticles, deep eutectic solvent, thermal evaporation, self-assembly, SERS based sensing.

[NSN-364] Low-temperature synthesis, enhanced reaction times and characterization of TiO2 nanoparticles by a microwave assisted sol-gel method for its application in green industry.

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In the present work, TiO_2 nanoparticles were prepared by the microwave-assisted sol-gel method and their link with the green industrial sector was evaluated. The synthesis was carried out without the presence of any catalyst or surfactant agent. The resulting products were subsequently dispersed using sodium dodecyl sulfate (SDS) and sodium chloride (NaCl) as surfactant agents and ethyl alcohol as solvent (EtOH). The TiO_2 dispersions were subsequently deposited on glass substrates as thin films using the spin coating technique. Through UV-Vis characterization a band gap energy of 3.9 eV was determined for the TiO_2 nanoparticles; FTIR technique confirmed the presence of O-Ti-O bond characteristic of titanium dioxide; SEM results showed that nanoparticles morphology is spherical and their size is approximately 20 nm; EDS technique confirmed the presence of Ti and O elements present in analyzed nanoparticles samples; finally, through XRD technique, it was confirmed the presence of anatase phase for the TiO_2 nanoparticles. Based on the information obtained through the bibliographic review and patent analysis, it was concluded that the materials reported here are a viable option for their application in wastewater treatment and developing solar cells, according to the resulting properties.

[NSN-383] The effect of silver loading on Au nanoparticles in the catalytic transformation of toxic nitroaromatics

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Nowadays, many cancer-types diseases have been correlated to the presence of nitro compounds commonly in several water effluents from the chemical industries. Thus, their safe transformation into useful products is a necessity. The catalytic reduction of 4-nitrophenol into 4-aminophenol, the precursor of acetaminophen (paracetamol, a famous analgesic), has been widely studied and described as a model reaction to evaluate the efficiency of catalysts in the transformation of toxic nitroaromatic compounds. It is well known that bimetallic nanoparticles are characterized by a better catalytic performance than the monometallic ones. The later is mainly attributed to a synergetic effect among the metals. Herein, we present the synthesis and catalytic activity of bimetallic Ag-Au colloidal nanoparticles characterized by different Ag loadings on the Au nanoparticles surface.
Bimetallic colloidal nanoparticles were prepared via the seed method, using Au nanoparticles as seeds. Different amounts of Ag were loaded on the Au surface, this was corroborated by the blue-shift of the surface plasmon resonance peak as the Ag content increased, measured by UV-Vis spectroscopy. It was found that as the Ag content increases, the particles tend to reduce their stability, which was observed by evaluating the Z potential. The bimetallic nanoparticles were tested in the 4-nitrophenol reduction as model reactions with $NaBH_4$ excess at 30°C. The reaction progress was monitored by UV-Vis spectroscopy in situ were every UV-Vis spectra was collected each 2 sec.
It was resolved the promotional effect of silver in the catalytic reduction of toxic nitroaromatic compounds. In addition, as the content of Ag increases, the catalytic activity also increases, reaching three times the value of the Au seeds for the colloid with 100% coverage.

[NSN-385] Solvothermal synthesis of nanoparticles for the SERS detection of chemical contaminants

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Metal oxide nanoparticles constitute an outstanding class of functional materials with potential applications in almost all fields of technology. Between the different approaches to its synthesis developed in recent years, non-aqueous or non-hydrolytic processes has been particularly successful with regard to achieving control on crystal size, shape and self-assembly. However, despite such progress, the preparation of metal oxides nanocrystals remains challenging due to some issues related to the reproducibility, functionalization and a substantial waste of precursor materials [2,3]. On the other hand, antibiotics are commonly used in excess by humans, which could trigger different problems such as water contamination. Metal oxide nanoparticles can be used in SERS measurements to detect these emerging pollutants that can be fatal to the environment [1].
In this work, we present a study of nanoparticles synthetized by solvothermal synthesis. Solvothermal synthesis is an efficient method to control sizes, shapes, and assembly behavior of nanoparticles with the advantages that it is reproducible and can be easily functionalized. Then the nanoparticles are used to analyze contaminants in the water by SERS. The study is carried out by using free-standing nanoparticles as well as a thin film of deposited nanoparticles used to fabricate a reusable substrate [1]. Atomic Force Microscopy (AFM) was used in order to examine surface ordering, Scanning electron microscopy (SEM) for size distribution, Transmission electron microscopy (TEM) for the sample structure and RAMAN and Surface-enhanced Raman (SERS) to analyze the signal enhancement due to the analyte in samples of contaminated water [2].

[1] Jumanji, C. (2019). Desarrollo de materiales nanoestructurados para la caracterización de contaminantes emergentes mediante Raman Aumentada en Superficies, Universidad Autónoma de Aguascalientes, Aguascalientes, México
[2] Bilecka, I, Djerdj, I, Niederberger, M. (2007). One-minute synthesis of crystalline binary and ternary metal oxide nanoparticles. *ChemComm*, 1, 1.
[3] Pedroza, G. (2012), Desarrollo de una metodología espectroscópica para la determinación de clembuterol, Universidad Autónoma de Aguascalientes, Aguascalientes, México

[NSN-392] PEG-coated silver nanoparticles by ultrasound assisted colloidal synthesis

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Ultrasound assisted colloidal synthesis is one of the simplest and inexpensive methods for AgNPs preparation. In this work, we use this method to synthesize small size AgNPs using PEG as stabilizer and citric acid as reducer. The alkalinity effect of NaOH to pH control and silver oxidation limitation was studied. Also, PEG concentration and [citric acid]/[$AgNO_3$] molar ratio effect in size distribution was analyzed finding the significant parameters to control to achieve small size AgNPs. Theorical calculations of surface plasmon resonance were made over UV-Vis characterizations to obtain size diameter. Finally, growth phases of AgNPs were visualized by UV-Vis characterization and size distribution was obtained by the data collected in TEM characterization. SPR bands of the smallest AgNPs synthetized were located at 396 nm which defines the size of the spherical nanoparticle by theorical calculation less than 10 nm. The mean size obtained by TEM micrographs was 2.61 nm and Ag and PEG hydroxyl groups interaction was detected by 418 cm^{-1} FTIR band.

[NSN-400] Synthesis and Characterization of Gold-Copper plasmonic nanoalloy for SERS applications

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The importance of nanoalloys lies in the synergistic properties that both metals provide. Gold-Copper nanoalloys can be tunable composition and geometry, and both are plasmonic materials, so their applications in SERS will be demonstrate.
Gold-Copper nanoalloys were synthesized in aqueous phase through co-reduction of $HAuCl_4 3H_2O$ and $CuCl_2 2H_2O$ by glucose in presence of hexadecylamine at 100°C. By shifting molar ratio precursors, nanoparticles of different shapes stellated liked were observed. Morphological behavior of Au-Cu has been examined through transmission electron microscope and with Energy Dispersive X-ray Spectroscopy confirms the presence of Au and Cu in the nanostructures; the optical behavior corresponds to Au, Cu localized surface plasmon resonance syntonized from Ultraviolet to Infrared region. Finally, dopamine at different concentrations were detected in a micro Raman Spectrometer using Au-Cu nanoalloys as SERS substrate.

[NSN-409] Detection of volatile organic compounds using 30 MHz-QCM sensors with self-assembled ethylcellulose microparticles

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Polymeric films (PFs) and polymeric micro and nanoparticles (µPs and NPs) have a wide range of applications. Among them is sensing Volatile Organic Compounds (VOCs) vapors using quartz crystal microbalances (QCMs) as high precision sensors. The coated polymers are highly sensitive to VOCs, as well as having partial selectivity towards them. In this work, Ethylcellulose µPs (EC-µPs) were synthesized and self-assembled for the fabrication of 30 MHz-QCM sensors (EC-µPs/QCM). Then, the fabricated sensors were used for sensing three VOC vapors with different concentrations (ethanol at 2060, 4120, 6180 ppm; ethyl acetate at 1230, 2460, and 3690 ppm, and heptane at 710, 1420, 2130 ppm). The experimental conditions were carried out at T = 20 °C and 20 %RH. Their frequency responses and sensitivities were studied, and both were compared with QCM sensors with an EC film (EC/QCM). Our results showed an increase when EC-µPs/QCMs are used in comparison with the EC/QCMs ones, ranging from 39.5% for ethanol, 3.05% for ethyl acetate, and 1.25% for heptane vapors.

[NSN-419] Growth mechanism and optical characterization of cubic InxGa1-xN Quantum Wells grown by Plasma-Assisted Molecular Beam Epitaxy

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$In_xGa_{1-x}N$ is one of the most important semiconductor materials for the manufacture of light-emitting diodes [1,2], therefore the study and understanding of the optical and chemical properties of these materials is very important. In the present work, we present the growth and characterization of c-$In_xGa_{1-x}N$ quantum wells (QWs) on GaAs (001) substrates by Plasma-Assisted Molecular Beam Epitaxy (PA-MBE) technique. $In_xGa_{1-x}N$/GaN QWs were grown with a thickness of 10 nm and GaN barriers of 30 nm, with the same In flow of $BEP_{In}=1.8x10^{-7}$ Torr and Ga flow of $BEP_{Ga}=2.28x10^{-7}$ Torr, and varying the growth temperature (Tg) from 600 to 680 °C. We found by means of the X-Ray Photoelectron Spectrometry (XPS) that the growth mechanism of the QWs is constituted by In-N and Ga-N bonds. In addition, photoluminescence measurements obtained at different temperatures and powers, evidence excitonic emissions between 2.23 and 2.41 eV, which corresponding to emission in the visible light spectrum (green). The green emission of the QWs is very important for their implementation as an active layer in light emitting diodes (LEDs). Likewise, by Secondary Ion Mass Spectroscopy (SIMS) we determined the In concentration in these QWs is between 29 and 24 percent.

[1] Shu, G. W., Lin, C. C., Lin, H. T., et. al., Opt Express., **19** (2011) A195-A200.
[2] Pozina, G., Bergman, J. P. & Monemar, B., J Appl Phys., **88** (2000) 2677-2681.

[NSN-440] Characterization of the electrical and spectral properties of a sensor fabricated employing self-assembled silicon nanoparticles embedded in a ZnO matrix produced by reactive RF sputtering.*

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A procedure to produce silicon nanoparticles embedded within a zinc oxide matrix on p-silicon substrates by reactive RF sputtering was developed by Avila-Meza et al. [1]. Using this procedure Si nanostructures embedded within a ZnO matrix were deposited on a 4 inches p-type silicon substrate. A Si wafer was processed at CICTA-UACJ using a mask with circular 1 mm diameter Cr circles. Squared samples 2 mm side were diced and then bonded using Al wire on a rectangular 8 pin frame. Transport and spectral properties exploring the sensor capabilities of the prototype device were determined. Current-voltage (I-V) measurements were performed in the temperature range 10–300 K showing a rectifying structure. From the temperature dependent forward bias I-V characteristics, the barrier height, ideality factor and series resistance are calculated.

*: Partially funded by CONACyT-Mexico

[1]. Avila-Meza, M. F., Zelaya-Angel, O., Gallardo, S., Fernández-Muñoz, J. L., Alfaro-Flores, D. R., & Meléndez-Lira, M. A. (2018). Synthesis and Characterization of Self-Assembled ZnO Nanoparticles Embedded Within a SiO 2 Matrix Deposited on (111) p-Type Silicon By Reactive RF Sputtering Using Metallic Zinc Target As Precursor. *Journal of Electronic Materials*, *47*(11), 6607-6612.

[NSN-444] MIS structures with SRO-LPCVD and SRO-HFCVD films, using transparent and conductive films.

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This work presents the manufacturing and characterization process of two types of transparent conductive oxide films, Aluminum-doped zinc oxide (AZO) using the Sputtering technique and tin-doped indium oxide (ITO) using the pyrolysis spray technique, these transparent and conductors films were deposited on a film of silicon-rich oxide (SRO) deposited by two systems of chemical vapor deposition by low-pressure (LPCVD) and by hot filament (HFCVD), in order to build two Metal-Insulation-Semiconductor (MIS) structures and highlight its emission and electrical characteristics to elucidate the best. The precursors used are silane (SiH4) and nitrous oxide (N2O) for the LPCVD system and for the HFCVD system the gaseous precursors are obtained from a solid quartz source stripped with atomic hydrogen. As a first stage, the results of the optical characterizations of the transparent conductive oxide films are presented, observing that the AZO films have a transmittance greater than 80%, while the ITO films have a transmittance of 75%, later the structures MIS were electrically characterized with IV curves finding interesting results.

[NSN-447] Green synthesis of reduced graphene oxide via chemical reduction

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Reduced graphene oxide (RGO) was synthesized through the reduction of graphene oxide (GO) in water using hydrazine hydrate as reducing agent. The proposal of the present work was the reduction of the organic functional groups of the GO by a simple chemical method, placing in reflux a dispersion of GO in water with the reducer agent. The reduced product was characterized by infrared spectroscopy with Fourier Transform (FTIR), X-ray powder diffraction (XRD), Raman spectroscopy, and field emission scanning electron microscopy (FESEM). Once the reduction has been made, RGO was obtained as a suspension in water, which was separated and washed easily by means of filtration, getting a black powder, consisting of thin, wrinkled, and associated nanosheets that shown black body radiation, porous characteristics, and disperse crystallite size, fact that indicated the removal of hydrophilic groups present in the GO and the recovery of electronic density through chemical reduction.

[NSN-450] Contact angles on ZrO2 thin film surfaces.

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By placing a drop of liquid on a solid surface, it can remain concentrated as a fraction of a spherical body on the surface or spread out until it appears flat. Whatever the case, there is an angle between the boundary of the liquid drop and the solid surface. The analysis of this angle provides information on the structure of the material on which the drop is deposited, related to its surface energy and referring to parameters such as its roughness, permeability, affinity of adhesion to the liquid used and wettability.
Zirconium oxide (ZrO2) thin films were prepared by the sol-gel dip coating technique, in combination with annealing at different temperatures in air atmosphere, with the final goal of studying the water wettability of the surface. In this work the theory of the phenomenon is analyzed and compared with the experimental results of thin films of ZrO2. The annealing effects on the structural and optical properties of the ZrO2 films were investigated to check the characteristics of the material.

[NSN-452] Growth of GaN on vicinal GaAs(100) substrates by MBE technique

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The group-III nitrides have become one of the most important families of semiconductors for developing optoelectronic and microelectronic applications. Recently, the metastable phase (cubic) of the nitrides has generated great interest due to the absence of spontaneous polarization and piezoelectric fields. Additionally, the nitrides in this phase have higher carrier mobility and they are easier to cleave than the nitrides in stable phase (hexagonal).

We present an investigation of optical and structural properties of cubic GaN as grown by plasma-assisted molecular-beam epitaxy on vicinal (100) GaAs substrates misoriented by 10° toward [111]. The films were synthesized with different growth temperatures for the substrate and Ga beam equivalent pressure (BEP_{Ga}) of $1.95x10^{-7}$ Torr with flux of N_2=0.4 sccm and power 150 W. During growth, the surface of the layers was monitored by Reflection High Energy Electron Diffraction (RHEED). X-ray measurements determined the crystal structure of GaN/GaAs to be cubic. High resolution transmission electron microscopy reveled planar defects propagating along the GaN planes. The majority of the defects originated from disordered regions at the GaN/GaAs interface. The optical properties of the films were investigated by photoluminescence.

[NSN-453] Mg- and Si Doping of GaN layers by molecular beam epitaxy

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Cubic GaN semiconductor materials have attracted considerable attention for optoelectronic high temperature and high-power electronic component applications because of their wide band gap and high saturation velocity. Cubic GaN samples on GaAs (1 0 0) substrates were grown by molecular beam epitaxy (MBE). For the nucleating layer we used a nominal growth temperature range from 565 to 570 ºC, during 17s, and a Ga beam equivalent pressure (BEPGa) of $1.95x10^{-7}$ Torr, with a flux of N_2=0.4 sccm and a power of 150 W. GaN was doped with Mg or Si at different concentrations to obtain p- and n-type layers, respectively The nucleation layer of GaN films were monitored by Reflection High Energy Electron Diffraction (RHEED). The structural characteristics of the GaN films were evaluated using X-ray diffraction (XRD), where the samples exhibit a mixture of the hexagonal and cubic GaN phases. Electrical properties were obtained by Hall effect, the change in mobility is discussed in terms of doping density.

[NSN-454] Surface Recombination Velocity measurements of GaN/GaAs heterostructures obtained by photoacoustic techniques

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The Surface Recombination Velocity (SRV) of a semiconductor is important for the assessment of its quality and the design of electronic devices. Although it can be measured by some experimental techniques, such as time-resolved photoluminescence, it is difficult to discriminate the properties of the surface and bulk recombination. Nevertheless, the photoacoustic signal of a semiconductor, in a frequency range where the sample is thermally thick, can be used to differentiate between heat absorption at the surface and heat absortion other mechanisms. This can be used to obtain the SRV and the carrier lifetime of a semiconductor thin film. In this work, we used a photoacoustic experiment to study the transport properties of GaN/GaAs heterostructures, to find a correlation between the defects at the interface and the SRV.

PLASMA AND VACUUM

Chairmen:
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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-223] Molecular beam flux measuring retractable system: design and setting up for ultra-high vacuum applications

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For industry, research and technological applications the reproducibility of any processes is mandatory for manufacturing either at large or small scale. In this direction the implementation of apparatuses to control or monitoring becomes of outmost importance. For instance, in Ultra-High Vacuum (UHV) systems the flow meters are of great importance, since by means of these it is possible to calibrate the molecular beams fluxes, attain reproducible growth rates at with which the epitaxial growth of the layers is carried out, and to asses precise atomic concentration in alloys. [1] However, these flow meters use to be very expensive due to the complexity of the whole parts such as the retractable system, the Bayard Alpert ionization gauge, electrical feedthroughs, and what else needs to be mounted on a CF flange. The design of the retractable system of these flow meters is a great challenge because it must have the facility to move inside the chamber in UHV environment from its resting to the measurement location. At the resting point the ionization gauge must not interfere with the molecular beams, while at the measurement location if must be set very close to the zone where molecular beams of the knudsen cells are impinged to achieve the atomic layers growth. In this work, a Bayard Alpert flow meter retractable system was built and it was implemented in a Molecular Beam Epitaxy (MBE) chamber. After performing drawings on paper of the whole design and every piece, 3D modeling was performed using Computer Aided Design (CAD) software. Then the elements were created in a 3D printer with polylactic acid (PLA). The meter system was assembled, probed in the MBE chamber, and redesigned to improve its performance. Once the retractable system was optimized it was processed with the manufacture of the 3D printed parts now in aluminum.

[1] J. O. and T. Foxon, *Molecular Beam Epitaxy - A Short History*, First edit. Oxford University Press, 2015.

The author acknowledges the financial support of CONACYT, CeMIE-SOL 22, FRCUASLP, INFR-2015-01: 255489 and PNCPN2014-01: 248071.

[PLV-316] Characterization of ECR microwave and laser ablation plasmas

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The main aim of the present work is to report on the study of the combination of continuous plasma, formed by a microwave electron cyclotron resonance (ECR) discharge and pulsed plasma of laser ablation which allow studying the formation of materials in the form of thin films making use of the relatively high densities of the microwave discharge and the wide range of ion energies produced in the pulsed laser ablation plasmas. With this arrangement it is possible to deposit thin films of materials that in the usual microwave discharge require the use of pollutant and corrosive substances, as the required element is obtained from a pure solid target. Moreover, as the laser ablation process is carried out in plasma as the background gas, instead of a neutral gas, the presence of contaminants, such as oxygen can be significantly reduced. For the purpose of the present paper a nitrogen microwave ECR discharge was combined with the plasma created during the ablation of an aluminum target, in order to deposit AlN thin films. Plasma parameters were measured by a Langmuir probe, and the chemical species contained in the plasma were analyzed by optical emission spectroscopy (OES)

[PLV-166] Structural and optical properties of CuInS2 films prepared by pulsed laser deposition for photovoltaic applications

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Nowadays, energy production trough renewable resources, is an important issue. Within development of photovoltaic devices, some alternative materials have been studied in order to process toxic–free solar cells. Chalcopyrite family offer a high efficiency potential among thin-film-based materials, which has been of interest for use in photovoltaic applications. The $CuInS_2$ is an attractive ternary semiconductor compound, has a direct bandgap of 1.55 eV which lies in the optimum range for solar energy conversion; it has reached efficiencies at the laboratory level of up to 12%.

$CuInS_2$ films have been prepared by different methods, for instance, closed–spaced vapor transport (CSVT), electrodeposition, ion layer gas reaction (ILGAR), co–evaporation and spray pyrolysis. However, $CuInS_2$ semiconductor needs suitable conditions for the deposition of high–quality films. Pulsed laser deposition (PLD) or laser ablation is an important technique in the manufacture of films with a complex composition, it offers a faster synthesis of specific controlled stoichiometry compounds.

The present work focuses on the elaboration of films of the semiconductor compound $CuInS_2$, using the laser ablation technique. The main objective of this research is to obtain a semiconductor heterostructure on flexible substrates that can be applied as a photovoltaic device.

[PLV-323] Atomic nitrogen generation transition to molecular nitrogen excitation induced by N2 molecular flux in an inductively-coupled nitrogen plasma.

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Keywords : dissociation rate, nitrogen plasma, energy density, EEDF.
The growth of III-N semiconductors and their nanostructures has been attracted to scientific attention due to their optical properties in the visible to ultraviolet wavelength range, as well due to its thermal stability and electrical properties under extreme conditions compared to those supported by III-V alloys. Advances in molecular beam epitaxy technique has already prove that the use of nitrogen plasmas inductively coupled enable to growth nitride thin films with better crystalline quality than films grown by ammonia or ECR sources, due to a low ions content in the plasma. However, some key issues remain unclear such as if nitrogen incorporation is carried out by atomic nitrogen atoms or by N_2 molecules in the metastable state ($B^3ĐŸ_g$). In this work, we analyze the relative generation of both nitrogen species using optical emission spectroscopy as a function of the excitation power and the molecular flux in a nitrogen plasma. Results are presented in terms of a single parameter μ well related to the energy density per molecule within the volumetric cavity containing the plasma. Nitrogen plasma species were studied for a molecular flux range of 0.25 to 1.5 sccm and the excitation power in the range of 150 to 350 W. The nitrogen dissociation rate increases linearly with the excitation power for all considered N_2 flows. The slope of this linear dependence increases with the nitrogen flow in a range of 0.25 to 0.8 sccm and saturates at a constant value for N_2 flows above 0.9 sccm. On the other hand, a fixed excitation power P_o, the dissociation rate increases with nitrogen flow until a critical flow F_o and becomes decreasing for N_2 flows higher than this critical value. This can be explained considering that as the molecular flux of N_2 increases, the energy density μ per molecule decreases (at constant excitation power), so when μ decreases to the value of 9.756 eV/molecule, the dissociation rate become decreasing due to the only electrons in the plasma that can dissociate N_2 molecules are which has energies in the tail of the electron energy distribution function. On the other hand, the generation of N_2* molecules in the metastable state $B^3ĐŸ_g$ increases both with the excitation power and with the molecular flux because μ remains higher than the energy necessary to excite this metastable state (7.4 eV/molecule).
This work was partially supported by SIP-IPN project No. 20200459

[PLV-328] CuLaO2 and LaCuOS: Fabrication of target by two-step solid-state reaction/sulfurization process and p-type TSO films by PLD technique

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LaCuOS has a potential to be used as *p*-type transparent semiconductor oxides (TSO), due its wide and direct band gap of 3.1 eV and its conductivity. The application of *p*-type TSO films to electrodes in solar cells is very attractive for suppressing the electron-hole recombination at the interfase region between the TSO and the *p*-type layer. There are many techniques for the synthesis of semiconductors materials, in this work we proposed a two-step SSR (solid state reaction)/ sulfurization method to prepare LaCuOS ceramic target. First the synthesis of $CuLaO_2$ by SSR, later the sulfurization of the ternary compound, to finally the manufacture of a LaCuOS target. We prepared $CuLaO_2$ and LaCuOS films on glass substrates by pulsed laser deposition (PLD). The X-ray diffraction analysis shows that polycrystalline structure for the $CuLaO_2$ target, and the Raman spectroscopy indicates the presence of vibrational modes characteristic of the $CuLaO_2$, E_g and A_{1g}. Spectroscopy UV-VIS indicates that the optical transmission of the $CuLaO_2$ films is greater than 50 percent, the E_g values for the films are close to 2.2-2.3 eV. For the LaCuOS, the Raman spectroscopy show the presence of modes vibrational associated of certain phases of sulfur, that indicates the insertion of sulfur into the $CuLaO_2$ target.

The authors acknowledge the technical support of Marcela Guerrero, A. García-Sotelo, and Zacarias Rivera from the Physics Department of the CINVESTAV-IPN. The authors acknowledge partial financial support for this work from CONACyT under Contract No. INFR-2014-01-230183. The authors also acknowledge financial support for this work from Universidad Autónoma de Querétaro through FOPES-UAQ 2019.

[PLV-351] A novel method for the fabrication of wrinkle-like plasma polymer film using dielectric barrier discharge

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In recent years, patterned polymer thin films, have attracted a considerable attention, in particular, in tissue engineering as well as in cell attachment for various biomedical applications. The overall methods for structuring polymer films surfaces can be classified into two main categories: (i) top-down and (ii) bottom-up. In most of cases, both methods require pre- and post-process complicating the overall process [1-3].

In this context, here, we introduce a novel bottom-up approach for the fabrication of a patterned polymer film without needing any post process. Our approach is based on the plasma deposition process using $C_2H_4/CF_4/Ar$ gas mixture in a filamentary and homogeneous dielectric barrier discharge at nearly medium pressure (200 mbar). Optimizing the deposition parameters (i.e. gas mixture, power applied, distance between electrodes) results in the spontaneous formation of a wrinkled surface. The roughness of the pattern is found to evolve from 0.18 to 0.13 µm when increasing the thickness of the plasma polymer film (PPF) from 1.6 to 2.5 µm. A further increase in the thickness of the PPF (i.e. 3.5 µm) leads to an increase in the roughness to a value of 0.17 µm. This behavior is explained through the growth of the wrinkles with the thickness at the PFF at first stage followed by their aggregation at higher PPF thickness giving rise to spherical wrinkles. The whole set of our data unambiguously reveal the attractiveness of the presented method for structuring, at the nanoscale in one step, plasma polymer thin films.

References

[1] P. JuÅ™ík, P. SlepiÄ�ka, M. Nagyová, V. ŠvorÄ�ík, Surf. Coatings Technol. 311 (2017) 344–350.
[2] D. Thiry, N. Vinx, P. Damman, F.J. Aparicio, P.Y. Tessier, D. Moerman, P. Leclère, T. Godfroid, S. Deprez, R. Snyders, Plasma Process. Polym. (2020) 1–6.
[3] M. Li, D. Joung, B. Hughes, S.D. Waldman, J.A. Kozinski, D.K. Hwang, Sci. Rep. 6 (2016) 1–9.

[PLV-429] PHOTOCATALYTIC DEGRADATION OF LIGNIN UNDER VISIBLE ENERGY IRRADIATION USING ZnO-N, CdS-N COMPOUNDS IMPURIFIED BY NITROGEN PLASMA

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N-doping of semiconductors has been carried out using a variety of nitrogen precursors. Doping is considered a promising method to achieve the reduction of the energy bandgap (E_g) interval to shift its absorption spectrum to a lower energy level and also improving the separation of the photogenerated charge. These doped semiconductors, tested as photocatalysts, offer great potential for the degradation of organic pollutants dissolved in water. Typical procedures to induce nitrogen doping are based on chemical methods that use precursors which generate some residues from the synthesis processes, which in many cases are potentially polluting. An interesting alternative to induce doping is through the use of N_2 plasma. The production of plasma from N_2 gas is a novel, simple, and reliable technique. In the present work, a discharge system has been used to produce a nitrogen plasma to achieve the N-doping in ZnO and CdS structures. The synthesis of ZnO and CdS was carried out in a reactor heated by microwave radiation. The structures were used in a photocatalytic process to study the degradation of lignin and methylene blue (MB) molecules. Furthermore, the structural, morphological, and photochemical properties of the samples were determined by X-ray diffraction (XRD), UV-Vis spectroscopy, energy dispersion spectroscopy (EDS), scanning electron microscopy (SEM). In addition, X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy analyzes were achieved. Photocatalytic degradation studies confirm the improved efficiency of nitrogen-doped systems compared to ZnO and CdS. The maximum percentage of MB degradation under UV

energy irradiation using ZnO-N and CdS-N was 100% in 50 min. In the case of lignin, the degradation was 70% in 90 min for ZnO-N. The photocatalytic activity tests under irradiation with Vis energy showed 100% degradation of MB in 60 min and 60% degradation of lignin, in 90 min for ZnO-N. The results discussed here are promising with respect to the methodology to achieve nitrogen doping and also in terms of photocatalytic performance.

Acknowledgment
To W. Cauich for his technical assistance in XPS and SEM analysis. To D. Aguilar for his technical support in XRD analysis. To J. Bante and D. Macías for their technical support in optical spectroscopy measurements. To the LANBIO of CINVESTAV, Mérida unit. P. Quintana thanks the FOMIX-Yucatán projects 2008-108160 CONACYT-LAB-2009-01-123913, 292692, 294643. The SEP-CONACYT-221418 project. To CONACYT, for the scholarship granted in call 291236

RENEWABLE ENERGY: MATERIALS AND DEVICES

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The symposium Renewable Energy: Materials and Devices, has the aim to provide a forum to present and discuss the research relating to the science and technology of energy generation, storage, and managements. An important theme is the research concerning to first generation solar cells, based on mono and poly-crystalline silicon; second generation cells, including CdTe, CIGS, CZTS, amorphous silicon, micro-crystalline and polymorphous silicon; third generation cells, based on the use of quantum dots, nanowires, carbon nanotubes, photo-electrochemical cells, polymer solar cells, nano-crystalline cells, dye-sensitized cells, perovskite solar cells, etc. Moreover, the symposium cover 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-160] CuO coatings on fiber glass mesh for combined CO2 capture and its photocatalytic conversion to solar fuels

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Photocatalytic reduction of CO_2 holds great promises for addressing the environmental and energy issues that are facing in the actuality. The major challenge of CO_2 photoreduction into solar fuels is the main objective of the research community. In this work, the deposition of thick films of CuO by a simple microwave-hydrothermal method on flexible substrates such as glass fibers to produce solar fuels (CH_3OH and HCOH) was studied such a strategy to mitigate the current problems. Three glass fibers with different chemical compositions and open area were selected as supports. The best performance for CO_2 adsorption was 3080 $mg_{COÃƒÂ¢Ã¢Â€ÂšÃ¢Â€Âš}$ g^{-1}, that could be attributed to the homogeneous distribution of CuO 1D architecture particles deposited over-rich in Na_2O and CaO substrates. In a possible mechanism proposed in this work, the CO_2 was adsorbed on the surface of coatings, CuO, exposed to visible LED light to carried out its conversion to HCOH and CH_3OH. According to the results, a higher CuO content in the surface and a higher open area in the glass fibers favored a higher CO_2 photocatalyst reduction to HCOH (382 µmol $g^{-1}h^{-1}$) and CH_3OH (187 µmol $g^{-1}h^{-1}$). The photocatalytic performance of the CuO thick films was also affected by the presence of Na_2O, which played an important role as a hole scavenger, preventing the re-oxidation of the products. The use of glass fibers as support of CuO promoted efficiencies up to 10 times higher than other materials used in these processes.

[RWE-163] FLUODYNAMIC SIMULATION OF A DRAINED BED BIOFILTER TO DETERMINE PERMEABILITY AND HYDRAULIC RETENTION TIME

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Biogas in the development of renewable energies will in the future have a demand of 25% of the bioenergy used worldwide and will be fundamental in the process of decarbonization and in the impulse towards a circular economy. Raw biogas production contains trace contaminants, including hydrogen sulfide (H2S) (1-3% v/v), which according to the World Health Organization, exposure to concentrations of 500 ppm can cause death and is highly corrosive. The biofiltration process is an effective and environmentally friendly technology. Biofilters can be packed with a great variety of organic and inorganic materials, however they have limited use, since they tend to become saturated by the accumulation of the products of the removed contaminant and the biomass. The hydraulic retention time (HRT) is the key parameter to guarantee a successful biofiltration operation. Consequently, it is necessary to understand the precise dynamic fluid mechanisms involved in the removal of H2S, in order to determine the role they play.
In this study, a drained bed filter on an industrial scale was analyzed under computer simulation to determine the operational variables (permeability of the porous medium, hydraulic retention time (HRT)). In order to obtain an effective elimination of the poisonous gas (hydrogen sulfide) that contaminates a whole mass of biogas, which is produced through a set of cattle waste biodigesters, located on the ranch the plows meoquia jimenez chihuahua. This is where a medium-scale biogas production plant is located. For the design of the computational modeling, the real dimensions of the biofilter in operation were used, as well as, the velocities and pressure drops obtained in real time. The results obtained through the computational modeling were highly favorable as a starting point for the development of future larger scale biofilters. It is worth mentioning that the parameters obtained under the computational modeling (permeability and retention time), cannot be parameterized as constants since both depend entirely on the dimensions of the biofilter and the interactions of the microbial consortia, which perform the removal of hydrogen sulfide from the biogas and generate a biofilm which obstructs the passage of biogas, decreasing the permeability and increasing the retention time of biogas in the biofilter. The implementation of these new technologies for the removal of trace contaminants in the production of biogas, will generate a great impact on reducing production costs.

[RWE-175] Synthesis and characterization of perovskite films of CsPbI3, CsPbBrxI3-x for application in solar cells

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With increasing energy consumption and environmental pollution, traditional fossil energy sources cannot meet the sustainable development of human society. Solar power is one of the most promising technologies. A solar cell is a device that converts light energy directly into electrical energy. Because of the high efficiency and low cost, perovskite solar cells have attracted attention from researchers worldwide. In this work, the synthesis and deposition of $CsPbI_3$, $CsPbBr_xI_{3-x}$ perovskites on TiO_2 layer by spin coating is reported. The compact (*c*) and porous (*p*) layer of TiO_2 were deposited on FTO substrates by spin coating, using a precursor solution of TiO_2 by the process of sol-gel using titanium tetraisopropoxide as precursor whit HNO_3 as a catalyst and applying a dispersion of TiO_2 nanoparticles in ethanol on theTiO_2 compact layer; both layers were treated to 450 ° C for 4 h. The perovskite films of $CsPbI_3$ y $CsPbBr_xI_{3-x}$ were also obtained by spin coating, using the one-step synthesis technique, PbI_2, CsI and $PbBr_2$ metal halides used has precursors were dissolved in DMSO at different concentration, under magnetic stirring at 300 rpm, at room conditions of humidity, pressure and temperature, followed by a heat treatment at 200 °C. The layers of TiO_2 and perovskites were characterized by X-ray diffraction, scanning electron microscopy, diffuse reflectance, and colorimetry. In all cases, the films obtained from TiO_2 (*c* and *p* layer) presented anatase phase, and the perovskites presented cubic phase. The chemical stability and the optical band gap value (E_g) of perovskites increase with bromine content, the Eg obtained values were between 1.7 y 2.2 eV.

[RWE-194] EFFECT OF THE SYNTHESIS METHOD ON PHOTOCATALYTIC PROPERTIES OF ZnTiO3 POWDERS

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In recent years, great interest has been focused on the production of H_2 by the photocatalytic water splitting, because it has a high energy capacity and can be obtained from clean and renewable water using solar energy. Many semiconductor oxides such as TiO_2, ZnO, Fe_2O_3, NiO, $SrTiO_3$, $CaTiO_3$, $ZnTiO_3$ and $NiTiO_3$ are used as photocatalysts to split water for hydrogen generation. Among these materials, titanium based ternary oxides ($ATiO_3$) have received significant interest for photocatalytic applications, due to their high stability and durability in the aqueous medium under UV–Vis irradiation. $ZnTiO_3$ is an ilmenite-type mineral based on the ZnO-TiO_2 simple oxides, which has a band gap of 2.88 eV and a high dielectric constant ($\varepsilon \approx 19$). $ZnTiO_3$ is conveniently prepared by solid-state reaction but for this is necessary a high calcination temperature, long processing times.

In this work, $ZnTiO_3$ powders were prepared by molten salts and coprecipitation methods to study their photocatalytic properties. Analysis by X-ray diffraction (XRD) was carried out to study the crystal structure. The morphology was analyzed by scanning electron spectroscopy (SEM). UV-Vis spectroscopy was performed to obtain the absorption spectra and determine the band gap. The relationship between the physicochemical properties and the photocatalytic activity was investigated. It is found that the photocatalytic activity is dependent on the phase of photocatalysts.

Keywords: Water splitting; Molten salt; Coprecipitation

[RWE-195] Biodiesel production using a basic heterogeneous catalyst, characterization and evaluation in diesel engines

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

[1] NikoliÄ‡ BD, Kegl B, MilanoviÄ‡ SM, JovanoviÄ‡ MM, SpasiÄ‡ Å½T. Effect of biodiesel on diesel engine emissions. Therm Sci 2018;22:S1483–98. https://doi.org/10.2298/TSCI18S5483N.

[2] Martínez A, Mijangos GE, Romero-Ibarra IC, Hernández-Altamirano R, Mena-Cervantes VY, Gutiérrez S. A novel green one-pot synthesis of biodiesel from Ricinus communis seeds by basic heterogeneous catalysis. J Clean Prod 2018;196:340–9. https://doi.org/10.1016/j.jclepro.2018.05.241.

[RWE-247] Synthesis and characterization of quaternary metal chalcogenides Ag2ZnSnX4 (X= S, Se) for photovoltaic applications

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The scarce efficiency of $Cu_2ZnSn(S,Se)_4$ (CZTSSe) solar cells has been associated to the band tailing and open circuit-voltage loss due to high densities of Cu_{Zn} and Zn_{Cu} antisites defects. Ag_2ZnSnX_4 (X= S, Se) are promising alternatives to CZTSSe with low Ag_{Zn} antisite defects concentration. In this sense, Ag_2ZnSnX_4 (X= S, Se) thin films were synthesized by spray pyrolysis technique combined with a post thermal annealing. The effect of annealing temperature on the structural, optical and morphological properties was investigated in both systems. The [Ag]/[Zn]+[Sn] and [Zn]/[Sn] molar ratios in the samples were verified by Energy-dispersive X-ray spectroscopy (EDS). Structural phase identification was performed using X-ray diffraction (XRD) and Raman spectroscopy. Scanning electronic microscopy (SEM) and Ultraviolet-Visible spectroscopy were used to know the morphology and absorption edge of the materials, respectively. X-ray photoelectron spectroscopy (XPS) was used to study the core levels of the constituent elements and surface contaminants. Firstly, stoichiometric Ag_2ZnSnS_4 (AZTS) thin films were obtained when the sulfurization process was carried out at 400 °C. Above of this temperature, the crystal-phases of samples are a mix of stannite Ag_2ZnSnS_4 and orthorhombic Ag_8SnS_6. Two bandgaps were found in the annealed samples at 1.3 eV and 2 eV attributed to Ag_8SnS_6 and Ag_2ZnSnS_4, respectively. On the other hand, $Ag_2ZnSnSe_4$ (AZTSe) thin films showed a tetragonal crystalline structure after the selenization process at 450 °C and 500 °C. The bandgap of this material was found to be 1.34 eV. Moreover, a substantial increment in the crystal (70 nm) and grain (2µm) sizes was observed with the increase of temperature. In this case, a little amount of elemental selenium at the surface was detected by XPS. Finally, in both systems the films were constituted by Ag^+ and Sn^{4+}, which were analyzed by XPS and corroborated by the Auger parameter. AZTSe material exhibited the best properties to be incorporated in a solar cell.

[RWE-277] SnO2/Graphene TCO as an electrode for CdSe Quantum Dot Solar Cells.

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TCO's were fabricated using tin dioxide and graphene (SnO_2/G) and applied as transparent electrodes on CdSe quantum dot solar cells (QDSC). The devices were compared to reference cells fabricated with fluorine doped tin dioxide (FTO). Short circuit current values were obtained around $3.76x10^{-03}$ A/cm^2 and open circuit voltage measured about 0.486 V for the best performing device, compared to reference values ($5.49x10^{-03}$ A/cm^2 and 0.544 V). Efficiency values for the SnO_2/G cells (0.53 %) and FTO cells (1.60 %) showed that the determining factor for the superior efficiency with FTO was due to the FF, 29.00 (SnO_2/G) and 53.86 (FTO).

[RWE-320] Morphological effect of VLS grown ZnO nanowires on photocatalytic water splitting performance

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In the present work, ZnO nanowires were grown using the Vapor-Liquid-Solid technique on gold coated AZO seed layers. Multiple variations in the growth parameters were explored to obtain 1D nanostructures with different aspect ratio and surface area. Afterwards, the effect of the morphological properties over the photocatalytic hydrogen production performance of the system was evaluated. The obtained ZnO nanowires were structurally and morphologically studied by X-ray diffraction (XRD) and Scanning electron microscopy (SEM), showing a diameter ranging from 57 to 85 nm and a principal crystal orientation along plane (002). The compositional profile of the nanostructures was determined both by Scanning transmission electron microscopy and EDS measurements, corroborating the presence of a gold nanoparticle on the tip of the ZnO structure. The optical characterizations (UV-Vis and PL measurements) showed the effect of structural and morphological properties on the absorption and emission spectra of the synthetized nanostructures, particularly in the visible region. Finally, the photocatalytic water splitting performance of was evaluated using a 300 W Xe lamp. Random orientated nanowires with higher surface area and optimal diameter distribution exhibited the highest photocatalytic activity.

[RWE-339] On the development limitations introduced by poor characterization often reported on solar cells research

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In the work "Characterization of dual-junction III-V on Si tandem solar cells with 23.7% efficiency under low concentration" (E. Veinberg-Vidal, L. Vauche, K. Medjoubi, C. Weick, C. Besançon, P. Garcia-Linares, A. Datas, A. Kaminski-Cachopo, P. Voarino, P. Mur, J. Decobert and C. Dupré, Prog. Photovolt. Res. Appl. 2019;27:652–661), monolithic 1 cm^2 two-terminal III-V on Si dual-junction solar cells were designed and fabricated with the III-V top cell a p-n heterojunction by an n-Ga0.5In0.5P and a p-Al0.2Ga0.8As layers. The two terminal solar cell displays efficiencies of 21.1 ± 1.5% at one sun and 23.7 ± 1.7% at 10 suns. Realizing such cell structure requires intensive and high quality and sophisticated clean room work, as well as a world class technical facilities and know how. The authors conclude that the obtained efficiency is limited by the bottom cell high surface and bulk recombination, without having done any proper measurements nor a full theoretical analysis of its behavior, not even an IV full curve at dark and under illumination is given. The authors provide just the cell's Jsc, Voc, fill factor and efficiecies at four different suns concentrations.
In this work it is shown that with the reported data: Jsc, Voc, and fill factor and utilizing the simplest theoretical PN junction models, much more physical information about this solar cell can be obtained. Our results demonstrate, for instance, that paramters as its main charge transport mechanism, series resistance, saturation current and ideality factor, among others, can be straightforward obtained. Such parameters constitute valuable feedback information to reshape the cell design and laboratory processes. The detailed procedure of the way to obtain such information will be clearly exposed in this work. Finally, our results also demonstrate that just measuring and reporting cells efficiency is not enough and more careful theoretical and experimental characterization should be done if better performance cells are to be produced.

[RWE-344] Electrochemical deposition and thermoelectric characterisation of a semiconducting 2-D metal-organic framework thin film

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In recent years, there has been special interest in developing devices capable to harvest and store energy from natural resources without the generation of pollution. Thermoelectric generator (TEG) is an emergent technology to harvest energy, especially in those environments in which heat waste is involved. These solid-state devices are capable of generating an output voltage as a function of a temperature difference. The conversion of thermal energy into electrical energy in these devices is attributed to the Seebeck effect. The efficiency of a TEG is evaluated through the dimensionless figure of merit, Z. In order to achieve a competitive the figure of merit, a material with a high Seebeck coefficient, electrical conductivity and low thermal conductivity is desirable.

Conductive metal organic frameworks (c-MOFs) are hybrid materials composed of inorganic and organic building blocks, in which metal nodes are coordinated to highly conjugated organic linkers.[1,2] The overlap between the metal and ligand frontier orbitals facilitates the charge transport in these materials. Porosity and heterogeneity in atomic species and linkers are features that have led to a predictably low thermal conductivity[3], a key aspect to optimize Z, making MOFs potential candidates for TEG. To implement their practical use, the synthesis and study of ultrathin c-MOFs nanosheets have recently been reported[4]; however, the processing at large scale of these materials is still a challenge.

In this work we present an electrochemical approach to the growth of conducting thin films of the 2D c-MOF $Cu_3(HHTP)_2$ (where HHTP = 2,3,6,7,10,11-hexahydroxytriphenylene). Bulk $Cu_3(HHTP)_2$ was synthesized solvothermally according to the literature[5] and we have subsequently fabricated thin films of this important framework by anodic electrochemical synthesis.[6] We report the first thermoelectric measurements of this framework both in bulk and thin film form which resulted in Seebeck coefficients of -7.24 $\mu V\ K^{-1}$ and -121.4 $\mu V\ K^{-1}$ with a power factor of $3.15x10^{-3}\ \mu W\ m^{-1}$ for the film respectively. The study of conducting MOFs and their performance as TEG is expected to expand and offer alternatives to non-toxic, scalable and high-efficiency novel TEG materials.

References

[1] P. Q. Liao, J. Q. Shen, J. P. Zhang, *Coord. Chem. Rev.* **373**, 22, 2018
[2] L. Sun, M. G. Campbell, M. DincÄƒ, *Angew. Chem. Int.* **55**, 3566, 2016
[3] Huang , A. McGaughey , M. Kaviany , Int. J. Heat Mass Transf. 50, 393, 2007
[4] W. Zhaoa, et al., *Coord. Chem. Rev.* **377**, 44, 2018
[5] M. Hmadeh, et al., *Chem. Mater.* **24**, 3511, 2012
[6] Ameloot, R. et al., *Chem. Mater*. **21**, 2580–2582, 2009

[RWE-379] Sodium Zincsilicate: A novel and efficient catalyst for biodiesel production from soybean oil.

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In this work, a ceramic material called "Sodium Zincsilicate" was developed with chemical formula Na_2ZnSiO_4, proposed as a new heterogeneous catalyst for the transesterification reaction of soybean oil to overcome the limitations of the alkaline silicate family of catalysts (hygroscopicity, lixiviation, etc.).
Sodium zincsilicate was characterized by X-ray diffraction techniques, volumetric nitrogen adsorption, scanning electron microscopy, energy dispersion x-ray spectroscopy, and isopropanol catalytic decomposition. The catalytic process was optimized through a Box-Behnken experimental design while keeping the temperature constant at 65ºC, varying the rate of agitation, the load of the catalyst relative to the oil, the molar ratio between methanol and soybean oil, and an evaluation of the reaction time, obtaining as optimal conditions 500rmp, 5.3%wt, 14:1 respectively at 45 minutes of reaction, obtaining a conversion rate greater than 99%. These conditions were repeated 10 times consecutively to evaluate the reusability of the catalyst.
The products obtained from the transesterification reaction were characterized through Fourier transformed infrared spectroscopy, proton nuclear magnetic resonance, and mass spectroscopy coupled to electrospray ionization, obtaining impurity-free biodiesel in the first three reaction cycles.

[RWE-394] Spray pyrolyzed p-CuCrO2/n-ZnO heterojunctions

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Thin films of $CuCrO_2$ and ZnO were deposited using the ultrasonic spray pyrolysis technique, the obtained results for $CuCrO_2$ show a delafossite structure with an energy bandgap of 2.96 eV, a *p*-type material with a resistivity of 1.42 x 10^{-1} â„¦ cm; the ZnO results show a typical wurtzite structure with an energy bandgap of 3.16 eV, an *n*-type material with a resistivity of 2.66 x 10^{2} â„¦ cm, these results are suitable to build a *p-n* diode. Three different *p-n* diodes were successfully elaborated by ultrasonic spray pyrolysis, varying the thickness of the ZnO and then, the obtained diodes were characterized by J-V measurements and impedance spectroscopy. The J-V measurements applied to the three diodes presents rectification, and by increasing the ZnO thickness, the rectification ratio seem to increase linearly until it reaches 7. The results obtained open up the possibility of diversifying their uses, by varying the deposition parameters, as solar cells or as part of technology for rectification processes.

[RWE-438] Unraveling amazing structural features of a highly efficient oxo-Co/phosphate catalyst for water oxidation

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The oxo-Co/phosphate based material (CoPi) developed by Kanan and Nocera in 2008 is among the most outstanding catalysts for water oxidation at neutral pH. The remarkable performance and striking properties of CoPi reside on its intriguing and unique structure. In the present contribution, TEM, SAED, UV-vis-NIR absorption and Raman spectroscopy were performed at 77 K, complemented by room temperature experiments, to unprecedentedly reveal that CoPi is composed by short-range ordered β-$NaCoPO_4$ (a solid ionic conductor) and expanded-lattice Co_3O_4 clusters with electronic structures, vibrational responses and catalytic properties quite deviated from those of their bulk counterparts. Internal morphological features of CoPi are also disclosed. Consequently, some aspects of the previously proposed structure and operating mechanisms are revised. This study derived in a deposition route which yields CoPi layers that outperforms, as water oxidation catalyst, the traditionally electrodeposited CoPi.

[RWE-445] Atomic scale model and electronic structure of Cu2O/CH3NH3PbI3 interfaces in perovskite solar cells

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Cu_2O has been proposed as hole transport layer in perovskite solar cells. Using density functional theory, we study the interfaces of $CH_3NH_3PbI_3$ with Cu_2O to assess their influence on device performance. Several atomic scale models of these interfaces are presented, considering different compositions of the interface atomic planes. The interface electronic properties are discussed on the basis of the optimal theoretical situation, in connection with the experimental realizations and device simulations. It is shown that the formation of vacancies in the Cu_2O terminating planes is essential to eliminate dangling bonds and trap states. The four interface models that fulfill this condition present a band alignment favorable for photovoltaic conversion. Energy of adhesion, and charge transfer across the interfaces are also studied. The termination of $CH_3NH_3PbI_3$ in PbI_2 atomic planes seems optimal to maximize the photoconversion efficiency.

[RWE-159] SYNTHESIS OF 1D ARCHITECTURES OF COPPER OXIDES TO PRODUCE RENEWABLE FUELS OF ZERO AND LOW CARBON CONTENT THROUGH THE PHOTOCATALYTIC DECOMPOSITION OF H2O AND THE PHOTOCATALYTIC REDUCTION OF CO2

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Due to the energy crisis and serious environmental concerns, there are alternative sources of energy being developed to replace fossil fuels. CO_2 capture photocatalytic conversion (CCPC) is one of the promising routes that could mitigate the CO_2 increasing concentration on the atmosphere and solve the energy crisis. The CCPC can be implemented via the direct CO_2 adsorption and photocatalytic reduction, to convert it into solar fuels such as CH_3OH, HCOH, CO/H_2, etc. 1D nanostructured copper oxides have attracted attention recently due to their potential use in several applications such as water splitting reaction and CO_2 photocatalytic reduction. These architectures can be obtained from simple and easily scalable methods such as thermal oxidation (OT) of metals such as copper, which is a cheap and an earth-abundant metal. Cu_2O-CuO 1D architectures were prepared in situ on copper mesh by thermal oxidation at 100-600 °C in air. Cu mesh, a 3D metallic skeleton, was selected as a substrate due to good light diffusion. Easy application and higher effective surface area in comparison with the Cu foil. For this reason, in this work is evaluated the thermal growth, shape, distribution of 1D architecture effect, and 1D nanoneedles obtained by thermal oxidation of a copper mesh, at 500 °C for 3 h in an atmosphere of air. Subsequently, the different CuO aquatinters were decorated with were synthesized on three different substrates with different physicochemical properties. According to the SEM/EDS analyzes, it was possible to identify a homogeneous growth of the 1D CuO nanoneedles on the copper mesh and good simple oxides dispersion, which favored a CO_2 photocatalytic reduction, whose best result to produce liquid phase CH_3OH was 0.3 µmol g^{-1} h^{-1}, HCOH was 7.1 µmol g^{-1} h^{-1}, and H_2 was 38 µmol g^{-1} h^{-1}. These efficiencies were up to 1.5 times greater than when using other materials as liquid phase photocatalysts, which was ascribed to the many advantages of the use of double-function materials in the CCPC process such as CO_2 affinity, rapid electron transport, a reduction of the shielding effect, as well as a homogeneous exposure of the materials.

[RWE-172] MODIFICATION OF PROPERTIES OF Sb2S3 BY THE FORMATION OF STRUCTURAL DEFFECTS DURING SOLVOTHERMAL SYNTHESIS

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In recent years, investigations on metal sulfides of group 15 elements of the type, Sb_2S_3 have been the subject of great interest due to their optical and electrical properties [1,2]. Antimony trisulfide (Sb_2S_3) with needle-bundles morphology were successfully synthesized by the solvothermal route using potassium antimony tartrate, $C_8H_{10}K_2O_{15}Sb_2$ as antimony precursor, and carbon disulfide as sulfur precursor with ethylene glycol as the solvent. The crystal structure corresponds to orthorhombic unit cell (Stibnite) and no secondary phases were observed. The introduction of structural defects caused by the intergrowth has been evidenced by Raman spectroscopy. The optical bandgap Eg, of 1.415, was determined by diffuse reflectance using UV-Vis spectroscopy. Finally needle-bundles were coated into thin films by mixing different amounts of Sb_2S_3/ PVDF (inorganic / organic composite) and its electric conductivity was measured by EIS or impedance spectroscopy.

[1] Lakade, S. D. (2020). *Purakala with ISSN 0971-2143 is an UGC CARE Journal*, *31*(25), 69-85.

[2] Radzwan, A., Ahmed, R., Shaari, A., & Lawal, A. (2019). *Physica B: Condensed Matter*, *557*, 17-22

[RWE-182] Study on the hydrophilic properties of Molybdenum- Oxide nanowires arrays obtained by thermal treatment and reactive ion etching

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This investigation is focused on the synthesis of Molybdenum oxide nanowires array by two different methods in order to find the relationship between the contact angles of water droplets on and the resulting morphology in the surface of samples. In order to synthesize the array, Molybdenum substrates (Mo, 99.99 %) were commercially obtained and mechanically polished till produce a mirror-like surface, then were ultrasonically cleaned in deionized water (18 MΩ) for 5 minutes, afterward in ethanol bath for 3 minutes and finally in acetone for 3 minutes, then the substrates were dry with Argon flux to avoid oxidation. Once the Mo substrates were cleaned, two different synthesis techniques were used. The first technique consists by a thermal treatment in which the substrate was oxidized into a furnace with a 20 wt. % oxygen atmosphere at 500 °C, 600 °C and 700 °C. Each experiment was performed for 1, 3 and 5 hours in order to determine the relationship between oxidation time exposure and the obtained structure morphology. The second technique was Reactive-Ion Etching, in which the Molybdenum was exposed 10, 20, 30, 40 and 50 minutes. The Scanning Electron Microscopy images confirmed the achievement of nanowires array, with an average diameter of 10 nm. Energy Dispersive X Ray Spectroscopy showed the presence of Mo and O as the unique elements in the sample, this is in good agreement with X-Ray diffraction results, which showed Mo-oxide as the main phase in the obtained samples. Images of a water droplet (5 µL) on the synthesized arrays were obtained by CCD camera and the analysis confirms that hydrophilic properties are enhanced when both temperature and time get rise, these properties are directly linked to the nanostructured morphology.

Keywords: Nanowires array, thermal treatment, Mo-Oxide, contact angle, RIE.

[RWE-183] Microwave-assisted synthesis of BiVO4 microstructures for hydrogen evolution reaction in the artificial photosyntehsis process

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$BiVO_4$ has been studied in recent years due its photocatalyst properties to the visible-light region for pollutant decomposing and relatively strong oxidation properties for water splitting. Those properties rely on phase composition, particle size and are strongly influenced by the synthesis method and crystal structure. Different methodologies have been used to synthesize monoclinic $BiVO_4$, such as hydrothermal, co-precipitation, flame spay, ultrasonic-assisted and microwave-assisted method.
In this work, $BiVO_4$ powder was synthesized by microwave-assisted method and thermal treatment as contribution to increase crystallinity and thus, enhance photocatalytic properties. In order to synthetized $BiVO_4$ powders, two solutions were prepared; Solution 1 (0.25M): NH_4VO_3 dissolved in deionized water, Solution 2 (0.25M): Bi $(NO_3)_3{\cdot}5H_2O$ dissolved in 4 M HNO_3. Both solutions were mixed in a ratio 1:1 and pH was adjusted to 7. $BiVO_4$ was synthesized by microwave-assisted hydrothermal. The obtained solution is then dried to obtained Bismuth Vanadate powders. Then, the powders are oxidized in 20% Oxygen atmosphere.
X ray diffraction shows $BiVO_4$ as main phase and Raman Spectroscopy confirms thermal treatment enhance crystallinity and scanning electron microscopy proves the obtention of no regular particles in micrometer range.
Keywords: $BiVO_4$, nanowire array, microwaved-assisted synthesis

[RWE-184] Electrochemical reactor to remove Cr (III) from real effluents

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The effluents from the tanning industry are characterized to present Cr(III) and Cr(VI), although this latter is 500 more toxic than the trivalent form, causing that a lower number of treatment methods have been developed to remove Cr(III). 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.

This study aims to tackle these issues by using a electrochemical reactor employing a steel anode. For this particular case, the reactor is made up of an inner cylinder as anode with large area that enhances the turbulence to facilitate the mass transference between reacting species, and multiple cathodes of DSA (dimensionally stable anode) concentrically attached to the reactor walls. This condition produces a uniform concentration profile within the reactor enhancing the efficiency of the reactions of interest of diverse applications. The present analysis also considers to evaluate the effects of different current densities upon the Cr(III) removal of a real tannery discharge containing 2600 mg/L. Residence times shorter than 2 h are regarded to guarantee the viability of its application at larger scales. A synthetic solution is initially assumed to determine the optimal conditions in the reactor, which are subsequently applied in the real effluent. Structural and morphological characterizations of the precipitates are carried out using Scanning Electron Microscopy (SEM) and X-ray Diffraction (XRD), respectively, to establish a possible electro-precipitation for the system. To our current standpoint, a process with similar characteristics has not been described, whereby it is expected that its easy implementation enables its scale-up to sustainably treat real Cr (III) effluents.

[RWE-200] Surface electric field modulation and effect in GaAs-based photovoltaic devices grown by molecular beam epitaxy

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GaAs has a notorious importance in the research of thin-film technology of photovoltaic systems by their bandgap energy which is close to the theoretically predicted 33.5% Shockley–Queisser efficiency limit for single junction solar cells. Moreover, this limit can be overcome with the addition in GaAs-based devices of low dimensional systems such as quantum well or quantum dots and with the development of the intermediate-band concept [1]. Nonetheless, one of the most important problems to rise the efficiency of GaAs-based solar cells is the nonideally of the surface, which becomes more important when thin-films reach nanoscale. In this work, the authors grew two set of GaAs-based samples by molecular beam epitaxy (MBE): (a) simple p-n junction device and (b) multilayered system where the FSF and BSF (Front Surface Field and Base Surface Field) layers where inserted and designed with the aim to reduce the effect of the SRH recombination. We found that (b) samples improved five times the efficiency contrasted with the (a) structure. The surface charge density was modulated by ex-situ sulfur treatments at room temperature which were performed on both samples to determine the impact of the surface in the measured efficiency of each photovoltaic structure design. First, the effect of the sulfur passivation process was studied by the behavior of the L- and LO vibrational modes measured by Raman spectroscopy, where changes in the LO/L- ratio was found in both samples, indicating that the surface charge density has been modified by the chemical treatment. The built-in electric field along the structures was studied through the Franz-Keldysh oscillation (FKO) behavior of the photoreflectance spectrum. The FKO for sample (a) was strongly modified with the passivation process, being their period reduced. On the other hand, FKO in samples (b) are slightly modified with the sulfur treatment, indicating that the FSF layer has a good performance avoiding the surface recombination since the FKO phenomena is very sensitive to this process. The electrical performance of the as-grown and passivated samples was analyzed under AM1.5 solar cell simulator where an increase of the short-circuit current was observed in conjunction with an increase in the absorption of blue wavelengths for treated samples. According to the results obtained we found a strategy to improve the efficiency of solar cells by controlling the effect of surface by both the passivation procedure and the insertion of the FSF layer. Additionally, we noticed that the FKO behavior can be employed to evaluate the performance of the FSF layer. Our experimental results have been supported by numerical analysis.

[1] DOI: 10.1002/adma.200902388

Acknowledgments: The authors acknowledge the financial support from FRC-UASLP, C19-FAI-05-18.18 and CONACYT-Mexico through grants: INFR-2015-01-255489, CB 2015-257358, PNCPN2014-01-248071 and the Catedras CONACyT (Project No. 44).

[RWE-213] Heterojunctions in base compound films ZnO-M (M = Ge, Ag, Al) through chemical and physical use deposit techniques and their application in photocatalytic and photoelectrochemical processes.

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Currently, multiple research efforts are focused on increasing the efficiency of the conversion energy solar into electrical energy through photovoltaic technologies and photoelectrochemical systems (PEC). The water splitting molecule into H_2 and O_2 in a PEC system is a highly promising technology to provide sustainable solutions in the area of clean energy generation. The doped development systems based on inorganic semiconductors is of great interest for this application because it makes it possible to take advantage of the different physicochemical properties of the materials, which play a fundamental role in the decomposition reaction of water. Considering the optical and electronic properties of semiconductors, there is design possibility and developing doped materials with different combinations to modulate and improve their performance as photo anodes.

In this work, the development of ZnO-M base compounds (M = Ge, Ag, Al) doped with different metals will be presented, with the aim of improving the efficiency materials compared to simple oxide systems. For this, physical and chemical deposition techniques will be used, which will allow the formation of semiconductor films that can be used as active photocatalytic materials and photoelectrochemical systems. The materials used were selected based on their abundance, economy, easy handling and non-toxicity, and they also have adequate potential for water oxidation. The characterization results show that all the films obtained are polycrystalline, with Eg values close to 3.3 eV, and of an n-type semiconductor nature. Furthermore, when efficiency photoelectrochemical tests, it was found that the presence of silver (Ag) increases the charge transport in the material, decreases its resistivity and increases its stability. In the photoelectrochemical tests, it was determined that the materials have a high photoconversion efficiency, close to 60 percent for the studied silver doped zinc oxide system. This result is due to the fact that the material has a higher volume of charges when irradiated that is, it has a greater number of electrons that go from the valence band to the conduction band at the same intensity of the incident radiation. The tests H_2 production by photocatalysis showed this system, that when the doping with silver increases, the hydrogen production increases linearly, with the 5% doped film being the one with the highest H_2 production.

[RWE-222] Synthesis of Na3V2(PO4)3/C and Na3V1.9Fe0.1(PO4)3/C by solvothermal method assisted with MOF and its electrochemical properties in sodium ion batteries

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Lithium ion batteries (LIBs) have been used for a variety of electronic devices due to their capacity and good efficiency. However, lithium is not readily available in the earth's crust, limiting its application to demand for energy storage. On the other hand, sodium ion batteries (SIBs) have generated great attention by research groups as it exhibits a working principle similar to lithium ion batteries, having great potential for energy storage and conversion.

Among the various electrodes, NASICON-type $Na_3V_2(PO_4)_3$ (NVP/C) has been widely studied as an advanced cathode material for sodium-ion batteries because of its good thermal stability and impressive energy density. It has a highly covalent three dimensional framework (3D), which can facilitate fast ionic diï¬€usion. Also, a lot of research has been performed reagarding applicability of metal organic frameworks (MOFs) in SIBs because of their high specific surface area and ultra-high porosity. MOFs are considered as promising precursors for deriving cathode materials with excellent electrochemical property. There is a challenge to depeloved a materials whit this characteristic and the substitution of vanadium by iron due of the performance in SIBs.

In the present work we report the solvothermal synthesis of two cathodes for sodium batteries, $Na_3V_2(PO_4)_3$/C and $Na_3V_{1.9}Fe_{0.1}(PO_4)_3$/C using as raw materials VCl_3, terephthalic acid, Na_2CO_3, $NH_4H_2PO_4$ and $FeCl_3$ with reaction temperature about 80 °C for 8 h. X-ray diffraction results showed the presence of the cathodes with NASICON related rhombohedral structure (space group *R3c*) with out impurity phases and preferential orientation of the planes (012), (104) and (113). The unit cell volumes lightly increases when Fe^{3+} partially replaces V^{3+} as expected from the ionic radii reported for these elements, V3+. SEM images of both materials, show an amorphus carbon layer with slight agglomeration and crystal growth was observed in three dimension (3D). Which is critical for long-term structural stability of the electrode material during cycling.The Raman spectrum for both cathodes are the characteristic two conspicuous peaks of D-band (the disorder-induced phonon mode) and G-band (the crystalline graphite band), wich suggest the existence of carbon in the sample. Galvanostatic test for Na batteries of both cathode materials are currently under progress into coin cells.

[RWE-271] Synthesis and characterization of materials for the elaboration of a solar cell sensitized with protoporphyrin IX

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In this research we have synthesized and characterized materials for the fabrication of a sensitized solar cell using the dye protoporphyrin IX. Nanoparticles of titanium dioxide, graphite oxide, reduced graphene oxide and the composite titanium dioxide-protoporphyrin IX were synthesized. Titanium dioxide nanoparticles used for the photoelectrode were synthesized by Sol-Gel technique, these nanoparticles were mixed with the dye protoporphyrin IX in order to increase the light absorption. For the counterelectrode we used reduced graphene oxide, which was obtained by two steps: 1) synthesizing graphite-based graphene oxide by the modified Hummers technique and 2) reducing graphite oxide by a sonication method. The materials were characterized by X-ray diffraction, scanning and transmission electron microscopy, Raman and infrared spectroscopy, UV-Visible spectroscopy, dynamic light scattering and electrical techniques. Titanium dioxide nanoparticles showed a representative diameter of 10 nm and 9 nm of cristallyte size. We have found evidence of molecular interactions between titanium showed by some shiftings in the wavenumbers of some bands in Raman spectroscopy, we confirmed this information by uv-visible and infrared spectroscopy. The graphene oxide obtained in the process for synthesizing reduced graphene oxide had a great amount of functional groups, evidenced by infrared spectroscopy. The reduced graphene oxide had a square resistance of 1.69 Ω. In the electrical characterization, the photosensitive behavior was observed as well as an increase in the conversion efficiency, from 0.09% for TiO2 to 5.6% for the TiO2+PIX compound.

[RWE-275] Supported in RGO, catalyst with High Activity and Stability of NiCu@Pt

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The catalyst of octahedral shaped NiCu cores were prepared through chemical reduction by method a modified polyol process with the right amount of oleylamine, oleic acid and precursor salts of non-noble metals, Cu(acac)2 and Ni(acac)2, using morpholine borane as reducing agent, while the shell of Pt was deposited by galvanic displacement on the Ni-Cu nanoparticles. The presence of alloy Ni-Cu in the core and Pt in the shell

To measure the catalytic activity and stability of the alloy catalyst (electrodes containing Pt loading of 0.02 mg/cm2, 20 wt.% Pt/C, E-TEK), the polarization curves were obtained. The alloy catalyst showed higher catalitic activities and stability than Pt/C. It can be concluded that in platinum formed alloy with transition metals, the electronic state of Pt and the nearest neighbor Pt–Pt distance changes, which significantly influence the electrocatalytic activity for oxygen reduction.

The aforementioned catalyst was shown to possess improved resistance to electrochemical surface area (ECSA) loss during accelerated aging tests relative to commercially available pure Pt electrocatalysts

[RWE-292] A NEW PASSIVATION SCHEME FOR THE PERFORMANCE ENHANCEMENT OF BLACK SILICON SOLAR CELLS

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It is well known that, in crystalline silicon solar cells, to reduce the front reflection and to improve light trapping, the top surface of the solar cell is modified by different treatments and annealing. The last are very important and have a great technological relevance in the final efficiency of the devices. Black silicon solar cells are the terminology commonly used for naming the crystalline silicon solar cells with complex grades of surfaces texturization schemes. Metal-assisted chemical etching (MACE) method is one of them, which form nanopillar, porous silicon and different pyramidical structures on the substrate surface. These structures have low surface reflectance and appear dark (black) and therefore referred to as 'black silicon'. On the other hand, the increase in the surface area, intensifies the recombination velocity and respectively increases the saturation current density "J_0". For that reason, it is very important to implement different passivation surface schemes. Surface plasma annealing combined with different thin films as antireflection coatings are some alternatives to this.

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

[RWE-373] Obtaining resin based on unicel waste

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Expanded polystyrene (EPS), commonly known in Mexico as unicel, is a foamed plastic material obtained from polystyrene, is employed in the construction and packaging sector. It is characterized by its lightness, resistance to moisture and above all hygiene, but being one of the least environmentally friendly materials to take up to 500 years to degrade, currently looking for alternatives for recycling.

In the present work an alternative to its recycling is proposed from the manufacture of a resin based on unicel, whose production consists in the dilution of unicel residue, previously collected and washed, to dilute in an organic solvent (ethyl acetate). Different concentrations was tested until obtaining the most suitable one based on a liquid silicone consistency, in a proportion of 3:6 g/ml, after this it was allowed to dry for approximately 5 days. The material obtained was studied by scanning electron microscopy (SEM) to obtain information on the morphology and size of the samples prepared, an X-ray dispersive energy spectroscopy (EDS) analysis was performed to obtain information on the chemical composition of the samples prepared. In addition, hardness tests were carried out to measure some mechanical properties of the different samples obtained.

[RWE-375] Application of CeO2:Gd buffer layer to a Sb2(S,Se)3 solar cell

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In recent years, the development of emerging materials applied to solar cells has been promoted [1, 2]. Materials such as perovskites and kesterites are the most promising at this moment, [3, 4] because they have reached conversion efficiency values (h) of 12.6 and 23 %, respectively. Among the emerging materials of the last decade we can find cerium oxide doped with gadolinium (CeO_2:Gd). In this work, the application of CeO_2:Gd thin films for application as a buffer layer in the CdS/$Sb_2(S,Se)_3$ solar cell is proposed. The spin coating technique was used for the elaboration of a CeO_2:Gd thin film and chemical bath deposition(CBD) technique for CdS and ($Sb_2(S,Se)_3$) thin films. The effect of the variation of the Gd concentration on the optical and electrical properties of CeO_2:Gd thin film and the influence in the performance of CdS/$Sb_2(S,Se)_3$ solar cells. An increase in open circuit voltage values (V_{OC}) was observed from 110 to 228 mV and the conversion efficiency (h) values increased from 0.06 to 0.19 % by incorporating the CeO_2:Gd thin film. I-V curves were analyzed following Hedegus et. al, to determinate the series resistance (R), shunt conductance (G), ideality factor (A) and diode current saturation (J_0). [5]

References

[1] L. H. Wong, A. Zakutayev, J. D. Major, X. Hao, A. Walsh, T. K. Todorov and E. Saucedo, J. Phys.: Energy1 (2019) 032001.
[2] M A Green, Y Hishikawa, E D Dunlop, D H Levi, J Hohl-Ebinger, M Yoshita and A W Y Ho-Baillie, Prog. Photovoltaics Res. Appl. (2019) **27**3.
[3] EH Jung, NJ Jeon, EY Park, et al; Nature (2019) **567 (7749), 511-515**
[4] W Wang, MT Winkler, O Gunawan, et al. Adv Energy Mater. (2013) https://doi.org/10.1002/aenm.201301465
[5] S. S. Hegedus and W. N. Shafarman, Prog. Photovolt: Res. Appl. (2004) **12**, 155–17

[RWE-422] Synthesis and characterization of gadolinium doped cerium oxide thin films for applications in solid oxide fuel cells.

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Cerium dioxide is one of the materials of great interest for application in solid oxide fuel cells and catalysis. In this sense, homogeneous thin films with controlled amount of vacancies are required. In this work, gadolinium doped cerium oxide thin films were prepared by the Ultrasonic Spray Pyrolysis technique, which is an economical and industry scalable technique. The influence of deposition conditions (air flows, substrate temperature and Gd concentration) on the morphology, optical and electrical properties of the films was evaluated. Films were prepared at gadolinium concentrations of 10, 15 and 20%, at substrate temperatures of 425, 450 and 475ºC and at 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. The films obtained were characterized by X-ray diffraction, UV-vis spectroscopy, scanning electron microscopy, and impedance spectroscopy. Variations in temperature and air flows modify the morphology, grain size and texture of the films. Increasing the temperature of the substrate produces an increase in the band gap of materials, but does not substantially modify the activation energy, except for samples grown at 10% Gd. The activation energy for ion conduction increases considerably when using low flows (0.5 and 1.0 L/min for the carrier and director gases respectively). Based on the obtained results, it is proposed that the ideal conditions for obtaining homogeneous and fracture-free films with low conductivity activation energies are medium flows and substrate temperatures of 450°C.

This work was supported by IPN under project 20201523 and SECTEI under project 289/2019.

[RWE-423] Nanostructured cerium oxide thin film for electrochemical applications

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Hydrogen is considered an important energy vector, that is, it is capable of storing or transporting energy. However, the energy efficiency of hydrogen production using water is still modest, which makes it necessary to develop electrocatalysts and photocatalysts with better performances. In this work, nanostructured cerium oxide thin films were prepared on FTO substrates, stainless steel and titanium, by means of ultrasonic pyrolytic spray, using cerium acetylacetonate as a metallo-organic precursor dissolved in anhydrous methanol. The temperature of the heating plate was set at 475 C, the deposition time was 30 min, the carrier and director gas flows, air in both cases, were set at 1.0 L / min and 1.5 L / min respectively. The morphological, structural, optical and vibrational properties were studied by means of scanning electron microscopy, X-ray diffraction (XRD), Raman spectroscopy and UV-Vis. Homogeneous thin films with fluorite structure of ceria of ceria are obtained in all cases. The calculated band gap was 3.2 eV. In electrochemical measurements, reduction processes are observed in potentials close to -0.5 V, -0.7 V and -1 V. In chronoamperometry a stationary current associated with the reduction of water is observed at a value of -1.7.

Acknowledgment:

I.Zumeta Dubé greatly acknowledge support and facilities from Laboratorio Nacional de Conversión y Almacenamiento de Energía (LNCAE). This work was supported by IPN under project 20201523 and SECTEI under project 289/2019 CDMX México.

SIMPOSIO DE 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-170] Control y automatización de un sistema para la fabricación de dispositivos electrónicos de película-delgada orientado a la industria 4.0

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En una época inmersa en la tecnología, la eficiencia de los sistemas productivos industriales parte del uso de asistentes inteligentes (mecánicos, virtuales y de simulación) que son una extensión de lo que uno o varios operadores tendrían que hacer manualmente, reduciendo los riesgos y retrasos. En TecNM/ITQ se desarrolló un sistema para la fabricación de dispositivos electrónicos de película delgada, controlando las variables más importantes en el crecimiento de recubrimientos semiconductores por baño químico como tiempo, temperatura y agitación. Dicho proceso es realizado mediante un brazo robótico configurable, creado para manipular con precisión sustratos a través de distintas etapas de la fabricación del material semiconductor, garantizando la reproducibilidad y repetitividad de las propiedades de cada producto, y siendo capaz de operar varias horas sin la necesidad de supervisión. Dicha herramienta es apta para esta tarea con la versatilidad para escalarse a diversos procesos productivos industriales similares.

Se diseñó una estructura mecánica óptima para este proceso, mediante una configuración de elementos más eficiente y segura. Se trata de una estructura piloto que puede manipularse fácilmente, manufacturada con materiales adecuados para la exposición a los vapores que se pueden producir en el reactor químico donde sucede la síntesis. Adicionalmente el sistema de depósito se constituye de sensores que proporcionan control del mismo. La configuración y monitoreo de los parámetros de operación se realizan por medio de una interfaz de usuario, compuesta de una interfaz física y una virtual. La interfaz virtual consta de una aplicación que provee control, retroalimentación en tiempo real e informes sobre la etapa del proceso de manera inalámbrica, acorde a la tendencia “Bring your own device” (BYOD, o en español “traiga su propio dispositivo”), uno de los conceptos de la industria moderna para la disminución del uso de dispositivos internos y el ahorro de tiempo e infraestructura.

Muchos dispositivos móviles con los que en la actualidad contamos, son capaces de suplir a los robustos dispositivos usados tradicionalmente para el control de ciertos procesos industriales; aprovechando tales tecnologías desarrollamos una aplicación móvil para el control del brazo a través de señales bluetooth. Una perspectiva muy cercana del proyecto, es la creación de una red que nos permitirá interconectar a distancia los dispositivos de control con el sistema a través de Wifi, teniendo un sistema embebido completo respondiendo a las exigencias de la industria 4.0, que apunta a la automatización, las tecnologías digitales y los sistemas ciberfísicos para el control de los procesos. Este escenario nos brindará mayor confiabilidad en la calidad de los procesos de producción de los recubrimientos y la posibilidad de predecirlos o rediseñarlos de acuerdo a las necesidades particulares.

[SCD-264] Síntesis de Nanopartículas Plasmónicas: diseñando un Manual de Prácticas

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Un reto importante en la formación a nivel Licenciatura es poder brindar los conceptos básicos de la carrera acompañados de experiencias prácticas que les permita a los estudiantes, no solo entender y visualizar los conceptos, sino que además les desarrolle habilidades mediante aprendizaje kinestésico. Esto se enfatiza más en carreras de carácter científico-tecnológico. Más aun, en áreas con tanta actividad en investigación como la Nanotecnología, resulta necesario acercar laboratorios de investigación e investigadores en áreas afines a la formación básica de los estudiantes de Licenciatura.

Por su parte, la Plasmónica es un área emergente de creciente importancia en la Nanotecnología. Su desarrollo apuntala a prometedoras alternativas para problemas en sectores prioritarios tales como la salud, fuentes de energía renovables o remediación ambiental. En particular la síntesis de nanopartículas plasmónicas le puede otorgar al estudiante en áreas de Materiales y Nanotecnología, herramientas de gran valor para el diseño de nuevos materiales.

El presente trabajo pretende compartir las experiencias obtenidas en el desarrollo de un programa sobre la síntesis de nanopartículas plasmónicas, que le permite al estudiante tener experiencias prácticas en el Laboratorio, para visualizar conceptos aprendidos en el salón de clases y desarrollar habilidades en el diseño de nuevos materiales. Para ello se diseñó un Manual de Prácticas como guía para impartir temas relacionados con la Plasmónica, la síntesis de nanopartículas plasmónicas y la caracterización de dichas nanoestructuras. Vale la pena resaltar que las prácticas incluidas en el manual antes mencionado, se basan en una recopilación de resultados recientemente publicados en la literatura en artículos de investigación científica. Estas prácticas fueron acompañadas con actividades complementarias como: Encuentros Académicos, donde los estudiantes presentaron un Cartel con sus resultados para promover el intercambio de ideas; y un Ciclo de Seminarios, donde se invitó a investigadores expertos en temas afines a la Plasmónica a dar charlas a nivel divulgación para estudiantes de Licenciatura.

Agradecimientos: Se agradece el apoyo económico por parte de la UNAM a través del proyecto DGAPA PAPIME PE108319, así como apoyos complementarios del proyecto CONACyT Fordecyt 272894. Es importante agradecer también el apoyo técnico obtenido de E. Aparicio, A. Mizques, F. Ruiz, J. Díaz, I. Gradilla y E. Murillo.

[SCD-369] Nano- y Micro-Tecnologías con Aplicaciones en Ciencias de la Salud

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"*Amor y atención al prójimo con ciencia y tecnología nacional*"

En la actualidad, las tecnologías de Circuitos Integrados (chips) ofrecen sistemas electrónicos con funcionalidades sorprendentes, con impacto creciente en nuestra vida cotidiana: primero las computadoras y tabletas, luego una diversidad de instrumentos a base de chips inteligentes (productos computarizados) tales como los teléfonos celulares, pantallas inteligentes, hornos de microondas, hasta las estratégicas telecomunicaciones satelitales.

Tomando como referencia las aplicaciones industriales y sistemas de navegación, ahora los chips abordan con gran impacto el sector salud, no sólo en sistemas de diagnóstico como los ultrasonidos, también en nuevos *sensores biomédicos*. Pero, ¿cómo es esto posible?, pues con base en la ciencia de materiales y las ciencias químicas, cuyos avances evolucionan los complejos procesos de fabricación de los chips hacia el campo de los sensores inteligentes, adaptables a un nuevo ámbito de uso cuando son implantados en el cuerpo humano. Esto es factible porque los sistemas electrónicos son recubiertos con algún tipo de polímero, logrando que el organismo no rechace el sistema electrónico implantado. Esta nueva funcionalidad se llama biocompatibilidad, los chips de uso biomédico deben ser encapsulados con algún material que les permita estar residentes, sin reacción de rechazo, en alguna parte del organismo vivo. Es importante señalar que la mayoría de los materiales y metales de uso común en los circuitos fabricados con técnicas de microelectrónica, son tóxicos para el organismo.

Estas técnicas de fabricación de sensores inteligentes suelen basarse en las ***Nano- y Micro-Tecnologías*** para el desarrollo de Sistemas MicroElectroMecánicos (***MEMS***). Ejemplo de MEMS implantables son los marcapasos para regular el ritmo cardiaco o bien los implantes cocleares para resolver problemas de sordera aguda. ¿Podemos desarrollar nuestras propias microtecnologías para el sector salud? La respuesta contundente es sí.

Para ello es necesario abordar las ciencias básicas y la ciencia de materiales.

[SCD-426] El sol una fuente inagotable de energía, calentamiento pasivo.*

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El sol es la fuente de energía que permite el ciclo de vida en la Tierra. Los hidrocarburos son una fuente con un contenido energético óptimo para su transporte y utilización en cualquier lugar. Sin embargo, hasta ahora, no se ha desarrollado una tecnología eficiente para que el uso de los hidrocarburos sea inocuo sobre el medio ambiente.
Hay una gran preocupación por el futuro de la especie humana debido a los efectos nocivos del calentamiento global, por lo que el desarrollo de fuentes de energía renovable tiene una importancia creciente.
Si bien la producción de energía eléctrica usando celdas solares tiene una gran importancia, recientemente se ha planteado la importancia de usar la energía térmica del sol para establecer sistemas de calentamiento y/o refrigeración pasivos.
En esta platica pondremos en relieve la importancia y relativa facilidad de implementar estos sistemas en México empleando los conocimientos en ciencia de materiales que permitirán generar un impacto positivo sobre el medio ambiente.

*:Trabajo financiado parcialmente por CONACyT

[SCD-432] El agua: La sustancia más maravillosa

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¿Qué tanto sabes del agua? ¿Cuántos tipos de agua existen? ¿Qué tan importante es el agua en la vida? En esta plática se contestarán estas y muchas otras preguntas referidas al agua. Es increíble como una sustancia tan sencilla y común tiene propiedades tan increíbles como para hacer posible la vida en el planeta tal y como la conocemos. Se comentará de por qué los hielos flotan y otras propiedades termodinámicas del agua y su impacto en el planeta. Se hablará del agua ligera y del agua pesada y sus aplicaciones. Veremos las diferencias entre el agua de mar, de los ríos y de lluvia. Hablaremos del agua y el COVID, junto a otras enfermedades. Y por supuesto, comentaremos la importancia del cuidado del agua y de contar con un agua de calidad para tener una buena calidad de vida.

Agradecimientos:
Se agradece el apoyo del Instituto Politécnico Nacional a través del proyecto SIP 20201523 y a SECTEI con el proyecto 289/2019.

[SCD-437] ¡¡¡Agua de uso, no de abuso!!!

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El desabasto y calidad del agua potable es uno de los problemas más importantes que enfrentamos en la actualidad. El cambio climático, la alteración de los mantos acuíferos entre otros han impactado en gran medida el ciclo del agua. Al hacer un análisis del consumo de agua, no tomamos conciencia de que el agua es de uso, no de abuso. La Comisión Nacional del Agua marca como una estrategia general mejorar la administración del recurso. La presencia de contaminantes en las aguas presenta numerosos desafíos técnicos e institucionales para la sociedad, el medio ambiente y los profesionales del sector. El desarrollo de tecnologías apropiadas de tratamiento de aguas contaminadas es cada vez más urgente. En los últimos años se han propuesto varias tecnologías como una alternativa para el tratamiento de aguas contaminadas. Esta charla versará sobre una estrategia para el tratamiento del agua, enfocándonos en el agua pluvial. De esta forma se logró el aprovechamiento *in-situ* del agua, el uso de energía solar, el monitoreo constante de la calidad del agua pluvial y tratada, así como la implementación de procesos innovadores en el tratamiento del líquido.

Agradecimientos:
Se agradece el apoyo del Instituto Politécnico Nacional a través del proyecto SIP 20201705 y a SECTEI con el proyecto 289/2019.

[SCD-442] Aplicación de la Ciencia e Ingeniería de Materiales en el Diseño y Optimización de Recubrimientos Avanzados (una mirada al grupo de investigación DORA-Lab)

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El área de Ciencia e Ingeniería de Materiales combina conocimientos básicos y aplicados en el estudio de los principales componentes de los sistemas de ingeniería: los sólidos. Por la parte científica, el enfoque recae en la relación existente entre la estructura, la composición química y las propiedades de los materiales con los efectos que los diferentes procesos de síntesis tienen sobre ellos; por la parte Ingenieril, los estudios se centran en la manera en que las propiedades de un determinado material pueden ser aprovechadas en una aplicación en particular, incluyendo su seguimiento hasta que sea parte de productos útiles para la sociedad. Por tal razón, esta área de las ciencias se considera de tipo multidisciplinaria.

Cuando pensamos en materiales, los recubrimientos ocupan un lugar especial debido a su amplia gama de aplicaciones que van desde proporcionar mayor durabilidad a una pieza metálica hasta ser parte esencial de un circuito electrónico. Es por ello, que el grupo de investigación DORA-Lab se dedica a estudiarlos, teniendo como objetivo: investigar conceptos científicos básicos para desarrollar recubrimientos avanzados o mejorar los ya existentes, a través de la combinación de métodos especializados de depósito que aseguren su alta reproducibilidad y de la caracterización detallada de sus propiedades lo que permitirá entender su comportamiento a nivel atómico y microestructural y así, estar en posición de proponer soluciones o alternativas con alto potencial de impacto en a problemáticas específicas a nivel industrial, en temas relacionados con el aprovechamiento de energía y remediación ambiental.

[SCD-443] ¿La luz puede curar?

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En esta plática discutiremos el uso de la luz para el diagnóstico y tratamiento de varias enfermedades. Se cubriran los fundamentos básicos de la interacción luz-material biológico y sus consecuencias. En particular, daremos detalles sobre la terapía fotodinámica y otras actividades de investigación del grupo de biofotónica del INAOE.

SEMICONDUCTORS

Chairmen:

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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-165] Synthesis of Bi3+ doped anatase by sol-gel. Structural analysis by Rietveld refinement method

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Catalyst today are of great interest due to its use in energy and environmental applications, among this materials TiO_2 has been widely used for wastewater treatment trough photocatalysis process. One of the main disadvantages of using this metal oxide is that it only absorbs light in the UV region, and the wastewater treatment process turns out to be more expensive compared if the process is carried out efficiently under visible or solar irradiation. For this reason, in recent years intensive research has been made on the chemical and structural modification of TiO_2 through doping with different chemical elements. In this work it is presented the synthesis of Bi^{3+} doped anatase by sol-gel method and its structural analysis in order to understand how the incorporation of bismuth change the properties of the anatase. The results of the structural analysis by Rietveld refinement method show an expansion of the anatase cell in the doped sample (135.935 $Å^3$) compared to the non – doped one (135.847 $Å^3$) due to the enlargement of the parameter *a*. The results of the UV-vis absorption experiments indicate that the Bi^{3+} doped anatase sample absorbs light in the visible region and for that it is a suitable candidate to be used in photocatalysis using light of less energy compared to the pristine sample.

Keywords: *anatase, Bi^{3+} doped, structural analysis*

[SEM-208] Synthesis of ZnO/CdS multilayers and powders for photocatalytic applications

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The synthesis of multilayers of ZnO and CdS on glass substrates using the dip-coating sol-gel and chemical bath deposition techniques respectively, is presented. The layers were grown changing the deposition order (CdS/ZnO or ZnO/CdS) and the thermal treatments applied to them. The multilayers were characterized using UV-vis spectroscopy and X-ray diffraction. The resulted layers were used for the photodegradation of methylene blue with UV radiation. Single CdS and ZnO layers were synthesized as control samples. The absorbance of methylene blue was measured every 30 minutes during a period of 180 minutes to quantify the decrease on the concentration of methylene blue. The highest percentage of degradation was 49.1% for a CdS/ZnO multilayer. Thus, the degradation of ZnO and CdS that resulted on 28.4% and 17.6%, respectively, was improved. Additionally, mixes of ZnO and CdS powders were fabricated under the same conditions than the multilayers to compare their photocatalytic activity. It was found that powders are much more active than multilayers, reaching a maximum value of degradation of 82.4% for a ZnO/CdS mixture.

[SEM-221] IMPROVED PHOTOCATALYTIC EFFICIENCY OF ZnO-SILICA-BASED MONOLITHIC FILTERS THROUGH EXPERIMENTAL DESIGN (DOE)

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The presence of organic pollutants in wastewater represents one of the most serious environmental threats to human health for carcinogenic and mutagenic relationship. This problem has been studied by several authors which have reported the application of different advanced water treatments, highlighting the heterogeneous photocatalysis for the mineralization capacity of a pollutant up to CO_2 and water. This is one of the most promising alternatives because the use of semiconductors in powder form is reported that improves adsorption processes, recyclability and reduces charge recombination and secondary pollution generated. Therefore, in the present study, we report the use of treated monolithic filters based on silicon oxide for the degradation of the methylene blue dye in aqueous solution. The filters are chemically treated by a hydrothermal method at different conditions, using a 2^k two-level factorial design of experiments (DOE) on approach. At the same time, the deposition of different ZnO on the monolithic filter was reported to test its photocatalytic performance. The XRD results revealed that the silica filters show the α-cristobalite, β-quartz and sodium oxide phases, showing an increase in the α-cristobalite phase of those monolithic filters subjected to a higher hydrothermal temperature. While SEM analyzes showed a correlation between surface cracking with increasing temperature and reaction time, favoring the shape of spherical particles grouped in a pyramidal shape. Concurrently, the exfoliation of the monolithic filter by the hydrothermal method allows the cultivation and crystallization of ZnO particles in the form of highly crystalline flowers. The photocatalytic activity of the monolithic silica filter revealed that the degradation of the dye reached 94% under UV-Visible light after 5 hours of reaction and after 3 cycle efficiency decreases until 60%. On the other hand, monolithic filters with ZnO showed a degradation of 79%, improving the stability of the filter by keeping its efficiency intact after 3 cycles. According to the results above mentioned, the photocatalytic activity is because of the superficial exfoliation caused by the hydrothermal method and to the increase in the α-cristobalite phase that allows a greater adsorption of the organic molecule. By the way, recyclability tests show that ZnO-deposited monolithic filters improve the material stability. In conclusion, ZnO-silica-based monolithic filters prove to be an innovative alternative on photocatalysis reactions because of its efficiency, practicability and reproducibility.

[SEM-280] Electrical characterization of electrodeposited indium silfide thin films by electrochemical impedance spectroscopy and electrical force microscopy.

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In this work, we present the use of impedance spectroscopy and electrostatic force microscopy for the electrical characterization of 100 nm indium sulfide thin films. We demonstrated the usefulness of impedance spectroscopy, as it was possible to characterize films with thickness so thin that was impossible to detect by X-ray diffraction or ultraviolet spectroscopy. Impedance spectroscopy was used also to characterize grain boundaries, as well as for determining the n-type conductivity of the material. On the other hand, using spreading resistance microscopy, we mapped the surface, and we located the points with higher current flow. Using electrostatic force microscopy we measured the phase angle, which in turn was correlated with voltage drops at the interphase substrate/film. In order to calculate the work function of indium sulfide, we have proposed a scheme for conduction band locations at the interphase between the fluorine tin oxide substrate and the indium sulfide film.

[SEM-337] Synthesis of ZnO/ZnSe heterostructures by microwave-assisted method for efficient photocatalytic degradation of organic dye.

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ZnO/ZnSe heterostructures were synthesized by microwave-assisted technique for the photocatalytic degradation of methylene blue under visible light. The heterostructures were synthesized in two-steps. First, the porosity of the ZnO powders was controlled using ascorbic acid ($C_6H_8O_6$) and hydrazine monohydrate ($N_2H_4{\cdot}H_2O$). In the next step, the heterostructures were successfully formed by the recrystallization process, wherein sodium selenite (Na_2SeO_3) was used as a source of Se. The synthesized ZnO/ZnSe heterostructures were characterized to research their structural, morphological, and optical properties by XRD, SEM, physisorption N_2, and UV-Vis. XRD data analysis confirmed the presence of ZnO (wurtzite) and ZnSe (blend) on the material. ZnO/ZnSe powders showed an increasing significantly in the specific surface area, and absorption UV-Vis compared to the pristine ZnO.

[SEM-353] Synthesis of ZnO, CeO2 and ZnO/CeO2 semiconductors by the sol-gel method and microwave-assisted sol-gel for their application as photocatalysts in the degradation of colorants.

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In this work, the coupling of ZnO/CeO_2 by the sol-gel method and microwave-assisted sol-gel is presented. The obtained samples were structurally characterized by X-Ray Diffraction (XRD). The results show that ZnO was obtained with a good crystallinity with the hexagonal wurzite structure according to the crystallographic chart (PDF 00-036-1451), on the other hand, the characteristic peaks of CeO_2, coincided with the cubic structure of the material (PDF 01-081-0792). The ZnO/CeO_2 coupling shows that all peaks can be indexed as a combination of both materials. The parameters of the unit cells of each semiconductor were calculated, indicating that the results of the samples of these materials have been obtained with a good crystallinity. On the other hand, from UV-Vis studies with absorbance as a function of wavelength, the forbidden band of pure and coupling materials was calculated and values of 3.1 eV, 2.81 eV and 3 eV were obtained for ZnO, CeO_2 and ZnO/CeO_2 respectively. Finally, with the results of the experiments of the photocatalytic activity of these semiconductors, it was obtained a photocatalytic performance in the degradation of the Methylene Blue (MB) of 90% of the MB molecules after 240 minutes.

[SEM-363] Thermodynamic analysis on effect of complexing agents to synthesis of ZnS thin films by chemical bath deposition.

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ZnS deposition by chemical bath method was studied from three different complexing agents due to their effects on the growth rate. The deposition conditions for ZnS were obtained through thermodynamic analysis on the formation of Zn-Ethanolamine, Zn-Triethanolamine, Zn-Citrate complexes and predominance zones. Theoretical analysis by molar fraction diagrams of Zn(II) shown that for 4<pH<6 the predominant species at 90°C are $[Zn(ETA)_2]^{2+}$, $[Zn(TEA)]^{2+}$ y $[Zn(Cit)]^{â"€}$ complexes for Zn-Ethanolamine, Zn-Triethanolamine and Zn-Citrate systems, respectively. For predominance diagrams of Zn(II)-Complexing agents-Thiourea systems at 90°C, the chemical stability diagrams established that the predominant specie is ZnO(cr). Subsequently, films were synthetized at 90°C at pH equal to 7 by keeping fixed the molar relationships complexing agent-metal and sulfur-metal. These conditions produced ZnO films with hexagonal crystal structure by ethanolamine and triethanolamine. Although chemical stability diagrams showed that ZnS does not predominate into aqueous solution, characterization of structural and optoelectronic properties revealed that ZnS fabricated by chemical bath deposition have cubic crystal structure, a direct band gap energy of 3.75 eV and n-type conductivity, using citrate as complexing agent.

Keywords: Thermodynamic analysis, complexing agents, equilibrium chemical, ZnS.

[SEM-154] Sol-gel synthesis of ZnO-SnO2 nanocomposites by sol-gel method at room temperature

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In the present work, we discuss the synthesis and deposit of zinc oxide-tin oxide ($ZnO\text{-}SnO_2$) nanocomposites. The $ZnO\text{-}SnO_2$ nanocomposites were synthesized by a simple sol-gel method at room temperature in two steps: i) the ZnO solution was synthesized by sol-gel method at room temperature, ii) after, an adequate tin chloride ($SnCl_2$) quantity was added to the ZnO solution in order to obtain the desired $ZnO\text{-}SnO_2$ nanocomposites solution. The $ZnO\text{-}SnO_2$ nanocomposites solution was deposited on glass substrates by spin-coating technique. After, the $ZnO\text{-}SnO_2$ nanocomposites films were annealed at several temperatures in order to get different surface morphologies. The deposited films showed a high transmittance on visible range. Also, the band gap was calculated transmittance measurements and it was 3.3 eV. Through X-ray diffraction patterns we observed the crystallinity of the $ZnO\text{-}SnO_2$ nanocomposites deposited and its relation with the annealing temperature. Finally, we conclude that in this work, we developed a simple method to synthesized $ZnO\text{-}SnO_2$ nanocomposites. Such nanocomposites according to the results have a great potential to be applied in photocatalysis and gas sensors.

[SEM-174] Study of homogeneous and heterogeneous reaction to obtain Nanostructured semiconductors II-VI

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The numbers of studies about material nanostructured synthesis are rise in last years, due to the necessity of modulation and control of properties. The control on crystal size or particles size leads the modification of properties, this effect is more appreciate in nanometric sizes, even in some cases can be reported quantic effect. These materials can be obtain on different presentations e.g. films, nanoparticles, quantum dot and core shell and can be synthetized by different techniques with good properties such as laser ablation, sol gel, SILAR (successive ionic layer adsorption and reaction) and controlled precipitation among others. In this research was synthetized CdS and CdSe y thin films and nanoparticles using the controlled precipitation technic. The reaction was carry out with a Temperature from 50 to 90°C, stirring rate 200, reaction time was 120 min. Nanoparticles and films exhibit a mixture of phase hexagonal and cubic in all materials it was obtain a Eg closed to theoretical value as increased the pH, respect to the morphology the nanoparticles are agglomerates semispherical in almost all conditions, which are grown in function of pH and temperature (from 100 to 500 nm). The reaction efficiency has an important effect with experimental parameters; as pH and temperature rise, quantity of precipitate is increase.

[SEM-181] Effects of RF power variation on properties of indium sulfide thin films processed by sputtering.

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Thin films of indium sulfide were processed with different radiofrequency (RF) powers were deposited on glass substrate by RF magnetron sputtering with average thickness of 85 nm. The thin films were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), spectroscopy UV-Vis (OA) and electrical resistivity. Diffractograms show preferred orientation of beta phase of indium sulfide, the energy band gap increase as the RF power increases and the electrical resistivity order was $10^3\ \Omega$ cm.

[SEM-198] Annealing effects on the optical and structural properties of coherent and relaxed GaNAs layers grown by MBE.

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In the classification of III-N-V semiconductors, also called diluted nitrides, the GaN_xAs_{1-x} alloy has been studied by research groups around the world because of the attractive and unusual behavior that its electronic band structure acquires when the nitrogen atoms are added to the GaAs lattice, splitting the conduction in two sub-bands labeled as E- and E+ [1]. This conduction band behavior makes the GaNAs alloy quite promising to be employed in the development of photovoltaic devices. Nevertheless, the optical, structural and transport properties are downgraded with the nitrogen incorporation. In this work, molecular beam epitaxy (MBE) was used to growth two set of samples of GaN_xAs_{1-x} on GaAs (100) substrates. Samples A were grown with x = 0.001 and 0.02 with width close to the critical thickness. On the other hand, 500 nm layers were grown with x = 0.007 and 0.015, value exceeding the estimated critical thickness. An ex-situ thermal annealing treatment was applied to the samples in a temperature range from 600 to 950°C during 60 seconds under a nitrogen atmosphere with the aim of altering the GaNAs layer properties. The effect of the annealing on the structural properties was explored by means of Raman Spectroscopy where the reduction of the LO/TO ratio indicates a rise in the lattice disorder as the temperature is increased. The LO phonon mode frequency was red shifted in the process, which is associated to lattice strain relief. On the other hand, the Raman scattering intensity of the GaN-like mode has been associated to the incorporation of nitrogen in the lattice. We determined that the relative intensity rise due to the thermal treatment indicates an improvement in the nitrogen lattice incorporation, which indeed is a promising effect. This behavior is stronger exhibited for x > 0.01. The notable modification in the structural properties of the GaNAs produces a modulation in the band structure of the alloy, which was measured with photoreflectance spectroscopy where a blue shift in the bandgap associated transition is measured. Through this research the authors explore the optimal temperature to improve the properties of GaNAs alloys, which strongly depends on the nitrogen percent in the alloy.

[1] 10.1016/j.ssc.2003.11.004.

Acknowledgments: The authors acknowledge the financial support from FRC-UASLP, C19-FAI-05-18.18 and CONACYT-Mexico through grants: INFR-2015-01-255489, CB 2015-257358, PNCPN2014-01-248071 and the Catedras CONACyT (Project No. 44).

[SEM-242] CO2 detector based on tungsten oxide nanostructures: Effect of synthesis route on gas sensing properties

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Experimental and theoretical investigations were performed to study the structural and optical properties of tungsten oxide (WO_3). WO_3 nanoparticles powders were obtained by thermal decomposition of precursors prepared using an ultrasonic-assisted sol-gel method at 500 ºC. X-ray powder diffraction and Raman spectroscopy confirmed the presence of a monoclinic phase alone. The band gap of WO_3 nanoparticles was calculated based on UV-Visible diffuse reflectance spectroscopy data and was 2.57 to 2.58 eV. To explain these experimental measurements, first-principles total energy calculations have been performed to determine the structural and optical properties of WO_3 (002) and (020) surfaces. Results indicate that the density of states of the WO_3 (002) surface, it was possible to observe that the electronic gap is ~1.5 eV, while the optical gap (imaginary part of epsilon) was ~2.4 eV. The theoretical study shows the optimized crystalline network as well as the atomic positions. This may help to explain the multiple crystal phases. Sensing tests were carried out on tungsten oxide films in the presence of CO_2 to analyze their performance as gas detecting devices and results were obtained that confirm the good properties of WO_3 as a semiconductor-based gas sensor.

[SEM-297] Marked trend in GaN obtained from nitriding GaAs deposited by CSVT

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Galium nitride (GaN) is a promising material when developing technologies that are related to the emission of the color blue, ultra violet or violet, such as LEDs or LCD screens and solar cells. This since its manufacture by MOCVD focused on the creation of the blue LED by Isamu Akasaki et. all. And the main reason is its direct bandgap energy Eg = 3.39eV

With the use of the CSVT (close space vapor transport) technique, GaAs are deposited on different substrates (high and low resistivity silicon, fused quartz). The behavior of GaAs in its deposition is fundamental for the properties of the GAN obtained from it by nitriding.

What was collected in this study is that the GaAs obtained by CSVT has a favored growth direction (111) corresponding to its Zinc Blenda structure. When nitriding, the GaN gain show as preferred growth direction depends on the substrate on which the GaAs was deposited. This possibly to the rearrangement of the structure that occurs in the heat treatment in an ammonia environment when nitriding

After nitriding, GaN obtained has growth directions (111) corresponding to the Zinc Blende structure of GaN and (002) corresponding to the Wurtzite structure of GaN coexisting. It is common for both faces to coexist due to the missmatching between the substrate and the material formed on it. In this study shown that depending on the substrate and the deposit parameters, one or another phase can be favored if the origin parameters are modified, we also see the appearance of other growth directions such as (110), (120), (311), among other; all belonging to GaN.

[SEM-350] Microwave irradiation synthesis of a-Fe2O3/TiO2 heterostructures and their application as a photocatalyst in the degradation of acetaminophen

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a-Fe_2O_3/TiO_2 heterostructures were synthesized via microwave irradiation method varying the a-Fe_2O_3 concentration in the TiO_2. The structural, morphological, and optical properties were analyzed by XRD, SEM, BET, PL y UV-vis techniques. The characterization results indicate that the heterostructures were formed with an anatase phase TiO_2 with hematite incorporation. Furthermore, there is an improvement in the light absorption of the semiconductors when moving towards the visible light range. The photocatalytic activity of the heterostructures was evaluated with respect to the degradation reactions of acetaminophen (ACE) under light irradiation (35 W Xe lamp). The highest activity was obtained by the sample 5% a-Fe_2O_3 reaching a percentage of 91%, which represents 3 more times than to the performance of the materials separately. These results indicate decreasing recombination of charges, which generates greater efficiency in photocatalytic degradation.

[SEM-366] Synthesis of core-shell nanostructures Si/SiOx embedded in ZnO.

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Si nanoparticles embedded in a ZnO matrix were synthesized sequentially by means of the radio frequency sputtering technique with an Ar/O2 reactive atmosphere at room temperature. Silicon and metallic Zn were used as precursor materials to the synthesis. The SEM and AFM micrographs confirm the formation of the ZnO nanoparticles; in addition, by means XRD was calculated the ZnO particle size in the thin film. The UV-VIS transmittance spectra show that the nanostructured silicon of the samples synthesized at room temperature have a high transparency and the Tauc plot shows a bandgap of 1.86 eV for silicon nanoparticles while the ZnO has a bandgap of 3.3 eV. The photoluminescent performance of ZnO was increased due to the presence of silicon confinement in the synthesized samples at room temperature. Regarding their electrical properties, the sample offers a better behavior in the current characteristics according to the I-V diagram. The ZnO/Si(np)/ZnO structure could potentially be used in the photovoltaic and optoelectronics industry, thus also like as a transparent conductive material and emitting light.

[SEM-367] Study of ZnO as buffer layer in thin film solar cells based on chalcogenide materials

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Recently, ZnO has taken importance due to its excellent optical, piezo-electric and electro-optical properties, which make it suitable for thin film optoelectronic applications such as blue light emitting devices, short wavelength laser diodes, detectors in the UV-Blue spectral region and buffer layers in photovoltaic devices. A PET / ITO / CdS / PbS / ZnO structure was developed for its application in photovoltaic devices. CdS and PbS thin films were deposited using the chemical bath deposition method The ZnO layer was deposited as a buffer layer using the spin coating technique, three different ways of deposition were investigated un order to compare which of them gave the best properties for the desired application first of them was carried out using a solution of ZnO; secondly, using 30 days aged ZnO nanoparticles and finally 20 minutes aged nanoparticles was applied. A thermal treatment was carried out layer by layer at 150ºC for 30 minutes in a tubular furnance in an ambient atmosphere. The raman spectroscopy analysis in the PET/ITO/CdS/PbS/ZnO TF structure shows dispersion peaks with values in 298 cm^{-1} and 596 cm^{-1} corresponding to the 1st and 2nd optical phonons of the CdS, in 143 cm^{-1} corresponding to the optical phonon (LO) of the PbS and in ~101 cm^{-1} this is attributed to the $E2^{Low}$ phonon and ~438 cm^{-1} this attributable to the characteristic phonon in $E2^{High}$ of the ZnO. In the other two structures, the dispersion peaks corresponding to CdS and PbS do not vary from those described above. However, in the structure PET/ITO/CdS/PbS/ZnO Nps aged 30 days it is possible to appreciate the peaks of dispersion corresponding to the ZnO at ~100 cm^{-1} and 433 cm^{-1}, which are attributed to the phonons $E2^{Low}$ and $E2^{High}$ respectively, in addition two peaks of dispersion are observed

at ~352 cm^{-1} and ~592 cm^{-1}, which correspond to the phonons A1(TO) and A1(LO)/E1(LO) respectively. And in the structure PET/ITO/CdS/PbS/ZnO Nps aged 20 minutes as in the 2 previous structures, the dispersion peaks attributed to the phonons $E2^{Low}$ and $E2^{High}$ are observed with a lower intensity, which indicates a lower degree of crystallization, also dispersion peaks at ~376 cm^{-1} and ~595 cm^{-1} attributable to the phonons A1(TO) and A1(LO)/E1(LO). The microstructural characterization given by X-ray diffraction shows in all three structures, the hexagonal crystalline structure of the CdS, the cubic rock salt crystalline structure of the PbS and the hexagonal zincite crystalline structure of the ZnO. The results of the electrical characterization of the PET/ITO/CdS/PbS/ZnO TF structure show a threshold voltage ~1.2V and a slight offset of ~0.7V. The structure PET/ITO/CdS/PbS/ZnO Nps aged 30 days shows a threshold voltage ~0.7V and an offset of ~0.3V. Finally, the structure PET/ITO/CdS/PbS/ZnO Nps aged 20 minutes shows a threshold voltage ~0.6 V.

[SEM-372] FABRICATION OF A MIS STRUCTURE BASED ON TWO-DIMENSIONAL ZnO NANOSTRUCTURES BY CHEMICAL ROUTES

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

Here, we report the fabrication of a metal-insulator-semiconductor (MIS) structure based on ZnO nanostructures grown on the surface of an anodized aluminum substrate (ZnO/Al2O3/Al) by chemical routes. Namely, while the ZnO nanostructures were obtained through a low-temperature hydrothermal route, the Al2O3/Al substrate was obtained by electropolishing and anodizing of aluminum foil. The used electrochemical techniques for obtaining the substrate involve soft reaction conditions, short reaction times, low cost and easy processing. The obtained ZnO/Al2O3/Al architecture was studied by x-ray diffraction (XRD), scanning electron microscopy (SEM), micro- Raman spectroscopy (µRS) and electrical measurements. The voltage-time plot acquired during the anodizing process indicates the formation of an insulating barrier (Al2O3) on the metallic substrate (Al). The SEM analysis reveals that the semiconductor layer grown on the insulator film is nanostructured in nature, constituted by leave- like structures with an average thickness of ~ 50 nm. According with the Raman spectrum, these ZnO nanostructures are well-crystalline. The formation of Al2O3 and ZnO phases was further confirmed by means of XRD. Finally, the characteristic rectifying response of a metal-oxide-semiconductor junction is observed in the curves I-V and C-V of the obtained architecture, indicating that it is possible to build a MIS structure based on ZnO nanostructures using exclusively chemical routes.

[SEM-424] BiOCl1-xIx solid solutions: tunable band gap and photocatalytic activity

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Bismuth-based semiconductors are a recently developed family of photocatalytic materials promising to work under visible light in degradation of organic pollutants, reduction of heavy metals and CO_2, as well as water splitting applications, among others. In addition to their physical and chemical properties, non-toxicity and stability. Bismuth oxyhalides such as BiOI, BiOBr and BiOCl can be combined to form solid solutions with band gaps in the range between 1.7 and 3.4 eV. This wide range of band gaps make them suitable for applications where a tunable band gap value is required.

In this work, solid solutions of $BiOCl_{1-x}I_x$ (x=0, 0.25, 0.5, 0.75, 1) were synthetized through hydrothermal synthesis. Optical properties were studied by UV-Vis spectroscopy. X-ray diffraction and Raman spectroscopy were used to study structural properties and scanning electron microscopy to study their morphology. Measurements of photocatalytic activity were carried out by degrading methyl orange dye (MO) under visible and UV light radiation. As reference sample, standard P25 TiO_2 was used. Regardless of band gap values of samples, we found that solid solution samples with both, Cl and I in their structures, presented a significant improvement of photocatalytic activity compared with the single halogen samples.

[SEM-431] UV thermal modulation of the refractive index of c-GaN prepared by MBE

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Oscillations in the reflectance spectra at lower energies than that of the bandgap of cubic GaN (c-GaN) were observed. These oscillations have their origin in the multiple reflections between the c-GaN surface and the c-GaN / GaAs substrate interface. Thus, the reflectance shows interference in the spectral region in which c-GaN is transparent. The Fresnel equations were used to simulate the reflectance, using the sample thickness as fitting parameter. A modulating beam with λ = 285 nm, 10 mW power, and chopped at 527 Hz was then employed to obtain Photoreflectance (PR) spectra. These PR spectra also show oscillatory behavior. It was found that the origin of this spectra is a thermo-optical effect, in which the sample is heated by the modulating beam, which in turn changes the refractive index. This change is an energy dependent function, which in this work was calculated to fit the experimental PR spectra.

SURFACES AND INTERFACES

This symposium aims at bringing together academics and to be a forum for providing an overview of the field of nano-engineered surfaces and interface where information and expertise on cutting-edge research and technology are disseminated.

Topics of interest are related to:

- Single crystal structures
- Thin film materials self-organized at the nanoscale such as functional thin films multilayered systems
- Nanolaminates
- Nanostructured coatings and surfaces.
- Nano-engineered surfaces and interfaces
- Methods for studing surface and interfases

[SIF-190] Alumina Nanofibers by Electrospinning

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The fabrication of dense alumina fibers at low cost by sol-gel and electrospinning, using aluminum nitrate as precursor is reported. Polyvinyl pyrrolidone was used as spinning polymer, while Pluronic 127 was used as additive to achieve a porous structure. The material was characterized at different stages of thermal treatment by SEM, EDS, FTIR, XRD, and thermal analyses. It was observed than the increase in precursor ratio is related to the formation of more stable fibers that retain their morphology after sintering at 1600°C. The fibers obtained from a solution with high mole ratio presented a mean diameter close to nanometric scale 153±39 nm. FTIR and XRD demonstrated that amorphous, γ-, and δ-Al_2O_3 polymorphs were present in fibers treated at 800°C, while α-Al_2O_3 was formed in samples at approximately 1000°C. EDS and XRD study demonstrated the high purity and crystalline form of the alumina fibers.

[SIF-427] Application of a factorial experimental design for the synthesis of CeO2 compounds to tailor high specific surface area compounds

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Cerium oxide generally reports specific surface area values of 50 to 80 m^2/g on average, which is why excellent results are usually obtained in catalytic reactions. It is because of this that this research work was carried out an experimental design to optimize the formulations and synthesis conditions of CeO_2, assisted by microwave heating, to obtain higher specific surface area values than those obtained in other investigations. An experimental design with three variables (2^3) was used, each one studied at two levels. The variables included in the experimental design were temperature, whose values were defined as 150 and 120 ºC; the concentration of polyvinylpyrrolidone (PVP) considering a 5 and 8% solution (%w/w). The reaction times established for the microwave heating were 30 and 20 minutes. The obtained compounds were characterized by the BET technique to measure their specific surface area. Different values were obtained, depending on the conditions for the synthesis of each compound. In general, those synthesized for a reaction time of 30 minutes were those that showed higher specific surface area, being the compound labeled as OCPVP 6, which was obtained at 120 ºC, for 30 minutes and 8% of PVP solution, was the one that resulted with the highest surface area (146.5 m^2/g). From the obtained results, it was concluded that the experimental design used to produce the CeO_2 compounds could be efficient to obtain catalysts with high specific surface area values. It is expected that the surface area obtained might synergistically influence the oxidative capacity of CeO_2.

[SIF-167] Graphenic oxides-compound nickel coating on the 450 Hardoxsteel by microjoining-laser

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Graphenic oxides-compound coatings via microjoining-laser process have been applied on small steel components in order to increase their tribological properties. Samples without filler metal and with a shell of GO-xerogel that contains Ni-powder as a filler metal were deposited by Pechini´s method at 110 °C for 24 h. The microjoining-laser process was applied using an experimental design considering frequency, pulse, power and forward speed, without and with graphene oxide (0.002% and 0.008%) on the surfaces of the samples to evaluate the elastic, mechanical and tribological properties, individually. The samples were characterized by metallographic techniques, scanning electron microscopy, X-ray diffraction and nanohardness tests under cyclic loads of 50, 100 and 200 Hz applying a load of 350 mN to evaluate the contact stiffness. The wear resistance was studied by a pin-on-disc tribometer under dry sliding condition. The results showed that the presence of graphenic oxide materials in the coatings has a beneficial effect on the wear resistance due to their high elastic module and the self-lubrication property. A dependency of the studied parameters and the quantity of the graphenic oxides in the coatings was observed.

[SIF-178] Improving corrosion resistance of magnesium by application of TiO2-MgO coatings

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Magnesium is a biocompatible and biodegradable material that has gained increased interest for application in resorbable orthopedic implants. However, to date many research is being conducted to overcome the main disadvantage: its low corrosion resistance. In this work, we report our findings on the development and application of TiO_2-MgO coatings for improving the corrosion resistance of magnesium pieces. TiO_2-MgO coatings were fabricated by means of the plasma electrolytic oxidation technique. The corrosion resistance was evaluated through the corrosion current (I_{corr}) measured at room temperature by the polarization technique (Tafel). Also, immersion tests were conducted by employing the Hank´s solution in order to simulate body fluids. Tafel curves showed an improvement of the corrosion resistance on coated magnesium pieces in contrast to control pieces (uncoated): corrosion currents were lower and the corrosion potential changed to positive values. It was observed that experimental parameters such as deposition current and time allows to regulate the protective capacity of the coatings. Immersion test showed a lower corrosion rate in coated surfaces than in uncoated ones. TiO_2-MgO coatings have been successfully employed to improve the corrosion resistance of magnesium pieces.

[SIF-199] Numerical design of high-speed signal processing electronic devices through surface states engineering

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Standard electronics have limited performance and reliability in applications in both low-power consumption and high-frequency operation. Consequently, developing alternative technologies is necessary to satisfy the current demand in many engineering applications such as space exploration or information technology. In this task, solutions to markedly increase the frequency cut-off or to reduce the power consumption are being researched in many laboratories throughout the world devoted to nanoscale semiconductor systems. In this work, the authors modify the concept of self-switching diode (SSD) to produce a field-effect transistor based in surface states engineering by numerical simulations [1]. We considered a two-dimensional electron gas embedded in a III-V heterostructure to achieve a self-switching transistor (SST) when both an extra groove and a control terminal are added to the SSD geometry. We obtained a experimentally realizable device where the typical IDS-VGS transistor response is observed. We explain the electrical performance of the SST by the modulation of the carrier's concentration inside the nanochannel by the field-effect of the bias applied to the control terminal. The impact of the trenches size, nanochannel width and length on the transconductance and threshold voltage parameter is examined. It is found that the channel width and trenches size define the DC performance. Additionally, the SSD and SST concepts are proposed to produce logic gates in planar technology where the power requirements and operation speed are designed by geometrical parameters, building devices which follow the Boolean Logic. The AND and OR logic gates based in SSD are showed with the aim to employ the SSD in the diode-resistor logic, being the NAND, NOR, and NOT behavior also exhibited following the transistor-transistor logic. The switching and high-speed operation properties are investigated by the transient response in an inverter circuit and employing a square waveform with period of 100 ps, proving that the concept of surface states-based logic gates in three SST array is capable to produce the Boolean function with feed and input voltages of 0.5 V. The numerical results showed some insights for the improvement of the surface-states engineering to signal processing by SST arrays embedded in III-V compound semiconductors heterostructures. On this way, we design a set of devices capable to operate with voltages in the range of 1 to 0.5 V and process square signals with period even of picoseconds, exhibiting delays lower than 5 picoseconds and offering a simple device to operate at extremely high frequency in room temperature.
[1] doi: 10.1117/12.609126
Acknowledgments: The authors acknowledge the financial support from FRC-UASLP, C19-FAI-05-18.18 and CONACYT-Mexico through grants: INFR-2015-01-255489, CB 2015-257358, PNCPN2014-01-248071 and the Catedras CONACyT (Project No. 44).

[SIF-308] Steel coating by means of plasma electrolytic oxidation for wastewater coffee treatment through photo-Fenton

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In the scalable application of advanced oxidation processes (AOP) using sunlight for the treatment of contaminated water, there is a need to fix the catalyst in order to reduce the cost for recovery and reactivation in the homogeneous configuration. This can be achieved by using the technique of plasma electrolytic oxidation (PEO) to generate coatings of the corresponding oxides on the surface of steel sheets for photo-Fenton process. PEO consists of applying an electrical voltage between a metal sheet (anode-substrate) and a cathode immersed in an electrolyte; when the anode's breaking voltage is exceeded, micro-discharges are generated on its surface, local pressure and temperature increase abruptly and microcavities are produced on the electrodes surface. In this work, 304 stainless steel substrates were coated, using this technique; from X-ray diffractograms the formation of iron oxides coating (Fe_2O_3 and Fe_3O_4) was proved and their catalytic activity was evaluated in the removal of organic load from contaminated water, produced during the demucilagination of coffee by fermentation. This coffee effluent generates problems due to the appearance of mosquitoes and bad odors and contains recalcitrant substances that are difficult to decompose by other methods. The efficiency of the steel coatings as reducing agents was evaluated through the measurement of the chemical oxygen demand (COD) by spectrophotometry. It was thus proven that the photo-Fenton process with the samples led to a 42 % decrease in the COD of the treated coffee wastewater. This strategy of removing organic load through AOP is a potential complement to chemical, physical and biological methods proposed for the treatment of waste water.

[SIF-324] Low pressure contactless electroreflectance of GaN Van Hoof structures.

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Keywords : Electroreflectance, Van Hoof structures, low pressure, GaN

The Fermi level position E_F on surface of thin films and heterostructures plays an essential role in the electrical and optical properties because induce a carrier dynamic from the surface to the bulk. Diverse studies have been carried out to understand the behavior of the E_F value under heat treatments and surface passivation of the samples. However, the mechanisms under which the pressure and temperature of the sample induce changes that modified the surface Fermi level are not yet clear. In this work we evaluate the Fermi level position of Van Hoof structures as a function sample-ambient pressure by means of contactless electroreflectance (CER). When CER spectroscopy is applied to the so called Van-Hoof structures i.e. an n-type (or p-type) layer capped by a thin (20-80 nm) undoped layer, it is possible to determine the Fermi level position on semiconductor surface. For such structures, a homogeneous electric field is expected inside the undoped layer. The value of this field can be determined by CER spectroscopy since CER spectra exhibit Franz-Keldysh oscillations, which periods depends on the amplitude of the build-in electric field in the undoped GaN layer. As ambient pressure was reduced CER spectra contracts due to surface electric field is reduced and therefore E_F decreases. E_F changes from 0.5 to 0.38 eV when the pressure is reduced from 1 atm to 4 µTorr. This behavior is induced due to the desorption of the surface oxygen as the pressure is reduced. The structures investigated within this work show a different level of sensitivity to changing ambient. Only a slight change (a decrease in vacuum) in Fermi level position at the surface of Ga-polar GaN is observed under low-light conditions. In contrast to that, in the same conditions N-polar and m-plane surfaces seem to be a lot more sensitive. There is also a noticeable difference in time in which a change in Fermi level position occurs between different orientations. Such a behavior is attributed to adsorption or desorption oxygen at the surface in air or vacuum ambient and will be discussed in detail in this paper.
This work was partially supported by SIP-IPN project No. 20200459

[SIF-354] Functional CdS/TiO2 Nps thin films obtained by soft chemistry applied in degradation of methyl orange by sunlight

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Abstract

This research reports the degradation of methyl orange (MO) by heterogeneous solar photocatalysis with CdS/TiO_2 Nps thin films as an alternative to wastewater treatment. CdS thin films were deposited by chemical bath deposition in one and two layers, while the TiO_2 nanoparticles (Nps) were obtained by sol-gel process -assisted by microwave method and deposited by spin coater technique on CdS. All applied techniques for the synthesis of these materials are considered of soft chemistry. The optical characterization of the CdS/TiO_2 Nps thin films was evaluated by Ultraviolet-Visible spectroscopy, and the calculated band gap for the films was 3.0-2.8 eV. Agglomerated TiO_2 nanoparticles were observed on homogeneous CdS thin films with polycrystalline structure. The degradation of MO was done with three replicates of CdS/TiO_2 Nps thin films exposed to sunlight for 60 minutes, resulting in a degradation of 22%.

Keywords: Nanoparticles, TiO_2, CdS, thin films, photocatalysis, water treatment.

[SIF-398] MnxOy THIN FILMS SYNTHESIZED BY SPUTTERING AND THE HETEROJUNCTION WITH ZnO:Zn FOR ADAPTIVE ELECTRONICS: 1) SYNTHESIS AND STRUCTURAL CHARACTERIZATION

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New ways of processing information are being developed as the reduction of the scale of the technology reaches the prediction of Moore's law. An approach to provide a solution is adaptive electronics, where an electronic device can be designed with different properties and incorporation of internal states that are capable of reconfiguration, thus, an external stimulus (like a certain waveform) will self-adjust the parameters of those properties to carry out certain operations. In this work, a study of Mn thin films (100 nm) deposited by sputtering on glass and Si (100) substrates is presented. The films are oxidized at different temperatures (250, 350 and 450 °C) and Raman spectroscopy as well as X-Ray Diffraction (XRD) is done to examine the phases of oxidation obtained. An experimental bandgap is calculated by specular Reflectance Spectroscopy for the MnSi samples in order to understand the transport phenomena of the Mn_xO_y layer. After the initial deposit and study of Mn oxides, a second layer of ZnO:Zn is deposited by co-sputtering on top of the as growth Mn deposition on glass, given the stability and reproducibility of the sample. The ZnO:Zn layer proves to be a n-type semiconductor surface and the combination with MnO allows for a p-n heterojunction at the interface. In part 1, the synthesis and the structural characterization of the samples is presented.

[SIF-399] MnxOy THIN FILMS SYNTHESIZED BY SPUTTERING AND THE HETEROJUNCTION WITH ZnO:Zn FOR ADAPTIVE ELECTRONICS: 2) TRANSPORT PHENOMENA, ELECTRICAL CHARACTERIZATION AND APPLICATION

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New ways of processing information are being developed as the reduction of the scale of the technology reaches the prediction of Moore's law. An approach to provide a solution is adaptive electronics, where an electronic device can be designed with different properties and incorporation of internal states that are capable of reconfiguration, thus, an external stimulus (like a certain waveform) will self-adjust the parameters of those properties to carry out certain operations. Part 2 of the work presents the transport phenomena that happen at the interface between the MnO and ZnO:Zn. An electrical characterization of the final structure is performed, and an adjoined band diagram is represented to observe the level of interaction between the materials as well as to explain the transport mechanisms. Finally, an application in electronic circuits is proposed to show the importance of how the investigations of these materials and the heterojunctions are valuable to describe how the internal states of the films can be of use for adaptive electronics.

[SIF-416] ARXPS study of the early stages of aluminum oxide

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Aluminum is the third most abundant element in the Earth's crust and is widely used the aerospace, building and semiconductor industries. Is remarkable due to its non-magnetic, ductile and density properties, it is also employed due to its ability to resist corrosion.
As metallic aluminum is highly reactive to oxygen it is important to know how oxidation works in films and/or interfaces when is applied in ultra-thin films. This can be done appropriately with X-ray photoelectron spectroscopy (XPS).
In this work we present the quantitative analysis for chemical assessment of the early stages of aluminum oxide thin films. We prepared the metallic films through sublimation employing a tungsten filament with metallic aluminum (99.99% pure Sigma Aldrich). The background pressure in the processing chamber was 1.5×10^{-7} Torr and the pressure during sublimation was $1.1\times10^{â€'6}$ Torr. The growing rate (measured with a MASTEK TM-350) was 0.8 Å/s and the total thickness was 100 nm. The film was characterized with an X-ray photoelectron spectroscopy (XPS) instrument with a monochromatic X-ray aluminum source (XR5, from ThermoFisher) and a 7-channeltron hemispherical spectrometer (Alpha110, from ThermoFisher) assembled by Intercovamex.
Films of metallic aluminum were oxidized under an oxygen-controlled environment at 1 kL, 10 kL, 100 kL, 1 ML and 10 ML. A quantitative study of the surface composition of aluminum oxide was carried out employed the ARXPS data. For an appropriate fitting of the Al 2*p* spectra in oxidized aluminum we employ the block method [1] which consider the differences on background of the metallic and oxidized aluminum. Also, the multilayer method [2] were used to analyze the composition and thickness of the oxidized layer. We found that the chemical composition obtained since its firsts stages of oxidation is Al_2O_3 and its oxidation kinetics is carried out by the formation of a protective oxide layer.

[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
[2] A. Herrera-Gomez, Internal Report. CINVESTAV-Unidad Querétaro. "Self-consistent ARXPS analysis for multilayer conformal films with abrupt interfaces," 2008.

[SIF-439] Improvement in the conductivity of transparent conductive thin films made with silver nanowires trough thermal and mechanical processes.

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The wide expansion and dependence of optoelectronical devices around the world has produced the massive exploitation of different materials and the achievement of new ones. Some of those devices demand conductive materials which on being synthesized in thin film shape have as high charge carrier density as possible in its conductive band while allow the transmission of visible light, that means, conductive and transparent layers that can be used as transparent electrodes in devices like solar cells, LEDs, OLEDs, and touch and flexible screens. Currently, the transparent conductive oxides have been used to this propose, specially the ITO (Indium Tin Oxide), a composition which has some drawbacks, like the fact that Indium is a scarce element and the films have ceramic properties that make them useless in flexible devices, a future technology. For that reason, it is necessary to find out a new alternative to replace it [1,2].

Within the candidates that have been studied are organic and nanostructured materials. By our side, we have worked with structures of silver nanowires (Ag NW) to make thin films over glass substrates, obtaining promising results. We fabricated the Ag NW thin films by the Spin Coating process, which is a cheap and easy method that allows the adjustment of several fabrication parameters to obtain different products. In this way, the Ag NW film physical properties depend of the solution composition as well as of the parameters used in the thin film fabrication, like solution viscosity, solvent evaporation rate, angular frequency, rotation time and drying temperature [2,3]. In Fig 1 it is shown a SEM image of a deposited film. One of the purposes is to find the best parameters of film fabrication, here each film was made with a quantity of three drops of material dissolved in ethanol, scattered over the glass by rotation with an angular frequency of 3000RPM for 3 min at room temperature. Just a solvent fraction is evaporated in the processes of rotation; therefore, the films are dried on a hotplate at 100 °C during 10 min. After fabrication, the films are characterized as follows: the electrical properties were measured by four-point probe technique, finding sheet resistances lower than 30 ?/sq, the optical properties by transmittance which gave an average value of 80% at 550 nm wavelength and the morphological and structural properties with SEM [3]. These results allow us to augur the nanostructured films as promissory candidates to replace the expensive and scarce ITO, the current material used to fabricate the transparent electrodes.
Despite these results, there are some drawbacks to solve, for example the high contact

resistance between nanowires. Because of this last, we have probed two different extra processes to try to improve the electrical contact between the nanowires. This processes pretend as well getting more homogenous films without affecting its light transmittance [4]. The first one is the nanowire welding by heat treatment. In this method the films are exposed to high temperatures (120-190 °C) during different time intervals, achieving a kind of junction in some of the contacts and reducing the sheet resistance in a percentage magnitude of up to 50,1%. In this process it was observed the material degradation after a certain temperature. The second applied method is the application of pressures on the films; in this method, we applied a force between 2 and 10 Ton-Force during different time intervals over the films surface achieving a sheet resistance decrease in a percentage magnitude of up to 75,9%. The results show an improvement in the electrical conductivity of the metallic nanowire films after the welding processes without apparent variations of thin film transmittance.

References

[1] Din, D. A., K. N. Hui, S. Hui, P. Kumar, J. Singh.(2013). *Silver nanowires a promising transparent conducting electrode material for optoelectronic applications*. ASP, 2, pp.1-21.

[2] Hossinzadeh Khaligh, H. (2013). *Silver nanowires electrodes fabrication characterization and device integration.* Thesis. Waterloo Ontario Canadá.

[3] F. Yakuphanoglu and R. S. Anand, (2010). *Charge transport properties of an organic solar cell*. Syn. Met, vol. 160, no. 21, pp. 2250–2254.

[4] Langley DP, Lagrange M, Giusti G, Jiménez C, Bréchet Y, Nguyen ND, Bellet D (2014). *Thermal annealing effects on silver nanowire networks*. Nanoscale. 6(22):13535-43.

THEORY AND SIMULATION 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
Oral and poster presentations are welcome.

TSM-219] Influence of Li insterstitial Doping on the Optoelectronic Properties of WO3 and NiO

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Electrochromic materials are materials that change their optical properties by ionic insertion/extraction through the application of an electric field. These materials can be used to control energy consumption and heat dissipation in devices such as smart windows, visors, touch screens, sunglases, rearviews, etc. In this talk we shall deal with the progress done in the last years in the development of these devices. We shall discuss the shortcomings and show the experimental and theoretical advances. Emphasis is given to theoretical research we have carried out, based on ab-initio calculations, on the optoelectronic properties of transition metal oxides doped with lithium, one of the most important ions inducing electrochromism. Our research, shows that lithium interstitial doping turns materials metallic and severely affects the optical absorption in the infrared and visible regions.

[TSM-240] NO2 adsorption on pristine and Pt deposited SrTiO3(110), a DFT study

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Total energy density functional theory (DFT) calculations were performed to investigate the nitrogen dioxide (NO_2) adsorption on pristine and platinum (Pt) deposited on strontium titanate ($SrTiO_3$) surface (110). NO_2 is one of the anthropomorphic generated atmosphere pollutants that produce health issues. In this work we studied the NO_2 adsorption with $SrTiO_3$ surface (110). Platinum adatom on the surface is considered in order to improve NO_2 adsorption. First, we studied the platinum adatom on different high symmetry sites. Due to NO_2 polarity van der Waals interactions were considered. PDOS, charge density maps and isosurfaces of pristine $SrTiO_3$, platinum most stable configuration and NO_2 structures with larger adsorption energies. As further work NO_2 degradation will be studied.

[TSM-241] NO2 adsorption on Pt/Graphene: a DFT study

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At the present, the environmental pollution is a problem of global interest, therefore, in this investigation we perform ab initio calculations of NO_2 adsorption on platinum deposited on graphene surface and platinum doped graphene. Effective adsorption is helpful for removing NO_2 from air. The calculations were carried out by means of computational modeling using the Quantum ESPRESSO package. This software works within the framework of the Density Functional Theory (DFT). Ultrasoft pseudopotentials were used to model the electron-ion interaction. The exchange-correlation functional was treated by the generalized gradient approximation (GGA) with the parametrization of Perdew-Burke-Ernzerhof (PBE). We used an optimum value of K points of 6x6x1 and 60 Ry cutoff energy for the wave function. Several high symmetry sites were tested for platinum deposition and NO_2 molecule adsorption. The electronic properties of the most stables configurations were calculated. The adsorption energies values show that chemisorption take place on platinum doped graphene. This result suggest that platinum doped graphene could be used for removing NO_2.

Key words: Graphene, NO_2, platinum, adsorption, DFT.

[TSM-245] First-principles calculations of the structural, magnetic and electronic properties of AlN (0001)-(2x2) surface with Ni absorption and incorporation.

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Structural, electronic and magnetic properties of the nickel doped AlN (0001)-(2×2) surfaces are investigated using spin polarized periodic density functional theory calculations as developed in the PWscf code of the quantum ESPRESSO package. The surface is treated according to the supercell approach with a 2x2 surface periodicity. Four high symmetry sites were considered, taking into account different coverage: ¼, ½, ¾ and 1 monolayer (ML). The Ni adsorption exhibits the H3 site as the most favorable structure in all different coverages from ¼ to 1 ML. When coverage is in the range from ½ to 1 ML, structures show ferromagnetic (FM) phase. The reconstructions exhibit the formation of dimers, trimers and atomic chains in the ½, ¾ and 1ML coverage, respectively. In the incorporation, T4 site is the most stable structure with a non-magnetic behavior in all the systems. The deposit of Ni into substitutional sites suggests the possibility of growing NiN epitaxially. The ¼ ML exhibits a FM behavior, in the ½ ML the structure is AFM and higher coverages are non-magnetic. We employed the surface formation energy formalism to investigate the different structures stability. Results indicate that the Ni doping is favorable under Ni-rich conditions in all the range of chemical potential ÃƒÂ¢Ã‹Â†Ã¢Â€Â µAlN. The density of states shows that only the 1st ML of surfaces is metallic, in contrast layers beneath the first layer are semiconductor, where the valence and conductions bands are mainly formed by the N-p and Al-p orbitals, respectively.

[TSM-255] Thiolated Gold clusters: a polyhedra approach to explain their structure

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The nanotechnology field has in the thiolated gold clusters its main candidates to potential applications with a promise to improve our lives. On the experimental side, thiolated gold clusters are easy to synthesize but the main difficulty is found in their size separation. Regarding the theoretical side, it is neccesary to propose a simplification to explain all the reported structures (more than 80) so far. In this talk, I will deliver a study and an update of a recent approach proposed to explain the structure and size of thiolated gold clusters. Our approach is able to explain the thiolated gold clusters in terms of assembly of tetrahedra and octahedra. Interestingly, the dispersion on angle and bond distances values can be quantified and used to characterize them. Moreover, the importance of this study is that new models of thiolated gold clusters can be proposed based on our new geometricla approach.

[TSM-267] Structural and electronic properties of pollutant molecules adsorption on blue phosphorene

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Since the discovery of the two-dimensional (2D) materials such as Graphene, silicene, germanene, etc., with unique optical, electrical, mechanical, transport and gas sensing properties, the interest in the study of these 2D systems has increased significantly. Searching for new alternatives of gas sensing devices, it has been found that one of the most stable allotropes of phosphorus, the blue phosphorene, is a good candidate for such applications. Blue phosphorene is an indirect gap semiconductor with an energy gap of the order of 2 eV, with buckled honeycomb lattice and zigzag ridges. In this work, the density functional theory (DFT) is applied as implemented in the computational code SIESTA, to investigate molecules adsorption on pristine, Al- doped and a single vacancy blue phosphorene. Four molecules in the four high symmetry points are considered to explore the efficiency and versatility of the blue phosphorene. We show that Al-doped system improve the reactivity of the blue phosphorene, according to the interaction energy calculations, we obtain chemisorption in most of the cases. On the other hand, single vacancy systems present interaction energies between the pristine and Al-doped systems with magnetic properties in all cases. Finally, the pristine blue phosphorene exhibits the weakest interaction energies; in most of the cases we achieve physisorption with no magnetic properties. In the Al-doped and single vacancy, it is noted that they depend on the orientation of the molecule and the symmetry point where the molecule is. However it tends to dissociate, therefore we consider those systems as unstable. The density of states, show the decrease in the bandgap in all the cases and for the single vacancy systems, we can observe the difference in the states for spin-up and spin-down, and which elements and orbitals are the main responsible for the magnetic properties.

[TSM-281] Spin-polarized study in MoTe2 monolayer semiconductor

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Abstract—Using total energy calculations we found an intrinsic Zeeman splitting appearing when the inversion symmetry breaks in the $MoTe_2$ monolayer system. The Zeeman splitting causes out-plane spin polarization around K and K' high symmetry with points opposite spin direction.

I. INTRODUCTION.

Transition metal dichalcogenides (TMDs) have the general formula MX_2 (M = W, Mo; X = S, Se, Te) with an intrinsic direct band gap in the range of some 500 meV to 2 eV. In their monolayer form, these systems exhibit a giant spin-orbit interaction [1]. Spin–orbit coupling (SOC) is a relativistic effect that originates from the coupling between spin and momentum (p→) of particles in an internal electric field (E→). The SOC Hamiltonian has the form:

$$H^{SO} \sim \mu B(E\rightarrow \times p\rightarrow)\cdot \sigma\rightarrow mc2$$

where μB is the Bohr magneton, $\sigma\rightarrow$ is the vector of Pauli spin matrices, m is the mass of electrons and c is the speed of light, when an electron moves in the internal E→ field it experiences an effective magnetic field (Beff~(E→ × p→)/mc2) [2]. In low dimensional TMDs systems the SOC is a consequence of inversion symmetry broken. TMDs films with an even number of layers (including bulk and bilayers) exhibit inversion symmetry, which is explicitly broken in systems with an odd number of layers where the SOC increases when thenumber of layer decreases [3].

II. RESULTS

We calculated electronic structure of $MoTe_2$ monolayer(1L) with hexagonal space group D3h1 (#187) within the density functional theory using the full potential linear augmented plane waves method (WIEN2K) [5], the exchange–correlation energy calculations are used from thePerdew–Burke–Ernzerhof (PBE) functional form of the generalized gradient approximation (GGA) [6]. We found that the $MoTe_2$-1L has a direct band gap of 1.09 eV at

K symmetry point, as was reported experimentally by Ruppert et al. [7]. When we introduced the SOC to $MoTe_2$-1L system its valence band split around K and K' high symmetry points. Figure 1 shows the calculated in-plane electronic band structure for the $MoTe_2$-1L system, in our calculations we included the spin polarization effect. In the Fig.1 the atomic Mo-4d orbitals contribution to the electronic bands are showed by circles, where a large circle size corresponds to more charge within the atomic sphere, qualitatively showing thes pin-up and spin-down contributions to each electronic band [5]. The left panel shows the spin-up Mo-4d orbitals, where the calculated electronic bands from the M-K-Gamma directionthe spin-up Mo-4d orbitals are at the top of the valence bands, while Gamma-K'-M direction the Mo-4d orbitals are at the second bands below the top of valence bands. The right panel shows apposite results for the spin-down 4d-orbitals, namely: The spin-down 4d-orbitals are at the top of valence bands in the Gamma-K-M direction, while in the M-K-Gamma direction are the second band below the top of valence bands. The inset in the figure shows the in-plane path used. Our calculation shows that although the K and K' high symmetry points are equivalent in the reciprocal space, the calculated electronic bands show an asymmetry as a function of spin polarization. This asymmetry found of the calculated electronic band structure is due to the coupling between electron spin and anintrinsic effective magnetic field that translates to a Zeeman splitting.

III. CONCLUSION

$MoTe_2$ system has a high potential for spintronics and flexible electronics applications due to the intrinsic spin polarized effect in its monolayer form.

ACKNOWLEDGMENT

This work has been support by CONACYT

REFERENCES

[1] Kuc, A. and Heine, T. (2015). Chemical Society Reviews, 44(9), 2603-2614.

[2] Manchon, A., Koo, H. C., Nitta, J., Frolov, S. M., and Duine, R. A.(2015). Nature materials, 14(9), 871-882.

[3] Kuc, A. and Zibouche, N. and Heine, T. (2011). Phys. Rev. B 83, 245213.

[4] Zibouche, N., Philipsen, P., Kuc, A., and Heine, T. (2014). PhysicalReview B, 90(12), 125440.

[5] P. Blaha, K. Schwarz, G.K. Madsen, D. Kvasnicka, J. Luitz.: wien2k.Vienna, Austria (2001).

[6] Perdew, J. P., Burke, K., and Ernzerhof, M. (1996). Physical review letters,77(18), 3865.

[7] Ruppert, C., Aslan, O. B., and Heinz, T. F. (2014). Nano letters, 14(11),6231-6236

[TSM-282] The Electronic States of MoS2-ITO: Experiment and Theory

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The electronic states for indium-tin-oxide/molybdenum disulfide ($In_2Sn_2O_7/MoS_2$) crystal interface have been calculated by meaning of density functional theory using CASTEP code with ultrasoft pseudopotentials and revised Perdew-Burke-Ernzerhof (RPBE) functional in General Gradient Approximation (GGA). All molecular models were built using experimental information from atom probe tomography measurements on ITO-MoS_2 thin films as previously reported [1,2]. The experimental APT data indicates no segregation between species; however, some oxygen-molybdenum chemical bonding was detected corresponding to vertical <101>-direction growth of 2H-MoS_2 crystallites onto ITO during RF-sputtering deposits. The density of states indicate a semi-metallic character which are in agreement with Ohmic behavior of resistivity values of ρ ~24-27 (Ω/m) as measured by four-point probe in ITO/MoS_2 thin film samples.

References

[1] Manuel Ramos *et al.*, "Mechanical properties of RF-sputtering MoS_2 thin films", IOP: Surf. Topogr.: Metrol. Prop. 5 (2017) 025003.

[2] Manuel Ramos *et al.*, "Study of indium tin oxide MoS_2 interface by atom probe tomography", MRS Communications, doi:10.1557/mrc.2019.150

[TSM-300] Adsorption and incorporation of Cr atoms in the GaN(111) surface

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Structural, electronic and magnetic properties of the Cr adsorption and incorporation into the GaN(111)-(2x2) structure yields a CrN epitaxial growth. Spin-polarized total energy calculations have been done using the periodic density functional theory plus Hubbard correction (GGA+U) with 1<U<7 eV, as developed in the PAW (projector-augmented wave method and a plane wave bases set) of the VASP code. Different coverage of Cr is considered from ¼ monolayer (ML) up to a full ML. Highest symmetry sites are considered to explore the Cr adsorption: H3, T4, Top and Bridge. Surface formation energy calculations indicate that in all the chemical potential range, from N-rich to Ga-rich conditions, CrN bilayer formation is the most stable structure due to Cr incorporation into GaN. Epitaxial growth of the CrN(111)//GaN(111)-(2X2) is observed at the NaCl structural phase. Electronic properties of the most stable structures were investigated by calculating the total density of states (DOS) and projected DOS. The DOS calculations showed a metallic behavior of CrN(111), the main contribution around the Fermi level are obtained from *p* and *d* orbitals of N and Cr atoms, respectively. Moreover, the CrN(111) displays a ferromagnetic behavior as a result of the strain present in the coupling structure.

[TSM-319] Rigidity on chemical bonds of carbon nanostructures under strain

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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 (0*D*), nanotubes (1*D*), graphene (2*D*) and diamond (3*D*), are just a few examples that demonstrate the structural versatility of carbon, which can form a wide variety of nanostructures based on theirs hybridizations, with some of the type; *sp–, sp^2–, sp^3–* or *sp^2–sp^3*. The stretching bond force constants ($\boldsymbol{K_r}$) 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, $\boldsymbol{K_r}$ values describe the stiffness of the chemical bond when the bonds are under strain. In this study, $\boldsymbol{K_r}$ values calculated with Density Functional Theory for different carbon nanostructures are analysed. The results showing to *sp* hybridization with the largest $\boldsymbol{K_r}$ value.

[TSM-331] Electromagnetic simulations of gold nanorod optical properties.

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We are presenting the analytic comparison of electromagnetic absorption simulations of gold nanorods by discrete dipole approximation (DDA), finite difference time domain (FDTD), T-Matrix and finite element methods (FEM). A linear correlation is presented between the experimental data as well as FEM simulations to show the nanorod dependence respect to the size (minor – major semi-axis).

[TSM-332] Surface structures of magnetostrictive D03-Fe3Ga(001)

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First-principles total energy calculations and scanning tunneling microscopy experiments were performed to study the surface reconstruction on the magnetostrictive Fe_3Ga alloy. The inverse magnetostrictive behavior was evaluated in the bulk by compressing and stretching its lattice parameter, showing an increase in magnetic moments as strain increases. Surface analysis demonstrates two thermodynamically stable surfaces, the 1×1 and 3×1. The 1×1 is an ideal FeGa terminated surface, whereas the 3×1 is also FeGa terminated but it has a first-layer Fe atom substituted by a Ga atom every three unit-cells, forming a row-like surface structure. Tersoff–Hamann scanning tunneling microscopy simulations were obtained and compared with experimental results. We found excellent agreement between theory and experiment, in which the distance between rows is ~12.3 Å. Theoretical findings suggest that the substrate-induced strain may increase the stability of the 3×1 reconstruction. Analysis of the magnetic moments in the reconstructions showed that their behavior is affected by a surface effect, as well as by the inverse magnetostriction of the structure. A good understanding of the atomic reconstructions of the magnetostrictive Fe_3Ga alloys is an important step towards the understanding of its surfaces. Also, Fe_3Ga is a potential candidate for perpendicular magnetic tunnel junctions due to the existing perpendicular magnetic anisotropy effect when grown on different substrates.

We thank DGAPA-UNAM projects IN101019 and IA100920 and CONACYT grants A1-S-9070 for partial financial support. Experimental part of this research supported by the US Department of Energy, Ofi¬ce of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-06ER46317. Calculations were performed in the DGTIC-UNAM supercomputing center project LANCAD-UNAM-DGTIC-368. The authors

thankfully acknowledge the computer resources, technical expertise and support provided by the *Laboratorio Nacional de Supercómputo del Sureste de México*, CONACYT member of the network of national laboratories. JGS acknowledges THUBAT KAAL IPICYT supercomputing center for computational resources. The authors would like to thank E. Murillo, and A. Rodriguez Guerrero for technical assistance and useful discussions. Image analysis was performed by Gwyddion software package.

[TSM-335] Analysis of the non-collinear antiferromagnetic IrMn3 surface and exchange-biased IrMn3/Fe heterostructure from first principles

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We provide a complete and systematic first-principles study on the thermodynamic stability, structural parameters and magnetic properties of the T1 non-collinear antiferromagnetic $L1_2$-$IrMn_3$ surface and exchange-biased $L1_2$-$IrMn_3$/Fe heterostructure. We compare four atomic configurations and propose four possible magnetic arrangements taking into consideration the symmetry breaking at the interface. We find two stable terminations for the surface and heterostructure, which are in good agreement with experimental HR-TEM data. Using a comparative approach, we analyzed the exchange-bias properties in the heterostructure, discovering that the number of Mn-Fe interactions at the interface is related to the exchange bias intensity. This finding could lead to novel exchange-bias tailoring methods by controlling the terminating layers. Finally, we are able to accurately describe the interface magentic coupling atom-by-atom, and we find a relationship between antiferromagnetic order near the interface and stability of the heterostructure. Our analysis provides a possible mechanism for the appearance of exchange bias in non-collinear/collinear heterostructures, and the results are in good agreement with experimental hysteresis measurements of the $IrMn_3$/Fe bilayer.

We thank DGAPA-UNAM projects IN101019 and IA100920, and Conacyt grant A1-S-9070 for partial financial support. Calculations were performed in the DGCTIC-UNAM supercomputing center through projects LANCAD-UNAMDGTIC-051 and LANCAD-UNAM-DGTIC-368. The authors thankfully acknowledge the computer resources, technical expertise and support provided by the Laboratorio Nacional de Supercómputo del Sureste de México, CONACYT member of the network of national laboratories. The authors acknowledge THUBAT KAAL IPICYT supercomputing center for computational resources. The authors would like to thank E. Murillo, and A. Rodriguez Guerrero for technical assistance and useful discussions.

[TSM-352] Looking for new physics of novel 2D materials

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The isolation of graphene using the mechanical exfoliation technique opened the posibility of obtaining other 2D crystals for the investigation of their physical properties [1,2]. Indeed, short after the first reports on the physical properties of graphene, other 2D materials were isolated and investigated [2]. Thanks to simulations, we have an estimate of potential 2D crystals that can be obtained by exfoliation which amount to ca. 1800 [3]. Although highthroughput computation has been an important tool to investigate all of these materials [4], the level of detail is somewhat deficient for investigating new physical properties. In this talk, I will present some of the interesting physical properties that we have found in new 2D materials.

[1] Novoselov, K. S. et al. Electric Field Effect in Atomically Thin Carbon Films. Science 306, 666669 (2004).
[2] Novoselov, K. S. et al. Two-dimensional atomic crystals. PNAS 102, 1045110453 (2005).
[3] Mounet, N. et al. Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. Nature Nanotech 13, 246252 (2018).
[4] Haastrup, S. et al. The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals. 2D Mater. 5, 042002 (2018).

[TSM-404] Study of Structural, Electronic and Optical properties of Armchair, Zigzag and Chiral Silicon/Germanium Alloy Nanotubes

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In this work, a theoretical study was held using density functional theory implemented in siesta code which utilizes linear combination of atomic orbitals and a Perdew-Burke-Ernzerhof norm-conserving generalized gradient approximation potential. For a collection of infinite nanotubes made up of silicon and germanium alloy (SiGeNTs), within which there were modeled armchair, zigzag, and chiral type structures, structural optimization was carried out until forces on atoms were lower than 0.0001 eV, also band structure, density of states, and cohesive energy were computed. Furthermore, aiming to obtained absorption spectrum, optical computation was setup in an interval of 0-10 eV and with a broaden of 0.05. Optimized structures of SiGeNTs exhibit deformation of the structure on surface, moreover, it seems that buckling of surface is related with stability. In another hand, armchair and zigzag tubes are direct semiconductor materials, while chiral ones shift from indirect(for systems with diameter lower than 1nm) to direct band gap(for systems with diameter grater than 1nm) semiconductors. Likewise, it was found that band gap depends on size. Finally, peaks in absorption curves were associated with density of states through Van Hove singularities. Previous results on structural and electronic properties elucidate the possible application of SiGeNTs in thermoelectrics, photovoltaics and nanoelectrics, plus the possibility of associate absorption curves with density of states provides a method for characterization.

Kerwords: Density Functional Theory, Silicon-Germanium Nanotubes.

[TSM-411] A DFT study on the austenitic Ni2MnGa (001) surfaces

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Through the use of spin-polarized density functional theory calculations we have studied the different (001) surface terminations of austenitic Ni2MnGa. The stability analysis revealed a preference to form MnGa terminated surfaces in a large range of growth conditions, Ni-terminated surfaces are stable as well. The dominant structure, is the one engineered to be Ga-terminated, but that appears under Ga-rich conditions. STM images were simulated for all surface terminations and compared with the images obtained experimentally by Leicht et al. New J. Phys. 13 (2011) 033021. We found a perfect match between theory and experiment for MnGa and Ni terminations. From the STM images of the MnGa termination, the Mn atoms are strongly imaged, while the Ga atoms are weak. Whereas for the Ni terminated surface, there is a large local density of states due to the Ni atoms with an appreciably contribution due to the second monolayer Mn atoms. Magnetic characterization revealed surface effects on the MnGa and Ni terminated surfaces, whereas the Ga terminated experienced no change. Our results give insight about what is observed in the experimental STM images

[TSM-413] First Principles Studies of optical properties of pure and doped hydroxyapatite.

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Hydroxyapatite (HAp) [Ca10 (PO4) 6 (OH) 2] is the main mineral component of bones, 70% by weight of human bone is a modified form of hydroxyapatite. HAp provides toughness and rigidity to bones, which is why it is used for filling and support, but its applications can be so wide that it is used in ocular prostheses, as a dermal filler, biosensor and even as a drug release, all thanks to its biocompatibility, but also to the contributions of impurifying elements that improve its properties [1]–[4].
The main objective of this work is to model the optical properties of HAp in its hexagonal and monoclinic phases in its pure state and in the presence of transition elements as doping agents, using atomic and molecular simulation using the Quantum Espresso code. The imaginary parts of the function were calculated using the dielectric Density Functional Theory (DFT). The form of the dielectric function obtained using the exchange-correlation function PBE. The imaginary part is proportional to the absorption coefficient [5], the highest pole of the dielectric function in both phases of pure HAp is about 8 eV, far from the visible spectrum, however, characteristic absorption peaks in the visible spectrum are between 1.91 and 2.01 eV, in addition to high energy visible light absorption bands between blue and violet at 2.71 and 2.91 eV were observed by adding Dy atoms and Mn atoms respectively. Weak absorption peaks in the visible were found by adding Fe and Sm at 2.41 and 271 eV respectively, but more significant absorption peaks were observed in the ultraviolet region> 3.26 eV.

Key words: DFT, hydroxyapatite, optical properties, doped , visible spectrum .
REFERENCIAS

[1] M. Shafaei, F. Ziaie, D. Sardari, and M. M. Larijani, "Thermoluminescence properties of gamma-irradiated nano-structure hydroxyapatite," *Luminescence*, vol. 31, no. 1, pp. 223–228, 2016.
[2] C. S. Ciobanu, S. L. Iconaru, C. L. Popa, M. Motelica-Heino, and D. Predoi, "Evaluation of Samarium Doped Hydroxyapatite, Ceramics for Medical Application: Antimicrobial Activity," *J. Nanomater.*, 2015.
[3] K. A. Gross and C. C. Berndt, "Biomedical Application of Apatites," *Rev. Mineral. Geochemistry*, 2002.
[4] M. E. Zilm *et al.*, "Hydroxyapatite substituted by transition metals: Experiment and theory," *Phys. Chem. Chem. Phys.*, vol. 18, no. 24, pp. 16457–16465, 2016.
[5] L. A. Avakyan, E. V. Paramonova, J. Coutinho, S. Öberg, V. S. Bystrov, and L. A. Bugaev, "Optoelectronics and defect levels in hydroxyapatite by first-principles," *J. Chem. Phys.*, vol. 148, no. 15, pp. 1–14, 2018.

[TSM-176] Electronic and vibrational properties of porous silicon carbide

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In recent years, silicon carbide (SiC) has been the subject of many studies due to its attractive properties, that allow devices with this material to operate in adverse conditions of high temperature owing to its high melting point (around 1700°C) and wide bandgap (between 2.36 eV and 3.3 eV). The nanostructures of this material have been studied widely, mainly focused in nanowires, and only a few on the properties of porous silicon carbide (pSiC), which is attractive for applications in H sensors and supercapacitors, due to its high surface to volume ratio. In this work, the study of the electronic and vibrational properties of pSiC was performed using DFT and DFPT, respectively. The nanopore was modeled by removing Si and C atoms in the direction [001] of a perfect SiC crystal, according to the supercell method. The SiC supercell was formed by 2x2x1 cubic unit cells with periodic boundary conditions.

For the modeling 3 cases were considered, depending of ρ. Where ρ indicates the relationship between the number of silicon and carbon atoms that exist on the surface of the pore(ρ=nSi/nC, where nSi is the number of Silicon and nC the number of carbon atoms respectively). Thus, the case rich in silicon (ρ = 2), the case rich in carbon (ρ = 0.5) and the case with the same proportion of silicon and carbon (ρ = 1) are presented.

The electron density of states and the band structures were calculated for the electronic study, and the density of phonon states and the infrared and Raman spectra for the vibrational study, obtaining results that indicate a clear dependence to ρ, since the properties between the case studies are completely different. These differences could be exploited for the development of electronic devices.

[TSM-224] Adsorption of acetic acid and benzoic acid on pristine and defect containing Graphene

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The modification of graphene with acetic acid (AA) and benzoic acid (BA) was performed through computational simulations using the density functional theory (DFT). Pristine graphene, graphene with vacancies and Stone-Wales defects were considered. Adsorption results on pristine and Stone-Wales defected grapehene show weak physical interactions with both molecules, as confirmed by the non-covalent interaction index. Functionalized graphene sheets have similar structural and electronic properties. On the other hand, by placing vacancies in its structure, graphene promotes strong molecule adsorption on the surface due to the dangling bonds in these systems. Chemical adsorption is present by having a stronger interaction between the acids and surface. Single vacancy graphene becomes metallic. However, upon functionalizing it with acetic acid and benzoic acid, the electronic properties become pristine-like, demonstrating that functionalization with weak acids does not change the electronic characteristics of graphene.

[TSM-225] SEMI-ANALYTIC FINITE ELEMENT METHOD APPLIED TO SHORT FIBER-REINFORCED PIEZOELECTRIC COMPOSITE

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In this work, the prediction of the effective properties of periodic transversely isotropic piezoelectric composites made of short piezoceramic unidirectional fibers (PZT) in a soft non-piezoelectric matrix (polymer) is presented. The effective properties are obtained by means of representative volume element method based on a semi-analytical approach of the finite element method (SAFEM). Here, in order to simplify the method, the calculations were done only in 1/8 part of the representative volume element, therefore, the focus is on an eighth of the square and hexagonal arrangements of cylindrical fibers in the composite. Three different approaches are proposed to calculate the effective coefficients: an analytical method based on the asymptotic homogenization method (AHM), a computational method linked to ANSYS mechanical APDL-SAFEM, and a numerical using finite element method (FEM). Special attention is given on definition of appropriate boundary conditions for the representative volume element and SAFEM to ensure periodicity. Finally, numerical computations by the three methods were performed and the results were compared and discussed.

Keywords: Short fiber-reinforced composites, piezoelectric composite, effective properties, finite element method, asymptotic homogenization method.

[TSM-229] Effective transport properties for periodic multiphase fiber-reinforced composites with complex constituents and parallelogram unit cells

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The two-scale asymptotic homogenization method (AHM) is used to find closed-form formulas for effective transport complex properties of periodic multi-phase fiber-reinforced composites (FRC). Examples for three- and four-phase composites with complex constituents and periodic parallelogram unit cells (PUCs) are considered. Anisotropic interphase effects on effective properties quality in relation to complex shear and anisotropic conductivity of biological tissue comprising tubular cells, such as skeletal muscle, are studied as a multi-phase FRC. Numerical validations are carried out through comparisons with other methods. Good agreement is obtained. The formulas may be useful as benchmarks for checking experimental and numerical results.

Keywords: multi-phase fiber-reinforced composites; interface/interphase; asymptotic homogenization method; effective complex permittivity; transport problems

[TSM-237] Germanium adsorption on TiO2-terminated LaTiO3 (001) surface

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For this work was modelled a TiO_2-terminated $LaTiO_3$ (001) surface (LTO), and Ge atoms were placed at different adsorption sites (Ti_{top}, O_{top}, Hollow, O_{valley} and Bridge) to study the effects of Ge chemical deposition on the electronic properties of such systems. The calculations were performed in the Density Functional Theory scheme, using the Hubbard-corrected Local Density Approximation. After the geometric optimization of each model, it was found that the Ge atoms are more strongly attached to the LTO at the O_{top} site: two Ge-Ti covalent bonds and one with ionic character (Ge-O) were formed. Besides, the system exhibits a ferrimagnetic order and has associated a greater electronic band gap (1.091 eV) than another of the studied systems. Likewise, the systems for the Ti_{top}, Hollow, O_{valley} and Bridge cases were ferromagnetic. Finally, it was found that the electronic density transfer between Ge atoms and LTO is the main mechanism to modulate the physical and adsorption properties of those systems. **Acknowledgments:** This work was partially supported by the multidisciplinary project IPN-SIP-2020-1114. J. M. Cervantes and J. E. Antonio would like to acknowledge the graduate scholarship from CONACYT and support from BEIFI-IPN.

[TSM-258] Cellular Automaton growth simulation and investigation on low- and high-index high anisotropy substrates

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MBE growth of GaAs on the surfaces with different orientations has been studied by kinetic Monte Carlo simulations. The models allow taking into account the most relevant processes and reconstructions on the surfaces. The simulations show that islands grown on the (111)A surface have a chaotic shape whereas those on the (001) and (110) surfaces have more ordered structure due to the features of the surface structure. The diffusion length of Ga adatoms is observed to be dependent on the growth rate and V/III flux ratio. [2]. In this work we apply a cellular automaton model that has been applied to urban growth simulation and has been able to explain similar phenomena that occurs in crystal growth like self-assembly processes [1]. The model is used to explore the growth process over the GaAs (631) surface and to make comparison with low index substrates. The MBE growth of GaAs on the surfaces with high index orientations has always being a challenging terrain but it has a full weight potential for application in high performance optoelectronic devices due to their special properties. In specific, the GaAs(631) has proved to have intrinsic anisotropic and kinetic properties of this ideal to achieve nanocorrugation and 1D QWs, whose geometry essentially depends on the growth temperature and III/V BEP ratio that is denoted by Π. Nevertheless, there are few studies about its growth process and a lot of mysteries and unrevealed growth parameters that are necessary to have a decent control and rightful power of analysis over this MBE template. These are the main reasons why we propose the application of a dynamic automaton model to simulate its growth processes. We seek to gain knowledge over the grow rate and the way the adatoms are distributed as a function of the Π = III/V BEP ratio. One of the outstanding results is to relate the growth simulation to the RHEED patterns observed and documented on the work In situ monitoring previously presented by this work group.

1REFERENCES

[1] A. A. Ontiveros Ciudades como tableros de ajedrez (2002) Introducción al.
[2] S.V Balakirev. Journal of Physics: Conf. Series 917 (2017) 03203

ACKNOWLEDGMENTS: The authors acknowledge the financial support from CEMIE-SOL 22, FRC-UASLP and CONACYT-Mexico through grants: CB 2015- 257358 and PNCPN2014-01-248071.

[TSM-266] Effect of electrical charge on the structural and vibrational properties of Au60

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Obtaining metallic structures with high symmetry at nanometric scales is highly desired due to its physical and chemical properties that will allow us to improve the understanding of the behavior of the metallic bonds, of the constituent elements and of their future applications; for example, self-assembly, drug distribution and medical therapy, molecular recognition and electronics, and catalysis. In this study we determined the structural and vibrational differences that the Au_{60} presents with different electric charges that go from a charge of +2 to -1, through a neutral one and finally that it presents two structures despite their difference in electric charge. Furthermore, the structures were characterized by vibrational calculation and their IR / Raman spectra show characteristics that allow them to be distinguished. Structurally we determine that a structure has triangles (being the most symmetric), while the other two have a compact part where distorted tetrahedra and octahedra can explain their atomic distribution.

[TSM-284] Determining the electronic structure of Indium-Tin-Oxide/MoS2 interface

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We report density functional theory (DFT) investigations to determine electronic structure on indium-tin-oxide/molybdenum disulfide ($In_2Sn_2O_7/MoS_2$) interface using DFT code CASTEP and with aid of experimental information from atom probe tomography (APT) measurements. All molecular models were built using experimental information from APT in $In_2Sn_2O_7/MoS_2$ tin films synthesized by RF sputtering. Experimental APT evidence indicates no segregation between species; however, oxygen-molybdenum bonding was detected corresponding to vertically aligned MoS_2 layers of 2H-MoS_2 onto $In_2Sn_2O_7$. Interface models show us that molybdenum disulfide creates a van der Waals interface with indium-tin-oxide with an adsorption distance of 3 Å, similar to graphene interlayer distance. Density of states analysis indicates a semimetallic character at the interface a result from the interaction of d and p orbitals which in turn reduces the work function of the interface system.

[TSM-289] Novel carbon nitride nanotubes featuring spikes-like structures whith potencial aplication as a drug delivery system for cisplatin (anticancer drug): A DFT study

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We present two new carbon nitride nanotubes, designed from a new two dimensional carbon nitride allotrope with 1:1 stoichiometry featuring Spikes-like structures. The nanotubes present the same Spike-like structures which are the more reactive parts of the nanotubes. The sp3 -like C atoms are bonded to isocyano groups projecting out of its surface and resembling spike-like formations.In terms of Hamada index we calculate the Nanotube CN (3,0) and Nanotube CN (5,0).

The adsorption Energy for the Nanotube CN (3,0) whit Cisplatin was -0.53 eV wich does a candidate for a drug delivery system for cisplatin. Adsorption energy around -1.30 eV is suitable for adsorption and administration of slow release drugs (Kotzabasaki et al). The IR spectrum of the Nanotube CN (3,0) shows a large intensity in the frecuencies due to the Spikes structures. Also the IR spectrum of the Nanotube (5,0) shows a large intensity in the frecuencies due to the Spike structures so we expect a favorable adsoption energy for this nanotube whith cisplatin and his potential aplication as a drug delivery system.We are currently expanding the study to another quiralities

[TSM-290] Study of dissociation and/or adsorption of NOx in new materials to defeat the pollution

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Nitrogen oxides (NOx) are polluting compounds that degrade air quality, this affect the society and the environment, and it is responsible of a variety of problems as the eutrophication, acid rain, cardiovascular diseases, for mentioning only few. How the fuel process produces circa of 95% of nitrogen oxides, they were taken as a basis for this study, where we simulated the interaction of these compounds with three recent fullerene-like structures. The first of them is called volleyballene (Sc20C60), and this material interacts with NO producing a little modification in its bond length, making it shorter. The other two structures were obtained by replacing 12 carbon atoms by 12 P or 12 N atoms obtaining tetrahedral and icosahedral structures, respectively. When we study the interaction of Sc20C48N12 with one or six NO molecules located inside, we observed the dissociation of three molecules of NO, and the bond length are modified in the rest of those molecules. For the case of volleyballene doped with P atoms (Sc20C48P12), we observed tge formation of P-P bond, making the structure more stable when it interacted with one, two and four molecules of NO, and it displayed dissociation of up to three molecules of NO.

[TSM-304] Effect of ligands in NO2 absorption on porphyrin

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In this study, the potential applications of Porphyrin complexes as gas sensors at room temperature are addressed. It is analyzed the modification of their related structures, with an emphasis on the displayed bonding, adsorption energies, and vibrational properties. We showed using the ORCA's geometric optimization that Porphyrin-Ruthenium (Por(Ru)) is able to absorb CO and NO with an absorption energy of -2.95eV and -2.04eV respectively. However, it is not able to absorb NO2. To solve this, it is proposed the modification of the Por(Ru) ligands. In this case, we added four new ligands and we analyze them. Porphyrin-Ruthenium-ligands complexes are able to absorb NO2 (with lowest adsorption energy -1.11eV) . Further, we analyze the contributions of CO-OH and NH2 groups interacting with phenyls as ligands, and similarly simpler ligands. It is presented the assignment of their IR/Raman signals is carried out in order to facilitate their experimental detection. Finally we discuss the change of Porphyrin complexes HUMO-LUMO gap when a gas is absorbed.

[TSM-305] The Au22-xAgx(SR)17 clusters: doping and ligand effects on their structural and vibracional properties

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In this work, a DFT study of bimetallic thiolated gold clusters is addressed. We substitute 1 and 2 gold atoms by silver atoms in the parent $Au_{22}(SR)_{17}$ cluster. The isomers of minima energy were determined, and the ligands were varied. When –SH, $-CH_3$ y -Ph were considered a major/minor distortion was obtained with respect to -SH ligand. Calculated IR/Raman profiles showed more intense peaks when the -Ph ligand was used IR/Raman and it can be correlated with the induced distortion

[TSM-306] Raman spectrum and density of states of graphite and graphene layers, a DFT study.

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The study of materials with applications in solar cells or for hydrogen storage is one of the most important topic in the last three decades. In particular the study of carbon materials have discovered important structures, such as carbon nanotubes or graphene. In this DFT study we begins with the build up of a hexagonal closed packed crystal structure of graphite. Then we create graphene with one two and three parallel layers. With Castep module, geometric optimization are realized for graphite and their different layers. For graphite and the three layers we report the result of their optimized lattice parameter, electronic density of states, vibrational frequencies and Raman spectrum. Our results are in good agreement with experimental results reported in the literature.

Keywords: graphite, graphene, Raman spectrum, DFT study.

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[TSM-314] Exposed Surface and Confinement Effects on the Electronic, Magnetic and Mechanical Properties of LaTiO3 Slabs

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The search for new materials, that fulfill the more demanding functions associated to novel electrochemical systems, lead to explore the free surfaces of certain compounds. Then, for this work, were studied the quantum confinement and surface effects on the structural, electronic, magnetic and mechanical properties of $LaTiO_3$ (LTO) slabs using the Density Functional Theory. LTO slab models were proposed varying the thickness and the exposed surface, with LaO- and TiO_2-terminations. Results showed that all LTO slabs are semiconductors, regardless of the thickness of the exposed surface, contrasting with the bulk. Besides, thicker LTO slabs are ferrimagnetic, while thinner ones are antiferromagnetic. Furthermore, Young´s modulus increases gradually with increasing the thickness of the slabs, while the G/B ratio indicates the slabs are brittle as well as Poisson´s ratio indicates their bonds are covalent.

Acknowledgments: This work was partially supported by the multidisciplinary project IPN-SIP-2020-2106. J. E. Antonio would like to acknowledge the graduate scholarship from CONACYT and support from BEIFI-IPN.

[TSM-333] New modelling and map process design of the Laser Cladding phenomenon

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The laser cladding process was simulated using a mathematical model and a finite element analysis software. The laser cladding parameters used to obtain the melt pool characteristics where the scanning speed of the laser and the laser power.
The model was used to create a map process for the Laser Cladding phenomenon by describing different variations of the laser power and scanning speed and their effect on the characteristics of the melt pool created. Regions with defects such as keyholing and undermelting where identified as functions of the energy deposited.

[TSM-336] Stress influence on the electronic properties of zigzag carbon nanowires

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

[TSM-359] A density functional theory study on the stretching bond force constants of boron and boron nitride chains

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Using density functional calculations, the stretching bond force constants (kr) describing a bond stiffness of linear chains of boron (LBC), and boron nitride (LBNC) are determined. The effect of employing different exchange-correlation functionals for kr calculation is discussed using the local density approximation (LDA), the generalized gradient approximation (GGA) and two nonlocal hybrid density functionals (PBE0 and HSE06). A comparison between the kr values for LBNC of 10.56, 10.35, 10.99 and 11.00 mdyn/Å were presented using LDA, GGA, PBE0 and HSE06 respectively. Such comparison between these linear chains allowed for the elucidation of the effect and differences in bond stiffness of atomic boron substitution by boron nitride atoms inside an atomic linear arrangement. Our theoretical calculations suggest that under tension, linear boron nitride chains are highly stiffest nanomaterials.

[TSM-360] A density functional theory study on the bond force constants of benzene

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Density functional calculations are employed to determine stretching (kr) and bending (kθ) bond force constants appropriate to describe the bond stiffness of a benzene molecule. The effects of employing different exchange-correlation functionals for the calculation of kr and kθ is discussed using the generalised gradient approximation (GGA) and the local density approximation (LDA). We obtain a kr of 7.93 mdyn Å-1 and a kθ of 0.859 mdyn Å rad-2 using LDA, while kr = 7.67 mdyn Å-1 and kθ = 0.875 mdyn Å rad-2 using GGA. The parameters kr and kθ computed here can serve as an input to molecular mechanics or finite element codes of larger carbon molecules, which in the past had frequently assumed the same bond force constants for benzene and other carbon structures such as graphene and carbon nanotubes.

[TSM-403] Electronic Properties of N-doped ZnO

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ZnO structures with N doping at different concentrations were simulated through Ab Initio calculations to determine the electronic properties of the doped configurations, ranging from 3.125 to 12.5 %. At these concentrations, different configurations were used to check how the band structure and DOS are changing, affecting the typical ZnO DOS. It was found that depending on the configurations, changes on DOS are observed as the N was incorporated, depending on the position of the impurity and the percentage. The results showed that ZnO band gap energy is also affected directly and most of these structural configurations give states near to the top of the valence band, resulting in expected p-type semiconductor.

[TSM-408] Ab initio elastic constants for BaTiO3 and PbTiO3

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The Global Industry report in 2016, reported that the market for piezoelectric devices globally was valued at 1.17 billion us dollars. It is also important to highlight from the report that 60% of the piezoelectric devices are made of ceramic materials. the electronic industry is the main employer of this type of materials. In the field of research, piezo electrics are studied for their properties of energy conversion, both on a macro and micro scale. A simple way to determine the piezoelectric quality of a material is through the coupling coefficient, which determines the fraction of mechanical energy which is transformed into electrical energy. Classic piezoelectric materials such as quartz have a low coefficient, compared with composite materials such as barium titanate, $BaTiO_3$. These materials have a higher coefficient and therefore are more appropriate for conversion and obtaining uses of energy. In this work we present the elastic constants C_{11}, C_{33}, C_{44}, C_{66}, C_{12} and C_{13} for $BatiO_3$ and $PbTiO_3$ calculated with ab-initio DFT VASP code with PBESol approximation for exchange correlation approximation. Results are in good concordance with experimental values and other calculations.

THIN FILMS

Chairmen:
Dr. Alberto Duarte Moller (Universidad de La Salle Bajío), jduarte@delasalle.edu.mx

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

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

[THF-253] Influence of the deposition conditions and thermal treatment of ZnO by RF sputtering on the photovoltaic response of CdTe solar cells

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ZnO thin films grown by RF sputtering (Sp-RF) as a function of the deposition conditions: source power (P_s), deposition pressure (P), substrate temperature (T_s), partial pressure oxygen (P_{po}) and post thermal treatment (TT) were studied. ZnO thin films were characterized through profile thickness, optical measurements (Transmittance and absorptions), electrical resistivity measurements, X-Ray Diffraction (XRD), Energy Dispersive Spectrometry (EDS) and Scanning Electron Microscopy (SEM). As a part, buffer front layer, of the CdTe-based Solar Cell, Current-Voltage (I-V) as well as External Quantum Efficiency (EQE) measurements were carried out. Our results indicate that at major temperature the RF sputtered ZnO are polycrystalline without less in the transmittance response. The set of samples showed a resistivity of the order of 10^{o}-10^{2} â„¦-cm. The incorporation of the ZnO buffer layer film in the front contact improves the solar cell efficiency close to 7.4%, when the optimal conditions with a source power of 230W, 20 mTorr of deposition pressures and 300°C substrate temperature into the growth chamber, as compared to the CdTe-based solar cell, 6.0% efficiency, with the ZnO base layer with a P_s=140W, P=10 mTorr and T_s=250°C. When we use the optimal deposition conditions mentioned above, but without TT in the ZnO and combine them with a high heat treatment temperature to the thin film of ZnO+CdS of 500°C we obtain a photovoltaic efficiency of 10%.
Keywords: ZnO, buffer layer, thermal treatment, Sputtering RF, CdTe solar cells.

[THF-273] Characterization of MoO3 thin films deposited by laser ablation

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Molybdenum oxide thin films were deposited using the laser ablation technique, at three values of working pressure and four values of the mean kinetic energy (E_k) of the plasma ions. The structural characterization of the films performed by X-ray diffraction and Raman spectroscopies showed the presence of the α–MoO_3 phase in all cases. On the other hand, the value of the band-gap varied from 2.8 to 3.3 eV, depending on the experimental conditions. The XPS analysis showed a variation of the stoichiometry from $MoO_{2.5}$ to $MoO_{3.4}$ which could explain the variation of the band-gap.

[THF-302] ZnO:Al thin films prepared by sputtering using a target made by sol-gel

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ZnO is an n-type semiconductor with excellent physicochemical properties that can be applied in different devices. Taking advantage of some properties, like conductivity, and interaction with some chemicals as organic compounds, it could be used as a biosensor. Some works use chemical synthesis to get targets for sputtering and got a low conductivity and 90% of transmission in the visible region. In this research we made ZnO:Al thin films by sputtering using a pressed target of powders got by the sol-gel method. The precursor solution was made using ethanol as solvent, zinc acetate dihydrate, diethanolamine and aluminum as aluminum nitrate nonahydrate. Then, the solution was dried and calcinated to remove the remaining organic subproducts. Finally, the powders were pressed and sintered at 1000 °C. ZnO:Al thin films were compared with ZnO thin films obtained with the same process. The films were deposited by rf-magnetron sputtering using a power of 100 and 150 W, the distance between the target and substrate was 7 cm, and the argon pressure was 2x10-2 mbar. The structure identification agrees the zincite phase using x-ray diffraction and JADE software, the ZnO:Al target shows an increase for the (002) plane, the preferred orientation is more appreciable for the films. XRD shows an increase of crystallite when aluminum is added. The morphology was determined using scanning electron microscopy (SEM), the grain size grows with the increase of power. SEM analysis shows pinholes in ZnO thin films, these pinholes are not present in ZnO:Al thin films. The resistivity (ρ) of films was calculated by the transfer line method (TLM), the lowest ρ was 7x10-2 ohm cm for ZnO:Al thin film deposited at 150 W and the bigger is 1x105 ohm cm for the ZnO thin film deposited at 100 W, 7 orders of magnitude of difference, this can be explained by the decrease of defects and grains limits when we increase power and add aluminum. The results indicate that the addition of Al to ZnO and the increase of power in the deposition are important variables to get thin films with good physical properties. These thin films can be used to develop biosensors due its good physical properties and biocompatibility, this investigation is still in process.

[THF-365] Study of optoelectronic properties of hybrid heterojunction based on CdS and PVA/Phenyl boronic acids for sensing applications

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Organic small molecules as phenylboronic acids (PBA) have been used in flexible electronics in the last years, specially in optoelectronic devices due to it is optical properties, they are also used in electrochemical biosensors in combination with polymeric chains for thin films deposition as sensing layers. It is known that homogeneous thin films can be produced by the deposition of a complex based on phenylboronic acids and polymers as polyvinyl alcohol, SEM studies suggests that homogeneity and low thickness can be obtained. In this work, we present the study of the microstructural behavior of a controlled thin films deposition of phenylboronic acid molecules into a PVA matrix as a polymeric component deposited on CdS layer as a proposal for sensing applications. CdS thin films were deposited by chemical bath deposition. SEM micrographs verify high superficial homogeneity properties and low thin film thickness in transverse characterization mode. 300 nm to 900 nm emission-absorption analysis suggests homogeneous behavior on deposited thin films where absorbance intensities around 300 nm region shows variation according to deposition technique, and at 460 nm for photoluminescence. Also, electrical characterization shows current mobility over the hybrid heterojunction on different proposed structures.

[THF-410] Metals infiltration on copolymers for oxides obtention

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Nowadays polymer thin films infiltration is a little crowded area of study which offers a wide range of solutions to problems in optoelectronic industry. The study of polymer structures known as block copolymers due to its molecular accommodation infiltrated with metals as Al, Cu Ti and Zr. Obtaining metal oxides represent a huge advance in selective deposition techniques and a way to reduce time and investment cost in lithographic area. For this purpose, (Atomic Layer Deposition) ALD technique was used, some advantages of this technique are great conformity of deposited thin film and deposit thickness control, compared with other techniques such CVD or PVD. In addition, the metal infiltration was also made through wet chemistry with metal salt inclusion by using spin coating. The most important parameters to be considered for deposit were, in ALD: pulse time and substrate temperature. About Spin coating: rpm, viscosity, and precursor quantity. (X-Ray Photoelectron Spectroscopy) XPS characterization was made, this is optimal technique for qualitative and quantitative analysis. Last analysis allows the film thickness and composition trough the analysis of the sample at a different angle of incidence known as (Angle Resolve X-ray Photoelectron Spectroscopy) AR-XPS in addition FTIR and Raman were used for structural characterization, functional groups identification and molecular vibrational modes respectively.

[THF-446] THIN FILMS OF SEMICONDUCTOR NANOFIBERS WITH ELECTRONIC AND PHOTOCATALYTIC APPLICATIONS

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Electrospinning is a simple and versatile method for fabricating continuous fibers with diameters ranging from several nanometers to micrometers. This technique is typically applied to obtain polymer nanofibers. The combination of appropriate polymers with semiconductor precursors enables the formation of composite fibers, which after calcination results in crystalline semiconductor nanofibers. In this talk, we describe the electrospinning processes to obtain thin films of NiO-p and ZnO-n semiconductor nanofibers (NFs). We also analyze their main structural and morphological properties. Then, we describe the direct single step deposition of p-type NiO nanofibers on n–type Si substrate, which electrical response was analyzed in dark and under UV light illumination. The results show that the NiO-p NFs/Si-n heterostructure works as a self-powered photodetector of UV radiation. The responsivity of the fabricated photodetector was calculated to be 9.1 mA/ W-1 at zero bias. On the other hand, the ZnO-n NFs thin films deposited on glass substrates were homogeneous, crystalline with the intrinsic porosity of the fibers morphology and very well adhered to the glass substrates. The ZnO NFs thin films were then applied to the photodegradation of methylene blue (MB) in aqueous solutions activated by sunlight. The results show that the nanofibers thin films produce 96.4% degradation percentage of the MB solutions. After the photodegradation experiments, the photocatalytic thin films remained integral and well adhered to the substrate, then they were reutilized in subsequent photodegradation experiments.

[THF-448] The Effects of Variables like Humidity in Dip-coated Thin Films

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The technique of dip-coating is a time and cost efficient way to fabricate thin films, as is the sol-gel process for the synthesis of nanomaterials. Certain variations of factors such as temperature of calcination of the film, as well as environment humidity greatly impact the quality of the films created. The effects are visible when the films are characterized by the XRD or UV-VIS methods. The present work searches to explore and compare the films generated when these factors, especially humidity, have been further controll

[THF-149] Comparison on the structural and mechanical properties of TiN films with Zr inclusion produced by DC and RF magnetron co-sputtering

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Transition metal nitrides films are used as protective coatings to enhance properties of the substrate material. Particularly, titanium nitride (TiN) has been used for cutting and mechanical tools, and as diffusion barriers in the semiconductor industry. While, the zirconium nitride (ZrN) has drawn attention for its better corrosion resistance, lower electrical resistivity, better mechanical properties than the corresponding properties of the TiN. In the other hand, physical vapor deposition techniques, and especially magnetron sputtering deposition, have proven to be a versatile, environmentally friendly and industrially scalable route to grow such engineering materials.
In this regard, this work was focused on the synthesis and characterization of TiN coatings with the addition of Zr by dual confocal magnetron sputtering technique, starting from two independently driven targets. The stoichiometric of TiN was achieved by variations of the N2 percentage in the mixed atmosphere Ar: N2 in a fixed volumetric flow. After to obtain the optimum deposition condition for stoichiometric TiN coatings, Zr was included in the TiN using a co-sputtering process to identify the effects that it produced in terms of composition and structure, this was achieved varying the power applied to the Zr target (using DC power supplier) and fixing the radio-frequency power applied to the Ti. The composition, structure, and morphology of the films were characterized by X-ray photoelectron spectroscopy/ energy dispersive X-ray spectroscopy, XRD and SEM, respectively. The addition of Zr didn't modify the FCC structure of TiN, however the increase of Zr originated a change in the lattice parameter revealed by the shift of the XRD peaks. The coatings were nanocrystalline, the crystallite size diminished as the Zr concentration increased. The morphology of coatings changed at Zr concentrations up to 18%, which agrees with the decrease of the crystallite size estimated from the XRD results.

[THF-156] THIN FILM DEPOSITION OF CuS BY CHEMICAL BATH DEPOSITION

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Chalcogenide materials are promising semiconductors for electronic and optoelectronic devices due to their optical and electric properties. Copper Sulfide (CuS) is a *p*-type semiconductor which is composed with naturally abundant elements [1]. Copper sulfide thin films has been made by several techniques such as atomic layer deposition (ALD), chemical vapor deposition (CVD) and chemical bath deposition (CBD). CBD is a low-cost technique where the processing parameters (pH, temperature, deposition time, and molar ratios) can be controlled to deposit chalcogenide films of high quality. [2]. In this work, CuS thin films were deposited on glass substrates by the chemical bath deposition technique at 25 °C. The chemical reagents employed were triethanolamine as complexing agent, NaOH as reducing agent, copper sulphate ($CuSO_4{\cdot}5H_2O$) as Cu^{2+} ions source, and thiourea ($SC(NH_2)_2$) as S^{2-} ions source. Complexing agent concentration was fixed at 1M and 2M (Cu1 and Cu2), while the deposition time was varied to assess the thickness of CuS thin films. At the end, the films were washed with deionized water and dried in air atmosphere. The influence of the complexing agent concentration was assessed through characterizing its optical (UV-Vis), structural (Raman spectroscopy), and morphological (FESEM) properties.

Keywords: Chemical Bath Deposition, Raman spectroscopy, CuS thin films

[1] C. J. Diliegros-Godines, D. I. Lombardero-Juarez, R. Machorro-Mejía, R. S. González, y M. Pal, “Electrical properties and spectroscopic ellipsometry studies of covellite CuS thin films deposited from non ammoniacal chemical bath”, *Opt. Mater. (Amst).*, vol. 91, núm. December 2018, pp. 147–154, 2019.

[2] O. Erken, M. Gunes, F. Kirmizigul, y C. Gumus, “Investigation of properties the copper sulfide thin films prepared from different copper salts”, *Optik (Stuttg).*, vol. 168, núm. March, pp. 884–891, 2018.

[THF-171] Characterization of thin films semiconductor nanomaterials deposited in chemical bath and analysis of their growth mechanisms

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ZnS, CdS and PbS thin films have been deposited using the chemical bath deposition method in reactors composed of aqueous, alkaline and ammonia-free solutions, over glass substrates. The reaction solutions were composed by zinc, lead and cadmium salts as metal sources, thiourea as a sulphur source, KOH as a source of hydroxyl ions and a complexing agent for metal. The main contribution of this work is to obtain conditions of synthesis of this semiconductor films, with properties suitable for use such as buffer layer in solar cells based on SIGSSe or for electronic film-thin devices such as photodiodes, photoresistors or IR radiation sensors. We have studied the main reaction parameters (temperature, time, pH and composition), its relationship to the most likely deposit mechanism and its influence on the physical properties of this nanomaterials. Our discussion focuses on understanding the coating's growth mechanism, from molecular structure to final structure, from chemical reactions in the solution to precipitation and semiconductor deposit on the substrate. The correlation of these growth mechanisms with the optical, structural and morphological properties of these nanomaterials has been sought.

[THF-185] Structural and optical modifications on CBD-CdS thin films by metallic Au+ doping

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In the present work, we highlight the modifications of the crystalline structure of the IIB-VIA nanostructured semiconductor cadmium sulphur (CdS) associated to doping with gold metallic ion. Good quality thin films were obtained by chemical bath deposition (CBD) and doped in-synthesis with no additional steps required. A controlled thickness around 100 nm was confirmed for the films by ellipsometry. The binding energies of the CdS matrix and the interactions with the metallic ion were determined by X-ray photoelectronic spectroscopy (XPS). The material crystallinity was studied by X-ray diffraction (XRD). A change from monocrystalline to polycrystalline structure in the doped films was observed, this behaviour was confirmed by TEM micrographs. In addition of the different levels of quantum confinement promoted by transition metal. The Raman vibrational spectra allowed the analysis of the phononic interactions of the CdS binary where the Raman shift gives structural information and confirms the effects of quantum confinement. The UV-Vis optical characterization describes the effect of the structural modifications with shifts in the optical band gap of the evaluated samples, related with the different levels of confinement given by the dopant. Photoluminescence was measured at room temperature, which shows more recombination emissions of energetic excitons due to decrease in particle size and the defects created by the Au^{+} metallic ion in the doped sample. Also the pronounced stimulation of the luminescent spectrum of the semiconductor compound at room temperature.

[THF-186] Raman scattering study of the wurtzite-zinc blende phase transition of CdSe nanoparticles

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Structural and electronic properties characterization results show that the crystallographic structure of CdSe films, deposited by chemical bath synthesis, is controlled by the bath growth temperature. The synthesis parameters employed produced a set of nanostructured CdSe films on glass substrates with controlled crystal structure. The effect of bath temperature (T_b) on CdSe films was studied in the 0 £ T_b £ 80 °C range. The average crystal diameter (AD) of the films lies within the 7 £ AD £ 12 nm interval, where AD depends on the selected T_b. X-ray diffractograms (XRD) shown that at low T_b values the formation of the hexagonal wurtzite (WZ) is promoted while at the other extreme the cubic zinc-blende (ZB) crystalline structure dominates. It is observed that the WZ→ZB transition occurs at the critical temperature T_{bc} ~ 40 °C. The AD in each films for CdSe-NP's was obtained from XRD analysis employing the Scherrer-Debye formula. The values of the lattice interplanar spacing (IS), determined from XRD analysis, as function of T_b increases continuously except at temperatures around T_{bc} where a local minimum is observed. The presence of stress acting on CdSe NP's is identified by correlating the IS values with the crystalline structure: compression occurs for $0 \leq T_b \leq 40$ ° C, and tension for $50 \leq T_b \leq 80$ ° C. The band gap energy, obtained from optical absorption spectra, decreases monotonically but a local minimum is observed at T_{bc} = 40 °C. Results from Raman spectroscopy show that the CdSe Raman LO-mode hardens for T_{bc} as consequence of the WZ « ZB structural transition.

[THF-203] Water effect in the synthesis of nanostructured thin films of HfO2 deposited by the ultrasonic spray pyrolysis technique

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We report the effect generated by adding water during HfO_2 thin films synthesis on its structural and dielectric properties, for the high-k gate dielectric to replace SiO_2, especially for the fabrication of ultra large scale integration systems. The study of nanostructured hafnium oxide thin films (HfO_2) deposited on crystalline silicon wafers is presented by using the ultrasonic spray pyrolysis (USP) technique. For their synthesis, hafnium acetylacetonate was dissolved in dimethylformamide, as a hafnium source material. The deposits were made by varying the substrate temperature from 400 and up to 550 °C in steps of 50 °C and adding water during the process, favoring the formation of films with well-defined monoclinic structures as well as being polycrystalline. Employing the ellipsometry technique, refractive indexes have been obtained with values from 1.87 to 2.02 from different samples and an average thickness of ~21 nm for the thin films of HfO_2. In our analysis, the carbon and O-H bonds decrease considerably, and finally, the electrical characterization shows that the films deposited with the addition of water aerosol have a high dielectric constant and a very narrow temperature dependence, in particular that grown at the temperature of 450 ° C has a maximum value of 14.4, respectively. Showing that the addition of water during deposition allows thinner films with adequate dielectric properties to be obtained.

[THF-205] Optimization of the mechanical properties of hafnium (IV) oxide thin films as a function of the thickness using the finite element method.

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Evaluating the mechanical properties of thin films is essential for their integration into microelectromechanical systems (MEMS) applications. Hafnium (IV) oxide (HfO 2) or hafnia is an electroceramic with interesting properties that make it suitable for many applications.

This research project is divided into two parts: simulated and experimental. In the first part, different film thicknesses will be simulated using the finite element method to determine the values of the mechanical properties at different thicknesses. Then, in the experimental part, thin films of hafnium oxide (IV) will be grown on silica substrates (100) with different thicknesses with the atomic layer deposition technique. The composition will be characterized by Raman spectroscopy and energy-dispersive X-ray spectroscopy (EDX). The mechanical properties will be evaluated by microhardness and nanoindentation analysis; these mechanical properties are hardness, elastic modulus, shear modulus, thickness, and Poisson's ratio.

[THF-287] Synthesis of Pb10O(OH)6(CO3)6 by Successive Ionic Layer Adsorption and Reaction (SILAR) Technique

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Lead oxide (PbO) is a semiconductor that in recent years has had different uses such as gas sensors, pigment in paints and as an anode in secondary lithium batteries; due to its semiconductor and photoconductive properties, PbO has attractive potential to be applied in photovoltaic cells, imaging devices, and lasers. On the other hand, Plumbonacrite ($Pb_{10}O(OH)_6(CO_3)_6$) called lead carbonate, is an oxy-hydroxy-lead carbonate that is formed in lead pipes and in old organ pipes found in churches and museums. This material has been synthesized due its properties as a semiconductor.

There are several ways to prepare thin films of PbO and plumbonacrite, which are complicated due to their high volatility at relatively low processing temperatures, some of applied techniques are sputtering, spray pyrolysis, Autocalalytic Oxidation and Chemical Bath Deposition (CBD), being chemical bath the one that takes a simpler processing and avoids the use of sophisticated equipment, but even so it is a process that takes around 20 hours. In this work, using the Succesive Ionic Layer Adsorption and Reaction (SILAR) technique, the growth of a combination of lead oxide and plumbonacrite was carried out, using a thermal treatment, the carbonate is converted to lead oxide, taking time of processing of maximum 30 minutes, according to the given number of layers, using only two reagents: lead acetate and sodium citrate as complexing agent, taking a second step in boiling deionized water, achieving at 40 cycles to obtain a thickness of 1 micron.

[THF-348] CuS thin films coated with bioglass 45S5/TiO2 Nps and Zeolite ZMS5 thin films as a principle of an urea biosensor

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In recent years, the development of biosensors created from materials obtained through reproducible and low-cost methods has been of great interest. In the present work, we report the immobilization of urease in CuS thin films coated with bioglass and zeolite by adsorption method and the chemical and electrical characterizatiom of the thin films based in different concentrations of urea. These films were characterized by UV Vis spectroscopy and four probe method where an increasing of the ammonium curve and the resistivity of the thin films was observed in order of urea concentration. The synthesis of bioglass 45S5, zeolite ZMS5 and 1.5[Ti], titanium dioxide (TiO_2) nanoparticles (including the bioglass composite) were achieved by sol gel method and characterized by FTIR, and copper sulfide thin films were obtained by chemical bath deposition. For the deposition of biomaterial thin films, spin coating method was chosen, in order to deposit each biomaterial, the bioglass was scattered in methanol and the zeolite in acetone, and then the deposition of these materials was made over the CuS thin films. By characterizing these thin films with UV Vis, SEM it was obtained a homogeneity in the deposition and a porous structure adequate to immobilize the enzyme, were the view of the two phases of the depositio, the biomaterial and the semiconductor, was clear.

[THF-349] Process to manufacture thin film transistors by photolithography based of chalcogenide semiconductors deposited by CBD

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Chalcogenide semiconductors and transition metal oxides present a wide and interesting range of physical and chemical properties were the magnetic, electrical, optical, catalytic and energy harvesting ones stand out. These materials have been used in the development of devices such as flat screen TVs, smart gaseous windows, optical write-read-erase devices, sensors (gas, humidity and temperature) and for field emission and solar cells and Thin Film Transistors. This study reports the optimization of the gate dielectric etching process and the active semiconductor layer for the manufacture of a P-type thin film transistor (TFT) by photolithography. The manufacture of TFT uses Hafnium Oxide (HfO_2) as gate dielectric deposited by Atomic Layer Deposition (ALD), Copper Sulfide (CuS) as P-type active layer deposited by Chemical Bath Deposition (CBD) and Chromium (Cr) as gate metal (G), source metal (S) and drain metal (D) deposited by sputtering in a gate-bottom, top-contact (BGTC) structure. Hydrochloric acid (HCl) was used as an attacker of active layer of CuS. The etching of the dielectric layer was performed with optimized photolithography and negative photo-resin was deposited before depositing the HfO_2, avoiding the use of Buffered Oxide Etch (BOE). The electrical characterization of p-type TFT shows that the optimized manufacturing process is successful and scalable to any chalcogenide as active layer

[THF-389] The influence of hydrogen ion irradiation on the photoluminesce intensity of MoS2 nanoflowers

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Two-dimensional (2D) materials have been demonstrated to be promising candidates for active layer in next generation devices including luminescent devices. Their synthesis has been proposed by different methods including exfoliation, direct sulfurization of metal oxides and aerosol-assisted chemical vapor deposition. Here a one-step hydrothermal process was used to synthesize MoS_2 nanostructures and the influence of hydrogen ion irradiation in their luminescence intensity evaluated.

Based on the SEM and TEM images the resulting MoS2 nanostructures can be described as nanoflowers with 500 nm diameter composed of very thin 2D MoS2 petals. The XPS core level analysis reveals the presence of the 1T (metallic) and 2H (semi-conductor) MoS_2 crystal phases as well the MoO_x in the as synthesized nanoflowers.

The nanostructures were irradiated with low kinetic hydrogen ions, the effect of different irradiation time in the chemical composition, crystal phase and photoluminescence intensity was evaluated. The hydrogen ion irradiation process was performed at 2 KV energy under a pressure ≈ 1.24 × 10-5 mbar of H2 (Purity: 99.999 Vol.%) for 10min, 30 min and 60 min. The relative amount of oxygen decreased from 27.2 % to 19.8% after 60 minutes of irradiation. The crystal phase of the MoS2 nanoflowers changed from predominantly 2H to predominantly 1T. The photoluminescence spectra of the MoS2 nanoflowers recorded after each hydrogen ion irradiation was measured using photons of 532 nm as excitation source. In the photoluminescence spectra of the MoS2 nanoflowers, a broad (FWHM 2 eV) peak centered at 1.71 eV was observed. The intensity of this peak increased for increasing irradiation time; the intensity increase was near (x8) between in the as-synthetized MoS2 nanoflowers and the in sample irradiated by 60 min irradiated. The origin of the increase in the photoluminescence intensity will be discussed.

[THF-396] Study of electrical parameters in CdTe solar cell influenced by Te p+ region as part of the back contact

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The polycrystalline CdS/CdTe thin film solar cell is one of the most important photovoltaic devices for cost-effective generation of solar electricity for terrestrial applications. A typical superstrate structure of CdTe solar cell has been studied through current-voltage (J-V) and secondary ion mass spectroscopy (SIMS) measurements. A close correlation between quality of interfaces and its photovoltaic efficiency was determined. It was found that a high short circuit current (J_{SC}), open circuit voltage (V_{OC}) and fill factor (FF) can be achieved reducing CdS thickness around 60 nm and using an appropriated thermal annealing process for CdTe. An efficiency of 11% has been reached on solar cells with a Te p+ region as part of the back contact in this case all electrical parameters were improved. Diffusion and intermixing for n-p and semiconductor-metal junctions were analyzed.

[THF-428] NITROGEN-DOPED ZnO THIN FILMS FOR PHOTOCATALYTIC APPLICATIONS

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One of the most promising technologies in wastewater treatment is photocatalysis. This technique is based on the use of the surface of a semiconductor to change the rate of a chemical reaction when it is exposed to irradiation of UV or visible energy. ZnO is a promising semiconductor material in the field of photocatalysis due to its excellent physicochemical properties. Recently, the use of thin films has been chosen in the field of photocatalysis due to the advantages they offer such as their easy separation, recovery, and reuse. A crucial factor in determining the quality of thin films is the deposition technique. Among the different techniques, atomic layer deposition (ALD) occurs in a gas phase. It is characterized by self-limited surface reactions that are repeated a discrete number of times, until reaching a specific composition and thickness. The self-limited growth mechanism of this technique allows excellent control of those features, which are decisive for its physicochemical properties. Furthermore, the photocatalytic surface of the thin films could be improved by achieving doping with heteroatoms, including nitrogen doping in ZnO thin films.

In the present work, the physicochemical properties of ZnO films synthesized by the combined use of the ALD technique and hydrothermal methods were evaluated. Subsequently, the ZnO films were doped using a nitrogen plasma discharge. The synthesized thin films were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), Raman spectroscopy and, diffuse reflectance spectroscopy. The ZnO thin films shown interesting features for possible application as photocatalysts.

Authors thank the facilities provided by LANBIO-CINVESTAV-IPN, Merida. To W. Cauich, D. Huerta and D. Aguilar for their technical support in XPS, SEM and XRD analyzes. To J. Bante and D. Macías, for their support in the use diffuse reflectance and Raman analyses.

TRIBOLOGY

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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

[TRB-207] Pulsed laser deposition of SiC thin films by the simultaneous ablation of Si and C targets

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Silicon carbide is used as protective coating for cutting tools because of its mechanical properties such as high hardness, wear and corrosion resistance. The synthesis method is crucial in order to control SiC structure, composition, and thus, mechanical and tribological properties. In this work, amorphous SiC were grown by pulsed laser deposition by ablating independent Si and C targets. The plasma parameters were determined by the TOF curves obtained from Langmuir planar probe measurements. Films optical and structural properties were studied by UV-Vis and Raman spectroscopies, respectively. Influence of plasma parameters variation on the deposition rate was also evaluated.

[TRB-227] Tribocorrosion study of D2 steel subjected to different time of cryogenic treatment immersed in basic, neutral and acid environment

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Steel AISI D2 has a high chrome content, which provides it with high hardness and high resistance to corrosion, due to this qualities it is used in tools subjected to different environments, in food industry, this steel is used for molds and mandrels for the closure of cans which can be full of acid or basic media, so the steel is exposed to vapor of these substances. Cryogenic treatment is not an extended treatment although its profits are proved, in the increase of hardness and resistance to wear because transform retained austenite to martensite and favors the coalescence and growing of carbides.

In this work, samples of AISI D2 steel where subjected to cryogenic treatment during 4, 12 and 16 hours, its hardness was measured after treatment and the number and size of carbides was analyzed, samples were subjected to tribocorrosion test in acid, neutral and basic environments using buffer solutions, after the electrochemical equilibrium was reached, wear was simultaneously studied whit a pin on disc device applying load during 25 minutes.

An increase in the hardness value was observed with increment in time of cryogenic treatment, this is supported by the accounting of carbides and their sizes, while the sample without cryogenic treatment presented a large number of small carbides, this amount was diminishing for samples when the time of cryogenic treatment increase this behavior was explained with the account of carbides, which dimished as the time of cryogenic treatment increases. The tribocorrosion measurements shown that in acid environment, an increase in potential was measured during wear for all samples subjected to cryogenic treatment, showing a passivation during wear. For samples subjected to wear in neutral media, potential increase linearly during wear, due to removal of the passive film formed and their slow new formation. In the case of samples subjected to basic media, and abrupt fall in potential was observed, showing an intense electrons exchange. The observed behavior must been explained in terms of chemical reactions of the alloying elements particularly for chrome and the structures formed during cryogenic treatment.

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