BOOK OF ABSTRACTS

XVI-INTERNATIONAL CONFERENCE ON SURFACES, MATERIALS AND VACUUM


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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 XVI-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 XVI ICSMV

Organizing Committee SMCTSM

September 2023

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Maureen Lagos, PhD
McMaster University, Canada
Spectroscopy and Imaging of Phonons in the Electron Microscope

PLENARY TALKS

ANGUS ROCKET, PhD

BIO

Angus Rockett is a Professor and past Head of the Department of Metallurgy and Materials Engineering and the Colorado School of Mines and an Emeritus Professor in the Department of Materials Science and Engineering at the University of Illinois. He was President in 2011 and is a Fellow of the American Vacuum Society. He was the General Chair of the IEEE Photovoltaic Specialists Conference in 2016 and has held many positions with both the PVSC and the AVS. Since January 2021 he has been the Editor in Chief of the IEEE Journal of Photovoltaics. He received his B.S. in physics from Brown University and his Ph.D. in metallurgy from the University of Illinois.

His research involves defects in semiconductors, primarily focused on synthesis and characterization and theory and modeling of solar cell materials. He has applied a wide variety of materials microanalysis methods to study semiconductors. His group has done density functional theory, continuum elasticity, lattice Monte Carlo, and drift-diffusion modeling of materials and devices. He has also worked with reactive sputtering of nitrides and other materials. He is the author of one book (The Materials Science of Semiconductors), five book chapter contributions, more than 190 publications in archival journals, holds three sputtering- and/or photovoltaics-related patents, and has given more than 155 invited talks. Google Scholar currently gives his h-index as 58 with over 12,000 citations to his work. He teaches courses in electronic materials and processing in addition to general materials science courses. He has presented short courses and tutorials in sputtering, materials microanalysis, and solar cells and solar cell materials for a variety of professional societies and organizations around the world..

Current challenges for next generation photovoltaics

CARLOS A. MARTÍNEZ-HUITLE, PhD

BIO

He is graduated in Chemistry at Universidad de las Américas-Puebla (México) under supervision of Prof. Marco Antonio Quiroz Alfaro. After a work experience in Ciba-Specialty Chemicals (currently, BASF), he moved to Ferrara (Italy) where he received his PhD in Chemical Sciences at the University of Ferrara under supervision of Prof. Achille De Battisti. During the same period, he worked as visiting scientist in the group of Prof. Christos Comninellis at the EPFL Institute (Switzerland)

From since 2005 to 2008, he has served as faculty member in the Department of Chemistry at the University of Milan. In 2008, he also moved to Brazil where he currently is a Full Professor in the Institute of Chemistry at the Federal University of Rio Grande do Norte. He was awarded with the “Oronzio and Niccolò De Nora Foundation Prize” by the Italian Chemical Society (2005) and the “Oronzio and Niccolò De Nora Foundation Prize on Environmental Electrochemistry” by the International Society of Electrochemistry (2009). He was also recognized by German Government with the “Green Talent Award” for his contributions in the field of electrochemical water disinfection-treatment (2009). He is author and co-author of more than 450 scientific publications, including conference books, book chapters, books, more than 295 papers in peer-reviewed international scientific journals (h-index of 56, >16500 citations), papers in national scientific journals, more than 90 contributions in conference proceedings and a co-inventor of 4 patents. He is co-editor of the books entitled “Synthetic Diamond Films” (Wiley & Sons) and “Electrochemical Water and Wastewater Treatment” (Elsevier). He is an editorial member of several journals (Applied Catalysis B: Environmental (Elsevier), Current Opinion in Electrochemistry (Elsevier), ACS ES&T Water (American Chemical Society), Journal Chemistry (Hindawi-Springer), SN Applied Sciences (Springer), ChemElectroChem (Wiley), ChemPhysChem (Wiley), and Critical Reviews in Environmental Science and Technology (Taylor & Francis Group)) and an Associate Editor in Scientific Reports (Nature) and Chemistry Africa (Springer).

The integration of electrochemical approches with material science in the water-energy-climate nexus

JULIO CHACÓN, PhD

BIO

Julio Chacon obtained his B.Sc. in Mechatronics Engineering at Tecnologico de Monterrey, Mexico in 2008. He enrolled the graduated program of Applied Sciences at the Institute of Science and Technology of San Luis Potosi in Mexico and further moved to Vienna in 2010 where he conducted his PhD within a French-Austrian Cooperation program.

During his PhD he was funded by the Austrian Science Foundation (FWF) and the OEAD Amadeus Program. He graduated in November 2013 with a thesis entitled: "Theory and Spectroscopy on functionalized graphene and GICs". In May 2014 he was awarded a DRS Posdoctoral Fellowship at Freie Universität Berlin, Germany,

Revealing supramolecular interactions between Biomolecules and Carbon Nanostructures employing spectroscopic techniques.

Over the past few years, Chemistry, Physics, and Biotechnology have merged in order to develop novel methods for studying supramolecular surface interactions between carbon nanostructures and biomolecular systems and diverse functional groups. Raman spectroscopy combined with X-ray photoelectron spectroscopy (XPS) have become together the tools of choice to analyze these supramolecular interactions, doping, and functionalization, especially in carbon-based nanostructures. However, much less is known about the physicochemical interaction existing between biomolecular systems and carbon nanostructures. During this presentation I will try to convince you about the existence of a near-universal Raman response where charge transfer governs the electrochemical activation of carbon nanomaterials when exposed to potassium undergoing an electron doping (n-type doping) process. [1]–[3] More recently, we have disclosed inherent interactions between biopolymers such as chitosan and DNA inhibiting the fluorescence effects of the biomolecule, and enhancing the Raman response of the bio-composite under the presence of pristine graphene. Our results from XPS confirm the presence of the biomolecule on graphene, and our Raman analysis reveals a strong electrostatic surface interaction between the biomolecule and the graphene.

JORGE LÓPEZ, PhD

BIO

Dr. Jorge López Gallardo, distinguished as the Schumaker Chair in the Department of Physics at the University of Texas at El Paso (UTEP), has carved an illustrious path in the realms of nuclear and surface physics, among other scientific disciplines. His academic journey began at UTEP, where he completed his undergraduate studies, and culminated in a doctorate from Texas A&M University.

Following his doctoral achievements, Dr. López Gallardo embarked on postdoctoral research at two renowned institutions: the Niels Bohr Institute in Copenhagen, Denmark, in 1985, and the Lawrence Berkeley Laboratory in Berkeley, California, in 1987.

XPS Spectroscopy at UTEP

By serendipity, a nuclear theorist has been involved in studies of materials surfaces with undergraduate students. In this talk, XPS is briefly introduced and several studies (ranging from cleaning water with tea leaves all the way to determining the temperature achieved in the Columbia shuttle explosion) are presented and used to remark the benefit of its use to train undergraduate students in research.

JORGE VARONA, PhD

BIO

Jorge is currently Vicepresident of Engineering at Semtech Corporation (NASDAQ: SMTC) and General Manager at Semtech Mexico, a high-tech supplier of advanced semiconductor integrated circuits (ICs) and IoT systems. He has extensive experience in the design of VLSI integrated circuits and MEMS and has been co-founder of two technology companies.

Previously he has worked as a Design Engineer for Texas Instruments and Tecno-Ingeniería Aplicada. He is an adjunct professor at Universidad Panamericana and member of the Board of Directors of the Mexican Microsystems Consortium (CMM). He holds 4 patents and has authored/co-authored over 40 peer-reviewed technical papers and one textbook. Jorge received a Bachelor of Science degree in Electrical Engineering from Universidad Panamericana, Mexico, a Master in Science degree in analog circuit design from the University of Toronto, Canada, and a PhD degree in EE from the State University of Morelos, Mexico. Jorge has also completed executive programs at IPADE Business School, is a Senior Member of the IEEE (Institute of Electrical and Electronics Engineers), and a member of the Mexican System of Researchers (SNI-I) since 2011.

Adsorption and Nanoporous Materials for Energy, Environment and Health Applications

This presentation explores the significant progress made in materials and manufacturing processes in the integrated circuit (IC) industry, leading to a plethora of possibilities for designing and fabricating circuits using various substrates and structural materials. The integration of these advancements has opened new avenues for implementing devices and interconnections that constitute the circuitry of monolithic ICs. As a result, different commercially available manufacturing processes now offer distinct and specific characteristics, each presenting unique trade-offs suitable for several types of circuits and applications.

This talk will delve into real and practical examples of IC products that have leveraged diverse foundry processes for their development. The discussion will encompass a range of technologies including planar CMOS at different scales, BiCMOS, GaAs, SiGe, advanced FinFET, and SiPho. By analyzing each of these technologies, we aim to shed light on their respective advantages and disadvantages, providing valuable insights into the considerations when selecting the most appropriate process for a given IC design.

MARGARITA SÁNCHEZ DOMÍNGUEZ, PhD

BIO

Margarita Sánchez Domínguez is a Research Professor at CIMAV MONTERREY, she belongs to level 3 of the National Researchers System (SNI), and she is a regular member of the Mexican Academy of Sciences since 2020. She graduated from B.Sc. in Industrial Chemistry at the Autonomous University of Nuevo León (1997). She worked as a Product Engineer at PYOSA (1997-2000). She completed a PhD in Physical Chemistry specializing in surfactant systems at the University of Bristol (2004). She completed two postdoctoral stays, the first at the Institut Charles Sadron in Strasbourg (2004-2006), and the second at the Institute of Advanced Chemistry of Catalonia in Barcelona (2006-2010).

Plasmonic hierarchical superstructures as highly efficient SERS substrates and triboelectric nanogenerators

Currently there is a high demand for ultrasensitive sensors for both health and environmental applications. The detection of contaminants is essential since many of these are usually harmful to health. On the other hand, the detection of cancer cells and biomarkers in early stages of the disease is essential to have greater chances of survival. In recent years, plasmonic hierarchical superstructures have played an important role in the development of new sensors with high detection capacity. These materials can be used as SERS substrates, which base their detection principle on surface enhanced Raman scattering. In this talk, several strategies for the synthesis of plasmonic nano and superstructures will be presented, as well as the evaluation of their performance as SERS substrates for the sensing of model molecules, contaminants, drugs and cancer cell lines. The synthesis strategies used were chemical synthesis, electrodeposition, and galvanic replacement. Various superstructures such as nanostars, decorated nanodendrites, and nanostructured hollow polyhedrons, based on Au, Ag, Cu and their combinations, were synthesized. 1-3 Some of the molecules detected were: rhodamine 6G, 4- aminothiophenol, crystal violet, bisphenol A, triclosan, tetracycline, vancomycin, and tramadol.

María Sánchez, PhD

Surface Photovoltage Spectroscopy in characterization of materials and devices

Surface Photovoltage spectroscopy (SPS) is a widely used technique to study the electronic transitions and optical properties of semiconductor materials and nanostructures. This technique relies on measuring changes in the surface voltage as a function of the incident wavelength.

In this talk, the fundamentals and experimental details of SPS are presented. Results obtained in characterization of: p-Cu2O/n-ZnO nanojunctions, InxGa1-xN self-assembled nanostructures1 and MoO3 thin films2 are presented. Experiments on the temperature dependence of the surface photovoltage (SPV) in InxGa1-xAs QWs have been performed between 20 and 275 K, demonstrating that quantum well transitions and barriers can be clearly identified even at room temperature. A specially designed sample holder was used for the SPV measurements3. Finally, we report on an original application of SPV for characterization of fully metallized AlxGa1-xAs laser4 diodes and c-silicon solar cells demonstrating the effectiveness of this technique as a simple, contactless and non-destructive tool in the characterization not only of materials but also in semiconductor devices. Kelvin Probe Force Microscopy (KPFM) was used for direct measurement of surface potential maps.

MAUREEN LAGOS, PhD

BIO

Maureen Lagos is an Associate Professor at the Department of Materials Science and Engineering at McMaster University, Canada. His research is focused on the study of nanomaterial properties using advanced imaging and electron spectroscopy techniques implemented in transmission electron microscopes. In particular, he investigates elementary excitations (phonons, plasmons, excitons) and electronic transitions in novel materials with potential for infrared nanophotonics, heat transport, and quantum material applications.

His group also develops novel methodologies for nanoscale material characterization (e.g. thermometry). Besides his interest in phonons and electronic properties of nanomaterials using EELS, he has worked on temporal aspects of the inelastic electron scattering associated with collective excitations, quantum electronic transport, and mechanical elongation of nanostructures using in-situ TEM. He obtained his PhD in Physics from The State University of Campinas. He is Canada Research Chair in Imaging and Spectroscopy of Advanced Nanomaterials, and he currently serves as Associate Scientific Director of the Canadian Centre for Electron Microscopy.

Spectroscopy and Imaging of Phonons in the Electron Microscope

Scanning transmission electron microscopes (STEM) equipped with high energy resolution monochromators permits the realization of phonon spectroscopy studies in materials using atom-wide electron probes. Instrumental developments are still in progress and energy resolutions of 3.7 meV at 60 kV were recently obtained. As it is usual the case, phonon spectroscopy experiments are complex and data interpretation presents enormous challenges. But despite these barriers the electron microscopy community has made progress in obtaining a much deeper understanding of the inelastic electron scattering by phonons in nanoscale materials. This is permitting us to uncover new and exotic properties of materials. In this presentation, we will describe this progress by highlighting results in areas of nanophotonics and nanoscale heat transfer: (i) imaging surface and bulk phonon modes in a single nanoparticle, (ii) uncovering plasmon-phonon coupling in infrared antennas, (iii) mapping hyperbolic phonon polaritons in twisted low symmetry crystals, (iv) the development of a thermometry methodology to measure local temperature with nanoscale resolution, and (v) probing heat transfer channels across nanogaps. Our results provide progress towards understanding the role of surface and bulk phonons in physical process involving light-matter interaction and nanoscale heat transfer.

ATOMIC LAYER DEPOSITION

CHAIRMEN

Dr. Edgard López Luna: (UASLP), edgar.luna@uaslp.mx
Dr. Pierre Giovanni Mani González: (UACJ), pierre.mani@uacj.mx
Dr. Hugo Tiznado:(CNYN-UNAM), tiznado@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-73] DESIGN AND MANUFACTURING OF ATOMIC LAYER DEPOSITION SYSTEM TO DEPOSIT SEMICONDUCTOR AND DIELECTRIC THIN FILMS

Jackeline Navarro Rodríguez Ing.[1], Francisco David Mateos Anzaldo Dr.[1], Jesús Román Martínez Castelo Dr.[2], Armando Pérez Sánchez Dr.[3], Juan Ruiz Ochoa Dr.[3], Armando Gaytán Pérez Ing.[3], Hugo Jesús Tiznado Vázquez Dr.[4], Nicola Nedev Dr.[1]

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[4]Centro de Nanociencias y Nanotecnología-Universidad Nacional Autónoma de México, Baja California, Mexico.

Atomic layer deposition (ALD) is a technique for layer-by-layer growth of films with thickness in the nanometer scale with high precision control and excellent uniformity [1]. The purpose of this work is to describe the design and manufacture of a lab-made ALD system. In this system, the reactor is made of aluminum with an internal diameter of 3.5 inches, with two entries for precursors with a diameter of 1/64 inch, and one exit with a diameter of 1/2 inch. To dose the precursor and the oxidant, two 3-way diaphragm valves were used. This type of valve allow a continuous flow of nitrogen as carrier gas and permit the creation of a high- and low-pressure zones, which allow a high-speed deposit. To heat the system, a flat circular resistance controlled by a PID was used. The control of all the system is carried out using a graphical interface of LabView.

Keywords
ALD, system, lab-made, design, manufacture

Reference

[1] Puurunen, R. L. (2014). A short history of atomic layer deposition: Tuomo Suntola's atomic layer epitaxy. Chemical Vapor Deposition, 20(10-11-12), 332-344.

[ALD-56] EFFECT OF ANNEALING IN ELECTRICAL AND OPTICAL PROPERTIES OF MULTILAYER Al_2O_3/ZnO NANOLAMINATE STRUCTURES DEPOSITED BY ATOMIC LAYER DEPOSITION

Jesús Martínez Dr.[1], David Mateos Dr.[2], Hugo Borbón Dr.[3,4], Hugo Tiznado Dr.[3], Nicola Nedev Dr.[2]

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Multilayer nanolaminates of alternate Al_2O_3 and ZnO were deposited by atomic layer deposition using trimethylaluminum, diethylzinc and water as co-reactants, on a p-type silicon substrate at 200 °C in a Beneq TFS 200 system [1]. A set of four nanolaminates with a total thickness of approximately 100 nm were fabricated containing multiple Al_2O_3/ZnO bilayers with thicknesses of 2, 4, 10, and 20 nm. After deposition, the nanolaminates were thermally annealed at 400 °C for 1 hour in N_2 atmosphere to improve the electrical and optical properties of the structures. Optical constants and thicknesses were obtained by ellipsometry measurements. The Al/nanolaminate/p-Si/Al structures were electrically characterized by current-voltage (I-V) measurements. The obtained results indicate that these nanolaminates have potential for applications in electronic and optoelectronic devices.

Keywords
ALD, electrical properties, optical properties, nanolaminates, thermal annealing

Reference

[1] J.R. Martínez-Castelo, et al., Structural and electrical characterization of multilayer Al2O3/ZnO nanolaminates grown by atomic layer deposition, Materials Science in Semiconductor Processing, 71 (2017) 290-295, https://doi.org/10.1016/j.mssp.2017.08.007.

[ALD-230] THERMAL AND PLASMA ENHANCED ATOMIC LAYER DEPOSITION OF NiO_x WITH WATER AND OXYGEN AS OXIDATING AGENTS

Lilián Garay-Cervantes BEng[1], Eduardo Martínez-Guerra PhD[2], Isabel Mendivil-Palma PhD[2], Gerardo Silva-Vidaurri PhD[2], Mario Hidrogo-Rico MS[2], Alejandra García-García PhD[2], Angel Osuna BEng[2], Oscar Vega-Becerra PhD[2], Pierre Mani-Gonzalez PhD[2]

[1]Institute of Engineering and Technology, Department of Physics and Mathematics, Autonomous University of Ciudad Juárez, Chihuahua, Mexico.
[2]Center for Research in Advanced Materials, Nuevo León, Mexico.

The synthesis of NiO_x via an atomic layer deposition (ALD) process has involved the manipulation of complex organometallics. This has resulted in low growth per cycle (GPC). Nickel acetylacetonate ($Ni(ACAC)_2$) is a low toxicity oxygenated volatile organic compound which has been found to be reactive with both water and oxygen radicals. This reactivity has been taken advantage of by using the organometallic as a metal oxide precursor. Plasma-Enhanced ALD (PEALD) is then proposed to achieve greater GPCs and higher ratio of NiO_x regarding additional nickel species formed.

Windows for Thermal-H_2O and Plasma-H_2O process are presented with their respective X-ray Photoelectron Spectroscopy (XPS) spectra along the respective NiO_x stoichiometry. For Plasma-O_2 precursor temperature of 180°C has been found optimal with stoichiometry of $NiO_{0.88}$. Results have shown that metallic oxide and hydroxide species are obtained throughout all deposition process. After this, heat treatments of 300°C for 2 hours have been performed in order to oxidate the hydroxide phase into NiO_x. Cyclic voltammetry was performed to evaluate the capacitive response of the oxide thin film.

Keywords
atomic layer deposition, nickel oxide, window, plasma, growth per cycle

Reference

M. Napari et al., “Antiferromagnetism and p-type conductivity of nonstoichiometric nickel oxide thin films,” InfoMat, vol. 2, no. 4, pp. 769–774, Jul. 2020, doi: 10.1002/inf2.12076.

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Sesión Oral

[ALD-364] SEMICONDUCTORS AND INTEGRATED CIRCUIT FABRICATION TECHNOLOGY IN MEXICO

Joel Molina Dr.

Instituto Nacional de Astrofísica, Óptica y Electrónica, Puebla, Mexico.

As of today, only 5 countries in the world are able to mass-produce and commercialize modern integrated circuits with nanoscaled dimensions: Taiwan, South Korea, Japan, China and USA, in that order. Mexico does not figure in this list even though has developed integrated circuits with more than 1,000 transistorssince 1984 and where each transistor had dimensions of only 10 μm at that time. Now, the modern semiconductor industry is routinely mass-producing advanced transistors with designs of only 5 nm between source and drain. Some of the reasons behind this delay in developing nanoscaled semiconductor devices for Mexico are simple: Mexico did not have the economic, political nor enterprise capabilities that these 5 countries had and that enabled their fast-economic development in only a few decades. Also, there was only one institution in Mexico (INAOE) able to develop integrated circuits but whose infrastructure has reached its useful operational lifetime. Today, these conditions have changed since we have more national academic institutions doing excellent research on advanced electron materials and devices. Also, we at INAOE have initiated a national project aimed at renewing major equipment for developing advanced integrated circuits whose planar dimensions will be scaled down to 350 nm. In this talk, I will introduce some details behind the development of advanced integrated circuits, some of our old and new infrastructure to develop advanced electron devices at INAOE and some of the most representative results for logic, memory, sensing, photoactive and quantum technologies that are under continuous development even today. Since the pandemics brought difficult conditions for the global semiconductor industry (creating a shortage of integrated circuits in several industries), we believe that Mexico has the potential to fulfill some of these needs but this endeavor would not be possible without the national and international collaborations that we have and will further strength towards creating a national platform for the design, simulation, fabrication, characterization and application of integrated circuits for enhanced sensors in water, health, energy and other global emergent fields.

[ALD-11] ATOMIC LAYER DEPOSITION SUPERCYCLE APPROACH APPLIED TO THE Al-DOPING OF NEARLY SATURATED ZnO SURFACES.

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Current research on transparent conductive oxides deals with the development of environmentally friendly materials having competitive electrical and optical properties. Also, the synthesis methods need to be compatible with the state-of-the-art microelectronics and miniaturization. ZnO films doped with Al (AZO) via Atomic Layer Deposition (ALD) have been subjected to thorough investigation for the latter. However, the conventional doping schemes in ALD seem to have reached their limit and alternative approaches are currently being explored. This work contributes to the improvement of the Al-doping efficiency of ZnO by the ALD supercycle approach, applying the doping-cycle on nearly saturated ZnO surfaces. The electrical and optical properties demonstrated typical values obtained by others applying the supercycle methodology. However, the main finding of this work is the trend observed in the electrical and optical properties, which suggests that the Al solubility limit was not reached as a result of the interaction between the dopant agent and the nearly saturated ZnO surfaces. This is also evidence that the dopant atoms do not become inactive once the compensation effect between substitutional doping and structural defects, has been established. These results open the possibility of exploring the incorporation of more Al into the ZnO structure following and optimizing the doping scheme used here, which at the same time, promises materials that could substitute indium-tin-oxide in many optoelectronic applications, attending the well-known environmental and economic issues.

Keywords
Al doped ZnO, transparent conductive oxide, ALD supercycle

Reference

Ramírez-Esquivel, O. Y. et al. Ceramics International. 47, (2021).

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[ALD-18] COMPUTATIONAL-EXPERIMENTAL STUDY OF THE NUCLEATION PROCESS OF TiO2 ON GRAPHENE

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By the different fields of materials science and engineering, the key to scientific and technological progress is the understanding and the control of the properties of matter at the scale of individual atoms and molecules. However, conducting research and studies on these dimensions is a complicated challenge; This is because the equipment and techniques that allow us to carry out this type of study are few and limited. Likewise, there is a large barrier in terms of the knowledge with the reactions and phenomena that occur within the processes of these techniques, which is why the study of the processes involved in the methods and techniques that allow the manipulation of matter at this scale they have become a fundamental part of scientific development in its various areas. In the present work, a theoretical-computational study was carried out of the initial stages of ALD growth of the TiO_2-GR hybrid from functionalized graphene with hydroxyl groups (OH) as growth sites for the interaction with the main titanium precursors in ALD. through the density functional theory (DFT) and the elastic band method (NEB). It was demonstrated how the chemical nature of the precursor directly affects the reaction mechanism for each ALD growth interaction through the minimum energy trajectories. Through the minimum energy trajectories, it is executed through the energy barriers of each trajectory that TDMAT is the precursor that presents a greater affinity in the TiO_2 growth process in the different ALD stages. Likewise, through non-covalent interactions, the reactions produced by the minimum energy trajectories are completely shown and thus the complete reaction mechanism for each precursor was proposed. Finally, the effect of the water molecules occurs in the reduction of energy barriers and consequently the favorable tendency for the formation of TiO_2 films.

Keywords
ALD, TiO2, Graphene, DFT, Precursors

Reference

Borbón-Nuñez, H. A.; Muñiz, J.; El Hachimi, A. G.; Tiznado, H.; Cuentas-Gallegos, A. K. Effect of oxygen based functional groups on the nucleation of TiO2 by atomic layer deposition: A theoretical and experimental study, Materials Chemistry and Physics, 2021, 267.

This work was supported by

We thank DGAPA-UNAM El IA100822, and Conacyt Basic Scientifc Research A1-S-26789 of the Call of Proposals for Basic Scientific Research 2017- 2018. Calculations were performed in the DGCTIC-UNAM Supercomputing Center, projects LANCAD-UNAM-DGTIC-390, LANCAD-UNAM-DGTIC-368.

[ALD-192] TEMPERATURE DEPENDENT ANALYSIS OF TRAP-ASSISTED TUNNELING IN MIS CAPACITORS WITH Al2O3 DEPOSITED BY ALD

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Aluminum oxide (Al_2O_3) is a high-k dielectric material which has gained significant attention as an alternative to silicon dioxide (SiO_2) in advanced electronic devices and applications. Al_2O_3 thin films can be grown with a high level of purity and desirable properties like improved capacitance, lower gate leakage for CMOS devices, high thermal stability, and excellent electrical insulation properties. In this work, the objective was to model the conduction mechanisms in ultra-thin Al_2O_3 films deposited by atomic layer deposition (ALD) to obtain an understanding of the physics behind their electrical behavior within the temperature range in which integrated devices typically operate. To achieve this, Al/Al_2O_3/n-Si metal-insulator-semiconductor (MIS) capacitors with a 6 nm thin Al_2O_3 film were fabricated and electrically characterized. The dielectric thin films were grown using thermal ALD, and current-voltage (I-V) measurements were performed on the MIS capacitors at a temperature range of 300 - 400 K. The resulting current-voltage-temperature (I-V-T) curves display a behavior that can be accurately modeled by the inelastic trap-assisted tunneling conduction mechanism at electric fields from 2.5 to 5 MV/cm. A lowering of the trap energy level corresponding to this mechanism from 1.5 to 1.3 eV was found as temperature increases in the studied range. The activation energy of this trap energy level was also analyzed as a function of the temperature. The results of this study provide an explanation to the conduction mechanism that generates a leakage current through 6 nm Al_2O_3 films deposited by ALD that greatly adjusts to experimental data, contributing to the understanding of the electrical behavior of Al_2O_3 thin films for potential applications in advanced electronic devices.

Keywords
aluminum oxide thin films, ALD, high-k dielectrics, trap-assisted tunneling
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[ALD-300] THERMAL CONDUCTIVITY STUDY OF HfxTi1-xO2 MONOLAYER ALLOY.

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The ability to deposit high dielectric constant (high-k) films via ALD has allowed for their widespread use in optical, optoelectronic, and electronic devices, including in the integration into CMOS compatible platforms. As the thickness of these dielectric layers is reduced, the interfacial thermal resistance can dictate the overall thermal resistance of the material stack compared to the resistance due to the finite dielectric layer thickness. Thermal conductivity of hafnium oxide, titanium oxide and $Hf_xTi_{1-x}O_2$ films on silicon was determine. We calculate a representative design map of effective thermal resistances, as a function of Hafnium concentration, which will be of great importance in predicting the thermal resistances of current and future devices.

Keywords
Monoalloys, metal oxides, themal conductivity
Reference
APL MATERIALS 6, 058302 (2018)
This work was supported by
M. I. Perez-Valverde, CVU 557501 acknowledges posdoctoral financial support from CONAHCyT México.

[ALD-317] PROMISING NICKEL OXIDE (NiO_x) AS HOLE TRANSPORT LAYER IN PEROVSKITE SOLAR CELL SYNTHESIZED BY ATOMIC LAYER DEPOSITION

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Nickel oxide (NiO_x) thin films were prepared by atomic layer deposition using ozone (O_3), water (H_2O), and oxygen (O_2) as co-reactant in thermal or plasma-enhanced mode. Initially, we studied the growth per cycle (GPC) and density using X-Ray Refractometry. Here, we found a high GPC attributed to the synthesis of ALD using O_2 plasma as co-reactant (0.06 nm/cycle) with high density (~6 g/cm^3). On the other side, when the thermal mode was used, the density and GPC of NiO_x is lower with values around ~0.05 nm/cycle and ~1 g/cm^3. Then, all films present high optical transparency (>60%) and a wide band gap (~3.6 eV). Then, studies of spectroscopic using X-Ray Photoelectron Spectroscopy (XPS) and Ultraviolet Photoelectron Spectroscopy (UPS) were employed to determine the chemical surface and energy levels of NiO_x films synthesized. When plasma enhances ALD was used, the chemical surface showed low carbon content (~10%). In comparison with thermal ALD, the carbon content was increased, with values around ~23%. On the other hand, UPS showed an energy valence band (E_v) around ~4.7 eV for all films. Finally, all NiO_x thin films were added to perovskite solar cells using a P-I-N architecture.

Keywords
Nickel Oxide, atomic layer deposition, inorganic hole transport layer

Reference

Koushik, D., Jošt, M., Dučinskas, A., Burgess, C., Zardetto, V., Weijtens, C., ... & Creatore, M. (2019). Plasma-assisted atomic layer deposition of nickel oxide as hole transport layer for hybrid perovskite solar cells. Journal of Materials Chemistry C, 7(40), 12532-12543.

This work was supported by

This work was partially supported by the Proyecto Bilateral Conacyt-AFOSR CC0015-22016-05-279915 “SINGLE CRYSTAL AND THIN FILM HYBRID PEROVSKITE MATERIAL FOR OPTOELECTRONIC APPLICATIONS”.

BIOMATERIALS AND POLYMERS

CHAIRMEN

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

The XVI International Conference on Surface Materials and Vacuum takes immense pleasure & feel honored in inviting the contributors across the globe to attend in the symposium on Biomaterials and Polymers during September 25-September 29th, 2023, at Zacatecas, Zacatecas, México.

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

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

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

[BIO-63] ELABORATION OF PCL/GO AND PCL/CNT COMPOSITES AND THEIR MECHANICAL CHARACTERIZATION FOR APPLICATIONS AS BIOCOMPATIBLE SCAFFOLDS

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Polycaprolactone (PCL), PCL with graphene (GO) and PCL with carbon nanotubes (CNT) fibers were elaborated using the polymer melt-spinning technique. The electrospinning equipment was home-made built, and the temperature was controlled through a microcontroller, a strain gauge and an interface with LabVIEW. The fibers were elaborated by changing the winding speed of the fiber collection, thus varying its diameter. The obtained diameters ranged from 0.12 to 0.05 mm, using RPM from 5 to 30. The results showed that the inclusion of GO and CNT into the PCL fibers, changed the mechanical properties, obtaining a decrease in the tension at break for PCL/GO, and an increase for PCL/CNT, but also an increase in the melting temperature of 20% higher for PCL/GO and up to 30% for PCL/CNT, with respect to the PCL of 60°C was observed. In conclusion, it is possible to add GO, CNT and other nanomaterials to create composites, using the melt-spinning spinning technique. This inclusion generates changes in the mechanical properties of the base polymer. Possible applications of these composites is organic and inorganic biocompatible scaffolds in biomedicine.

Keywords: CNT, Composites, Graphene, LabVIEW.
Reference: D. Kumar, G. Babu, and S. Krishnan, Study on mechanical & thermal properties of PCL blended graphene biocomposites, Polímeros 29 (2019) e2019024. https://doi.org/10.1590/0104-1428.05318.
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[BIO-109] ADHESION OF OSTEOBLASTS ON NANOCRYSTALLINE HYDROXYAPATITE COATINGS FOR ORTHOPEDIC IMPLANTS

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To avoid the most common failures of orthopedic implants after their implantation, associated with infections and excessive wear of their surface, it is proposed to cover them with the calcium phosphate called (hydroxyapatite), due to its antibacterial characteristics, biocompatibility, anticorrosive behavior and its properties mechanical properties. The incorporation of impurities to hydroxyapatite such as Mg and Cu, and mixing it with other substances such as Aloxita, PVP, PCL and Amphiphilic Peptide Nanoparticles (APNPs) significantly improves its performance. Within the materials mixed with hydroxyapatite, the APNPs turned out to be the best candidates, since they increased the adherence of osteoblasts in a statistically significant way. Nanocrystalline hydroxyapatite coatings showed higher osteoblast adherence than conventional hydroxyapatite coatings.

Keywords: Amphiphilic Peptide Nanoparticles, Hydroxyapatite Coatings, Nanocrystalline hydroxyapatite, Osteoblasts, Orthopedic Implant.

Reference:

1. Wei G. et al (2004). Structure and properties of nano-hydroxyapatite/polymer composite scaffolds for bone tissue engineering. Biomaterials, 25(19), https://doi.org/10.1016/j.biomaterials.2003.12.005
2. Tang, S. et al (2014). Chitosan/carbonated hydroxyapatite composite coatings: Fabrication, structure and biocompatibility. 251(25), https://doi.org/10.1016/j.surfcoat.2014.04.028

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[BIO-121] SURFACE STRUCTURE AND PHYSICAL PROPERTIES OF A BIOMATERIALS: THE CUTICLE OF PRICKLY PEAR (OPUNTIA FICUS INDICA)

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The cuticle, in the cladode of prickly pear, is the external cover that delimits that organ and therefore protects it from the adverse environmental factors. It is a polymeric fatty matrix of cutin, on epidermis with associated waxes (intra and extra cuticle). The objective of the work was to characterize and analyze the microstructure, heat resistant capacity (heatR-capacity) and expansion-reduction process of cuticle in response to water. Cladodes (1.5-2.5 years) were selected to obtain the cuticle and it was inspected for quality, according to the patent process (Mxa2017_013218). The cuticle (th=0.13µm; ρ=13.67g/m2; humidity= 10.15%) was examined by SEM. The heatR-capacity of the cuticle was tested on circular pieces exposed to dry heat in a Fisher Johns equipment up to their ignition point. The expansion-reduction was evaluated, in dry cuticle samples of surface 100cm2, introduced in water (25-27 °C) for 2h, later they were extracted and dried in an oven at 40 °C. The SEM results revealed deterioration in the extra-cuticle waxes with a scaly and fragmented appearance, but a preserved structure for cuticle layer (cutin matrix, intra waxes) and highly organized epidermal cells. The flash point occurred between 200-220 °C. A high heatR-capacity for a biomaterial; however, congruent for a composition of waxes in plant cuticles, which could be used to protect against forest fires. Finally, a value of 6% was determined in the expansion capacity of the cuticle due to hydration and a reduction to the original size in 30 minutes at 40 °C. This refers to a material with useful intelligence to develop biological functionality in the cladode of prickly pear, by expanding, for example, in a short time to reserve rainwater after a season of extreme drought, without exploiting. The results of heatR-capacity and expansion of the cuticle are aspects that inspire potential technological developments.

Keywords: cuticle, surface, heat resistant capacity, expansion, prickly pear.

Reference: L. Gang Shuai et al., Composition, metabolism and postharvest function and regulation of fruit cuticle: a review, Food Chem. 411(2023) 135449 https://doi.org/10.1016/j.foodchem.2023.135449.

This work was supported by: This work was sipported by the University of Guanajuato through its campus Celaya-Salvatierra.

[BIO-197] COMPOSITION OF CALCIUM PHOSPHATE PASTES USED IN ADDITIVE PRINTING OF BONE SCAFFOLDS

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Calcium phosphate ceramics are of special interest in bone regeneration and repair investigations, because they mimic the inorganic component of natural human bone. These ceramics enhance bone formation depending on the crystalline phase used and the Ca/P ratio, which result in the calcium and phosphate ion necessary for bone mineralization. The characteristics of biomaterials and the requirements of bone scaffolds determine the additive manufacturing technologies available. This paper presents the composition of the ceramic powders that make up the ceramic paste for the best fluidity conditions, for the formation of bone scaffolds using the paste module of the 3DMM1 printer.

Keywords: Additive printing, Bone regeneration, Calcium phosphate pastes, Ceramics powders.
Reference: K. Lin, R. Sheikh, S. Romanazzo, and I. Roohani, “3D Printing of Bioceramic Scaffolds—Barriers to the Clinical Translation: From Promise to Reality, and Future Perspectives", Materials , vol. 12, no. 17. 2019.
This work was supported by Instituto Politécnico Nacional.

[BIO-281] WO3 THIN FILMS GROWN ON TRANSPARENT WOOD BY RF-SPUTTERING FOR APPLICATION IN ELECTRONIC DEVICES

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Transparent wood is obtained by removing the lignin of natural wood and infiltrating a polymer into the wood´s cell walls (Li et al., 2018) , this process ensures that light instead of being absorbed it is transmitted, as well as having improved properties such as mechanical and thermal. In-house processes have been developed to obtain good quality in transparent wood from local Chakà (Bursera Simaruba) trees. In this work WO3 thin films were grown on transparent wood by RF-Sputtering, by varying the growth time 3 samples with different thicknesses were obtained. Optical and morphological studies were performed on the samples to measure the performance of the coatings, by performing UV-Vis spectroscopy it is shown that the samples have good transmittance in the visible region and by Scanning Electron Microscopy (SEM) it is observed the infiltration of the polymer into the wood's cell walls, making the samples suitable for applications as electronic devices.

Keywords: Transparent wood, Electrochromic, Sputtering.
Reference: Li Y, Fu Q, Yang X, Berglund L. 2018 Transparent wood for functional and structural applications. Phil. Trans. R. Soc. A376: 20170182.
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[BIO-289] SIMULATION OF BRINELL HARDNESS TESTING FOR TI6AL4V USING NUMERICAL METHODS

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Nowadays, the use of biomaterials for the replacement of deteriorated joints in the human body has led to the use of alloys with good biocompatibility and mechanical properties suitable for long-term performance. Ti6Al4V alloy is considered as one of the most used alloys in prosthetic surgeries and aeronautical industry due to its low density, ductility, elastic modulus, corrosion resistance and good mechanical properties. Experimental tests were carried out to obtain the Brinell hardness of the titanium alloy. The measurement of the diameter and the area of the footprint left by the ball indenter was obtained by Scanning Electron Microscopy. A digital scanner AMETEC ® brand was used and the profile of the footprint was obtained to determine its topography and make the comparison with the numerical simulation. Therefore, the objective of this research is the verification of the Brinell hardness test for the Titanium Ale alloy by means of numerical simulation, using a nonlinear elastoplastic model of isotropic material. Demonstrating that the model used to simulate the test and the experiments performed with the hardness tester to measure the Brinell hardness has enough accuracy in the plastic deformation produced by the penetration of the 2.5mm spherical indenter with the material surfaces.

Keywords: Brinell hardness,Numerical simulation, Ti6Al4V Eli, MEB, 3D scanning
Reference: La presente investigación se llevó a cabo en los laboratorios del Tecnologico de estudios Superiores de Jocotitlán en colaboración con el grupo de investigación de Ciencia e Ingeniería de Materiales con sede en el UPVM
This work was supported by: Support from CONAHCYT to the Postgraduate Studies and Research Section of the IPN at ESIME Zacatenco. y the Tecnologico Nacional de México, Tecnológico de Estudios Superiores de Jocotitlán.

[BIO-110] OBTAINING NANOCRYSTALLINE HYDROXYAPATITE BY CONTINUOUS SYSTEM

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Nanorods with diameters between 15 and 25 nm were obtained in the sample and human dentin, with lengths of 50-80 nm and 50-70 nm, respectively. Culture of human osteoblasts suggested that the specific surface area and relative crystallinity of the samples are critical parameters for cell viability. The biocompatibility test suggested the feasible use of the hydroxyapatite obtained in the continuous system for biomedical applications.

Keywords: Continuous system, Biomedical applications, Human dentin, Osteoblasts, Nanocrystalline Hydroxyapatite.
Reference: Kothapalli, C.R., Wei, M., Legeros, R.Z. & Shaw, M.T. (2005). Influence of temperature and aging time on HA synthesized by the hydrothermal method. Journal of Materials Science. Materials in Medicine, 16(5): 441-446. doi:10.1007/s10856-005-6984-5.
This work was supported by Instituto Politécnico Nacional.

[BIO-250] BIODEGRADATION OF POLYURETHANE BY THE FILAMENTOUS FUNGI CLADOSPORIUM SP

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Polyurethane (PU) are a type of mostly biodegradable synthetic polymer with a wide range of applications such as biomedical, automotive, etc. But its high demand and use has generated a great problem of contamination and waste management. According to the above, there is a need to explore for alternative methods to minimize the problems due to the accumulation of PU residues. In this sense, there are studies that have reported that PU may be vulnerable to attack by microorganisms such as filamentous fungi. Therefore, in this study the search for fungal strains with the capacity to biodegrade PU is proposed. To achieve this, a biodegradable PU was synthesized, and a strain of microscopic fungus was isolated from soil. The strain was identified according to its main morphological characteristics. PU biodegradation experiments were performed on plates using potato dextrose agar (PDA). PU biodegradation was monitored at days 7, 21, and 35 by weight loss, light microscopy, and scanning electron microscopy (SEM). Based on the morphological characteristics, the strain was identified as Cladosporium sp. On day 35, the PU lost 6.22 ± 1.04% weight due to the effect of Cladosporium sp., while the control (PU without strain) lost 1.14 ± 0.39%, being statistically different. On the other hand, optical microscopy allowed us to observe that the control did not show visible changes. Cladosporium sp. it even generated holes in the polymer from day 7 of incubation. The SEM evidence confirms that the fungus accumulates on the surface of the PU, observing grooves, cracks and erosion on the surface. In addition, it was found that the cells of the fungus have a hydrophobicity of 64.31 ± 0.22 %. Therefore, we consider that the strain Cladosporium sp. isolated in this work shows potential for biodegradation of PU.

Keywords: filamentous fungi, polyurethane, biodegradation, Cladosporium sp., microscopic fungi
Reference: M. Osman Sadia, A. Satti, F. Hasan, S. Ziaullah, A. Aamer. Degradation of polyester polyurethane by Aspergillus sp. strain S45 isolated from soil. J Polym Environ. 26 (2018) 301–310. https://doi.org/10.1007/s10924-017-0954-0.

[BIO-252] MICROSTRUCTURAL CHARACTERIZATION OF POLY(VINYLIDENE FLUORIDE) FILMS BY SOLVENT CASTING METHOD

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This study presents the synthesis process of poly(vinylidene fluoride) (PVDF) films using dimethylsulfoxide (DMSO) as a solvent and establish that PVDF can be used as a dielectric material for energy storage devices. The synthesis of the films was prepared by solvent casting method applying specific temperature and pressure. PVDF films were annealed at 90, 100 and 150 °C at atmospheric pressure for 5 hours at each temperature. Other films were treated at a vacuum pressure of 0.04 MPa and 0.08 MPa at room temperature for 14 days. From X-Ray Diffraction (XRD) analysis of the films annealed at different temperatures, β and γ phases were identified coexisting between 90 °C and 100 °C. While, at the annealing temperature of 150 °C, phases α and γ were identified. Meanwhile, it was observed that the low solvent evaporation rate at a vacuum pressure favored formation of β-phase at room temperature, as previously indicated by Horibe et al. From Fourier transform infrared spectroscopy (FTIR) analysis, α-phase was identified at 760, 875, 985, 1402 and 1430 cm-1, β-phase at 1073, 1170, 1275 cm-1 and γ-phase at 773, 812 and 1234 cm-1. In addition, a peak at 840 cm-1 corresponding to the presence of the β and γ phases. The FTIR results agree with XRD analysis, determining that by this method of synthesis at a temperature of 100 °C the β phase is obtained. From these results a semi-quantification of the α, β and γ phases was performed, finding that at 100 °C there is 18.2% α-phase, 53.1% β-phase and 28.7% γ-phase. While, at 0.08 MPa there is 21.7% α-phase, 15.4% β-phase and 62.9% γ-phase, establishing that by applying an annealing treatment at 100 °C during 5 hours a higher proportion of β-phase can be obtained, which provides the dielectric property of the material.

Keywords: DMSO, FTIR, PVDF, solvent casting, XRD.

Reference: Horibe, Y. Sasaki, H. Oshiro, Y. Hosokawa, A. Kono, S. Takahashi, and T. Nishiyama, "Quantification of the solvent evaporation rate during the production of three PVDF crystalline structure types by solvent casting", Polymer Journal, vol. 46, no.2, pp. 104-110, 2014.

This work was supported by This work was supported by the 20230078 and 20232280 IPN SIP projects.

[BIO-256] OPTICAL ABSORPTION AND EMISSION PROPERTIES OF BROCCOLI INFUSIONS

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Broccoli is one of the vegetables that has a very good reputation for having several health benefits due to its high nutrient contents. Some of the most important components of broccoli are its antioxidant agents, which have demonstrated to help preventing several diseases including cancer. Furthermore, carbon quantum dots can be obtained by processing broccoli extracts with hydrothermal or calcination treatments. Obtained dots can be used as biomarkers, heavy metal ions detectors or photodynamic agents for therapy.

In the present work, a broccoli infusion was prepared by putting broccoli in boiling water during 10 minutes. The infusion was filtrated using commercial coffee filters in order to eliminate big particles. Afterwards, several aliquots were taken and they were mixed with different concentrations of commercial white vinegar in order to induce PH modifications.

Th optical absorption and transmission of the samples were studied by UV-Vis spectroscopy. It was found that addition of vinegar changes the infusion color from the original green-yellowish one to a transparent liquid. Optical transparency depends on the vinegar concentration.

The photoluminescence emission of the samples were studied by using 405 and 370 nm excitation sources in order to observe different radiative transitions that help to shed some light to the components responsible for the electronic transitions that help to design strategies to use this infusions for biomedical applications.

Keywords: Broccoli, photoluminescence, UV-Vis.
This work was supported by Universidad de Guadalajara under PRO-SNI program.

[BIO-312] ANTIMICROBIAL EFFECT OF SILVER NANOPARTICLES IN DENTAL BIOFILM OF PATIENTS WITH MOTOR AND INTELLECTUAL DISABILITIES

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Worldwide, dental caries and periodontal disease are the main diseases affecting public health, caused by microorganisms present in oral biofilm. Although silver nanoparticles have demonstrated their antimicrobial effect on various types of microorganisms, there are no studies that have determined the inhibition of bacterial growth in oral biofilms taken from patients with motor and intellectual disabilities.

Keywords: Nanoparticles silver, antimicrobial effect, down syndrome, cerebral palsy, mental retardation.
Reference: Espinosa-Cristóbal LF, Martínez-Castañón GA, Martínez-Martínez RE, Loyola-Rodríguez JP, N. Patiño-Marín, Reyes-Macías JF, et al. Antibacterial effect of silver nanoparticles against Streptococcus mutans. Mater Lett 2009;63:2603–6. https://doi.org/10.1016/J.MATLET.2009.09.018.

[BIO-342] BIOSENSORS BASED ON ZINC OXIDE THIN-FILM TRANSISTORS (ZNO-TFT) USING RECYCLABLE PLASTIC SUBSTRATES AS AN ALTERNATIVE FOR REAL-TIME PATHOGEN DETECTION

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The fabrication of biosensors has future applications mainly from the perspective of eco-friendly technologies. Label-free strategies, recyclable materials, and low-temperature processing are parameters to consider for the development of a new generation of biosensor devices. In this work, Zinc oxide (ZnO) Thin-film Transistors (TFTs) using recyclable plastic substrates were used for real-time enteropathogenic Escherichia coli detection for the development of bio-TFT biosensors. Fourier Transform Infrared Spectroscopy (FTIR) was used to verify the characteristic absorption peaks at the different steps of the bio-TFT assembly process, whereas bacterial detection was assessed by electrical characterization. Finally, detection was validated by a molecular strategy consisting of DNA extraction from bacteria attached in situ over bio-TFTs surface, and the development of the Polymerase Chain Reaction to amplify specific genes from enteropathogenic Escherichia coli [1]. This experimental strategy was able to couple the physics of TFTs, thin-film deposition at low temperature, and binding of the biological recognition element (antibody) without affecting the device functionality. The tested conditions of the biofunctionalization process are compatible with TFTs fabrication at low temperature, as observed by FTIR characteristic signals of amide I and II and disulfide bridges. From the detection stage, the electrical modifications are associated with bacterial concentration (1x108 cell/ml) and the related response showed an important variation compared to the base signal. The use of a recyclable plastic substrate PET enables compatibility with flexible electronics that could contribute to its use as a low-cost biosensor useful in rural communities that lack the necessary infrastructure and trained personnel for bacterial detection. This technology has the versatility to be extrapolated to different testing models under different environments, such as food and clinical samples, allowing the early detection of emerging diseases (bacterial or viral), to provide the opportunity of self-testing for end-users.

Keywords: ZnO, TFT, PET, Biosensors, E. coli EPEC.

Reference: (1) R.A. Salinas, A. Orduña-Díaz, O. Obregon-Hinostroza, M.A. Dominguez, Biosensors based on zinc oxide thin-film transistors using recyclable plastic substrates as an alternative for real-time pathogen detection, Talanta. 237 (2022). https://doi.org/10.1016/j.talanta.2021.122970.

This work was supported by Fondo Sectorial de Investigación para la Educación CONAHCyT-SEP (Grant Number: A1-S-7888), VIEP-BUAP (Grant Number: DJMA-EXC17-G), and Proyecto SIP-IPN 20210151. M. Dominguez thanks Filmtronics Inc. PA, USA, for the supplies provided. O.-Obregon would like to thank CONAHCyT-Mexico for the scholarships awarded.

Sesión Oral

[BIO-21] CHITOSAN/PVA BIOPOLYMER FUNCTIONALIZED WITH SELENIUM NANOPARTICLES, AS AN ANTIBACTERIAL AGENT FOR THE FOOD PACKAGING INDUSTRY

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Chitosan (Ch) is a natural polymer isolated from crustacean shell waste, which possesses antioxidant and antimicrobial properties. Polyvinyl Alcohol (PVA) it's a synthetic polymer with solubility in water, that exhibits properties such, low toxicity, biocompatibility and film forming properties. These properties are crucial for the food industry due that this biopolymer composite works as an active material. Selenium Nanoparticles (Se Nps) are known as a nanomaterial with antibacterial and biocompatibility properties. In this work, we demostrate the antibacterial potential of Ch/PVA films functionalized with Se Nps. Ch was extracted from shrimp shells from the specie Farfantepenaeus Californiensis a native shrimp from the Gulf of California, Se Nps were synthesized by a green method using Pluchea Sericea (Cachanilla) aqueous extract (a native plant of Baja California, Mexico) as reducing and stabilizing agents, respectively. In the case of the active polymer, transparency, permeability and stiffness were characterized by qualitative methods. Tensile Strength and Elongation at break were analyzed as mechanical properties in a universal testing machine and morphological properties of films were performed by Scanning Electron Microscope (SEM). For Se Nps characterization, shape, size, particle distribution, and Z potential were characterized by Dynamic Light Scattering (DLS), UV-VIS, and Scanning Electron Microscope (SEM). Finally, functionalized films were tested on strains of E. Coli and S. Aureus, bacteria recurrent in contaminated food in supermarkets. Also, the biopolymer was tested as a film packaging on green grapes to know the preservation quality during storage. The results suggest that the functionalized Ch/PVA films significantly reduce the growth effect of the bacteria evaluated, this will contribute to develop new materials for the food packaging industry. Furthermore, this work contributes to the environment by substituting synthetic plastic films with a biopolymer from shell waste.

Keywords: Chitosan, PVA, Biopolymer, selenium, packaging.

Reference: Hajji, S., Salem, R. B.S., Hamdi, M., Jellouli, K., Ayadi, W., Nasri, M., & Boufi, S. (2017). Nanocomposite films based on chitosan–poly(vinyl alcohol) and silver nanoparticles with high antibacterial and antioxidant activities. PSEP., 111, 112–121. https://doi.org/10.1016/j.psep.2017.06.018

This work was supported by Laboratorio de Corrosion y Materiales Avanzados, Laboratorio de Biologia Molecular y Cancer, del Instituto de Ingenieria de la Universidad Autonoma de Baja California y el CONAHCYT.

[BIO-66] RELEASE STUDY OF CHITOSAN AND THYME ESSENTIAL OIL-LOADED NANOPARTICLES CONTAINED IN NANOCOATINGS BY UV-VIS SPECTROSCOPY

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Nowadays agricultural products conservation using environmentally friendly compounds is of special interest. It is well known the antifungal and antibacterial properties of chitosan as a nontoxic and biodegradable polymer. Also, thyme essential oil (TEO) has a significant antimicrobial activity against phytopathogens present in fruit nd vegetables. However, due to its volatility, the encapsulation could prevent the loss of the volatiles. Therefore, chitosan is a good alternative as an encapsulating agent. In this work, chitosan nanoparticles (CSNPs) and thyme essential oil-loaded chitosan nanoparticles were prepared using the nanoprecipitation method. Thyme essential oil concentration were 1, 2, 3, 4, and 5%. The nanocoatings were elaborated based on 33% nanoparticles, 66.7% chitosan solution (1%), and 0.3% glycerol. The release profile of the encapsulated oil in CSNPs from the coating after 15 days at different oil concentrations was assessed by UV-vis spectroscopy. The samples were scanned from 190 to 300 nm. The maximum wavelength absorption for TEO was at 211.5 nm. Calibration curve was constructed. From the results, the release oil from the coating was observed over time. The percentage release after 15 days was 0.99 % (1 % TEO), 1.56 % (2 % TEO), 2.67 % (3 % TEO), 3.32 % (4 % TEO) and 3.67 % (15% TEO). Released time was based on shelf-life of horticultural products. The importance of this research was to set the basis for the controlled release of TEO from the CSNPs in the nanocoating for microorganism control to preserve postharvest quality of fruit and vegetables.

Keywords
Biodegradable, controlled release, preservation, concentration, bioactive agent

Reference

I. Brlek, A. Ludaš, and A. Sutlović, Synthesis and spectrophotometric analysis of microcapsules containing immortelle essential oil, Molecules 26 (2021) 2390. https://doi.org/10.3390/molecules26082390.

This work was supported by
IPN-SIP project 20231325.

[BIO-243] OBTAINING CARBON BLACK (CB) WITH TITANIUM DIOXIDE (TIO2) NANOPARTICLES THROUGH GREEN SYNTHESIS

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Nanotechnology is a rapidly growing field of research with a wide range of potential applications. Nanomaterials themselves possess unique physical and chemical properties that can be enhanced by combining them to form nanocomposites. Carbon black (CB) and titanium dioxide (TiO2) are two nanomaterials that have been extensively studied for their potential applications in a variety of fields. CB and TiO2 can be obtained in the form of nanoparticles, and there are a number of methods for synthesizing these materials. However, many of these methods have disadvantages, such as the use of sophisticated equipment, hazardous chemicals, or lengthy and expensive processes. This study presents a green synthesis method for the production of CB and TiO2 NPs using natural extract and waste tires. This method is environmentally friendly and relatively simple to implement, making it a promising alternative to conventional methods. Different heat treatments were made to the CB to obtain different degrees of oxidation, the CB and TiO2 NPs were characterized using SEM, EDS, Raman, and DLS techniques. The results showed that these materials have a high surface area and a narrow size distribution, making them well-suited for applications in water treatment. This study demonstrates the potential of green synthesis methods for the production of CB and TiO2 NPs to form a nanocomposite. These materials have a number of potential applications in water treatment and other fields, and they are a promising alternative to conventional methods.

Keywords: Carbon Black, TiO2 NPs, Green Synthesis, Enviromental Remediation.
Reference: R. Gómez Hernández, Y. Panecatl Bernal and M. A. Méndez Rojas, High yield and simple one-step production of carbon black nanoparticles from waste tires, Heliyon 5 (2019). https://doi.org/10.1016/j.heliyon.2019.e02139
This work was supported by CONAHCYT, Proyectos VIEP BUAP.

[BIO-163] PRODUCTION OF POLYESTER FIBER FUNCTIONALIZED WITH ZNO NANOPARTICLES USING VIRGIN AND RECYCLED PET

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The current study aimed to create antibacterial fibers utilizing polyethylene terephthalate (PET) sourced from discarded bottles. To provide antibacterial capabilities, the fibers underwent modification using zinc oxide (ZnO) nanoparticles synthesized through the sol-gel technique. The key processing parameters, encompassing raw material selection, pretreatment, and extrusion, were thoroughly examined to identify optimal manufacturing conditions for the recycled PET fibers functionalized with ZnO oxide nanoparticles. The resulting fibers were evaluated for their physical, thermal, mechanical, and antibacterial properties. The inclusion of nanoparticles in the fibers demonstrated antibacterial activity against Staphylococcus Aureus (S. Aureus).

Now a days, the demand for textiles with antimicrobial activity has significantly increased in recent years. Such textiles aim to prevent performance degradation caused by microbial degradation, limit bacterial growth, reduce unpleasant odors resulting from microbial activity, and prevent the transfer and spread of pathogenic microorganisms (Höfer, 2006). Nanotechnology has emerged as a valuable tool across various fields of study. Inorganic materials like metal oxides, specifically Zinc oxide nanoparticles (ZnO NPs), have garnered attention due to their non-toxic nature (Fu et al., 2005).

Keywords: recycling, PET fiber, ZnO nanoparticle, antibacterial, sol-gel.
Reference: C. Cabello-Alvarado et al., 2019. Revisión de métodos para la obtención de textiles técnicos. textiles técnicos y su obtención. Revista Iberoamericana de Polímeros y Materiales, Volumen 20 (3).
This work was supported by The authors are thankful for financial aid received from CONACyT (Consego Nacional de Ciancia y Tecnología) and INCyTEA (Instituto de Ciencia y Tecnología del Estado de Aguascalientes).

[BIO-113] CELLULOSE ACETATE NANOFIBERS DECORATED WITH USING ELECTROSPINNING TECHNIQUE

Aime Margarita Gutierrez Peralta Dra.[1], Karen Rodriguez Rosales Dra.[2], Ana Angelica Feregrino Perez Dra.[3], Alma Delia Bertadillo Jilote M. en C.[1], Joel Moreno Palmerín Dr.[4], Liliana Licea Jiménez Dra.[5], Claudia Elena Pérez García Dra.[1]

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Cellulose acetate is a polymer that comes from the acetylation of the hydroxyl groups of cellulose, the most abundant natural polymer on Earth. This biopolymer has several properties that depend on the length of the polymeric chain, the degree of acetylation of the cellulose, and the type and amount of plasticizer. Among the properties that stand out are compatibility with other materials, hydrophobic, good adhesion, moisture resistance, and low cost. Cellulose acetate has widely used as a base in varnish, adhesives, filters, textiles, and toys. The work aims to fabricate cellulose acetate fibers decorated with graphene oxide for future applications as a photocatalyst. In the GiGa electrospinning equipment, electrospun cellulose acetate fibers were fabricated and decorated with graphene oxide (GO). Cellulose acetate dissolved in an acetone-ethanol 9:1 mixture and graphene oxide dispersed in ethanol was added in the following amounts: 0.5, 1.0, and 1.5 ml. The polymer solution was electrospun by varying the deposition distance (5-15 cm) from the needle to the collector and the applied voltage. The obtained nanofibers present fiber or ribbon-like morphology depending on the synthesis conditions as observed in the SEM images. In addition, TGA analysis of the nanofibers reveals a rapid mass loss of 12% attributed to the water contained in the sample, and the fibers are thermally stable up to about 400°C followed by decomposition at 500°C. In this work, cellulose acetate fibers decorated with graphene oxide were fabricated, which demonstrated higher thermal stability than bulk cellulose acetate.

keywords: Cellulose acetate, Graphene oxide, nanofibers, electrospinning, nanocomposites.
Reference: Yuanyuan Li, Qing Hu, Rui Zhangm Wenmei Ma, Siwei Pan, Yaohong Zhao, Qing Wang and Pengfei Fang, Piezoelectric Nanogenerator Based on Electrospinning PVDF/Cellulose Acetate Composite Membranes for Energy Harvesting, Materials 15 (2022) 1-13.
https://doi.org/10.3390/ma15197026
This work was financed by: Estancias Posdoctorales por México 2022.

[BIO-129] SYNTHESIS AND CHARACTERIZATION OF BIODIESEL USING CARBON FIBERS

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The continuous use and harmful effects derived from fossil fuels on the environment dictate to think about renewable alternatives without having adverse effects on the ecosystem. In this way, biodiesel is presented as a replacement for conventional diesel due to its renewable, biodegradable and non-toxic nature (Gupta and Rathod, 2019). Biodiesel, which is an alkyl ester of fatty acid, is considered a clean biofuel source, produced from renewable sources such as vegetable oils and animal fats (Corro et al., 2015). In this sense, a design of experiments was carried out to characterize the synthesis of biofuels through carbon fibers. Particularly, the synthesis of transesterifications and esterifications was carried out by varying different parameters and reaction conditions. The carbon fibers were impregnated with KOH in the presence of the reactions to act as a catalyst. The results show characteristics consistent with those of the biodiesel produced, in addition to a yield greater than 75%. Thus, using carbon fibers for the production of biodiesel, the necessary parameters and conditions are established for the production of this biofuel, reducing the production pollution generated by traditional fossil fuels.

keywords: Biodiesel, Catalysis, Transesterification, Vegetable Oil, Fibers.
Reference: A.R.Gupta, V.K.Rathod. Energy. 182, 795-801 (2019).
G.Corro, N.Sánchez, U.Pal, F.Bañuelos. Waste management. 47, 105-113 (2016).
This work was financed by: Consejo Nacional de Ciencia y Tecnologia (CONACYT)

[BIO-58] USE OF HYBRID BIOFOAMS FOR THE REMOTION OF AGRICULTURAL POLLUTANTS ON WATER

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Mexico is a developing country where more than 70% of consumptive water use is concentrated in the agricultural sector. To meet the demand for food, vegetable production must be increased by increasing the application of agrochemicals, including pesticides, causing side effects on the environment. Water is the main polluted resource and due to its importance for humans, different strategies have been created for its decontamination that are friendly to the environment such as heterogeneous photocatalysis using nontoxic materials.

This talk presents information about the removal of neonicotinoid pesticides such as imidacloprid and thiacloprid, as well as a metal such as copper, which are very common compounds used in greenhouses for pest control. We will show the interaction of the aforementioned pollutants with a cellulose-based biofoam homogenously loaded with zeolites and zinc oxide which we call "hybrid biofoam". Finally, the phytotoxicity test and full disintegration in compost demonstrate the environmental friendliness of the synthesized hybrid biofoams.

Keywords: pesticides, biofoam, photocatalysis, phytotoxicity, composting.
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[BIO-190] IDENTIFICATION OF USEFUL CHARACTERISTICS OF ZEOLITE FOR ITS USE AS MAIN COMPONENT METARHIZIUM ANISOPLIAE FOR ENTOMOPATHOGENIC FUNGAL USED IN THE BIOLOGICAL CONTROL OF SUGARCANE PESTS

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In this work, we have characterized micronized sieved zeolite free of organic residues as a substrate of Metharizium anisopliae spores. A thermal drying process of the zeolite was done before inoculate the fungal cultures prepared on laboratory. We have studied the zeolite through Scanning Electron Microscopy (SEM) to identify and verify parameters of interest such as morphology, porosity, and particle size. To obtain the chemical content we have performed Energy-Dispersive X-ray Spectroscopy (EDS). We detected compositional content of oxygen, silicon, aluminum, and calcium. SEM images were digitally processed to obtain information concerning zeolite surface aimed to be used as biological substrate to provide the survival of entomopathogenic microorganisms, including Metarhizium anisopliae, remaining in a latent state before being activated. Results indicate zeolite substrate could be successfully applied as a biological control of pathogens in sugarcane culture.

Keywords: SEM, EDS, entomopathogenic, zeolite, Metarhizium anisopliae.
Reference: R. Alatorre y F. Hernández, Mosca Pinta (Hemiptera: Cercopidae), Casos de Control Biológico en México, editado por H. C. Arredondo-Bernal y L. A. Rodríguez del Bosque. Biblioteca Básica de Agricultura, Editorial del Colegio de Postgraduados, Vol 2, 141-164(2015).
This work was financed by: Instituto Politécnico Nacional, “Proyectos de Investigación Científica y Desarrollo Tecnológico”, Project No. 20232120.

[BIO-279] PREPARATION AND CHARACTERIZATION OF CONTROLLED RELEASE SYSTEMS OF BIOHERBICIDA@QUITOSANO

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The results of the encapsulation of a Puccina sp. Bioherbicide formulation are presented, using the drip extrusion technique and chitosan as encapsulating polymer. Bioherbicide precursor solutions containing sodium glutaraldehyde were prepared under ambient conditions and with rigorous agitation. By varying the percentage of glutaraldehyde 4.0, 3.0, 2.0 and 1.0% in the precursor solution containing the bioherbicide, it was possible to prepare bioherbicide capsules with sizes of 4 mm and control the porosity of the shells. The characterization by optical microscopy showed the formation of well-defined and homogeneous microcapsules. The SEM analysis reveals the formation of different morphologies in the cross section of the shells depending on the glutaraldehyde 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 by optical absorption spectroscopy in the UV-Vis range.

Keywords: controlled release system, bioherbicide, extrusion dripping.
Reference: G. L. Zabot, F. Schaefer Rodrigues, L. Polano Ody, M. Vinícius Tres, E. Herrera, H. Palacin,J. S. Córdova-Ramos, I. Best y L. Olivera-Montenegro, Encapsulation of Bioactive Compounds for Food and Agricultural Applications, Polymers, 14 (2022), https://doi.org/10.3390/polym14194194.

[BIO-31] ENZYMATIC FUNCTIONALIZATION DEVELOPMENT FOR SUBDERMAL GLUCOSE MONITORING

Estephanny Jocelyn Alvarado Muñoz M.C.[1], David Andrés Fernández Benavides Dr.[1], Alexis Cruz Zabalegui M.C.[1], Pablo Alfonso Tirado Cantú Dr.[1], Juan Ponce Hernández M.C.[1], Gilberto de Jésus León Muñoz M.C.[1], Jesus Javier Alcantar Peña Dr.[1], Ricardo Antonio Escalona Villalpando Dr.[2], Daniela Díaz Alonso Dr.[1], Iker Rodrigo Chavéz Urbiola Dr.[1]

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Diabetes is one of the non-communicable diseases that most affect the world's population, causing the death of one person every 5 seconds. This chronic metabolic disorder, characterized by high blood sugar levels (>126 mg/dl), poses challenges for individuals, healthcare systems, and societies alike. Several strategies have been proposed to mitigate the damage of this disease, including molecular/genetic techniques and tissue engineering, however, these strategies still require years of research before they can be really applied and therefore a short-term strategy is correct and simpler monitoring of the disease, as well as the supply of medication.

This work studies different techniques of enzymatic functionalization to improve mechanical properties. The obtained functionalization process was capable to remain pristine after repeated piercing tests and quantify glucose levels at a subdermal level. The enzymatic functionalized process was carried out with glucose oxidase on commercial stainless-steel needles, using as mechanical and enzymatic support, biocompatible amino polymers (polypyrrole and polyaniline) to determine the best technique for the permanence after puncture of the functionalized film as well as the best electrochemical response for the measurement of glucose.

Needles were soldered to a wire for conductivity measurements and then coated with a platinum layer. Once metalized, the needles were coated with electrochemical polypyrrole and polyaniline polymers, then they were enzymatically functionalized by three different methods: 1 and 2 by varying the glutaraldehyde and 3 by varying the amount of glucose oxidase and adding Nafion. The obtained needles were taken to a puncture test to evaluate the permanence of the enzyme functionalization film. Finally, measurements were performed with a potentiostat to obtain voltammograms and chronoamperograms at different glucose concentrations and to determine its response toward glucose.

Preliminary results showed improved mechanical support of the functionalization film by adding polymers beforehand and improved oxidation response using method 3.

Keywords: Functionalization, Glucose Oxidase, Polypirrole, Polyaniline, Biosensor, Microneedles.

Reference: Wingard LB Jr, et.al. Immobilized enzyme electrodes for the potentiometric measurement of glucose concentration: immobilization techniques and materials. J Biomed Mater Res. 1979 Nov;13(6):921-35. 10.1002/jbm.820130610. PMID: 117008.

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CHARACTERIZATION AND METROLOGY

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

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

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

[CHM-23] MORPHOLOGICAL AND STRUCTURAL CHARACTERIZATION OF CATALYSTS SYNTHESIZED FROM FLY ASHES TO BE USED DURING THE HYDRODESULFURIZATION OF STRAIGHT-RUN GAS OIL

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Nowadays, environmental regulations are more stringent worldwide and refineries are required to produce low-sulfur fuels to meet the specifications. In this research, fly ash (FA) was converted into aluminosilicates by hydrothermal synthesis using sodium hydroxide (NaOH) with a FA/NaOH ratio of 1:6. In addition, aluminosilicates were used as supports to synthesize NiMo and CoMo catalysts, which are commonly used to remove sulfur from crude oil and petroleum derivatives. Metal impregnation of the support was carried out by two methods: 1) hydrothermal synthesis at 195°C using Ni, Co, and Mo salts and thiourea as the sulfur source, and 2) incipient wettnes at 400°C using Ni, Co, and Mo salts to obtain metal oxides that are further sulfided. The supports (aluminosilicate) and catalysts (NiMo/aluminosilicate, CoMo/aluminosilicate) were characterized by scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), and X-ray diffraction (XRD). The micrographs obtained by SEM showed that the fly ash and catalysts have similar morphology, while the presence of Ni, Co, Mo, Al and Si on the materials were detected by EDS. The conversion of fly ash by hydrothermal synthesis yields mainly zeolite P, followed by zeolite K and unconverted mullite as determined by XRD. In addition, the presence of molybdenum oxide and cobalt and/or nickel were observed in higher amount in the catalysts obtained by incipient wetness compared to those obtained by hydrothermal synthesis. Finally, the catalysts were evaluated in the hydrodesulfurization of straight-run gas oil to select the most active material for the reaction.

Keywords
hydrodesulfurization, hydrothermal synthesis, fly ash, zeolite
This work was supported by
Instituto Politécnico Nacional, Consejo Nacional de Humanidades Ciencias y Tecnologías (Conahcyt)

[CHM-75] CHARACTERIZATION OF A SILICON PHOTOMULTIPLIER FOR ITS IMPLEMENTATION IN A PARTICLE DETECTOR

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Silicon photomultipliers (SiPM) are devices widely used in many fields of applied science and engineering, like medical technology, environmental cleaning, and particle physics. In recent years, they have been implemented in particle detection technology; due to their high precision photodetection capability, they can detect single photons, which makes them an excellent option to analyze non-charged particles that produce photons in specific reactions with baryonic matter. The characterization of these devices is important since they work under specific temperature conditions that can tell us some notable SiPM parameters like breakdown voltage, and gain. The main purpose of this project was the obtain the parameters mentioned above, for this requirement, we used the I-V curve methodology to determine the breakdown voltage and calculate the gain to finally set the parameters to build a particle detection module.

Keywords
Silicon Photomultiplier, Characterization, I-V Curve Method, Particle detection

[CHM-97] SOLAR ABSORTANCE OF N- TYPE POROUS SILICON ELABORATED BY ELECTROCHEMICAL ANODIZATION

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We report the solar absorptance determination of porous silicon (PSi) samples elaborated with different substrates and several attack times to determine this parameter for a potential application as a photothermal material. The PSi samples were elaborated by electrochemical anodization from non-degenerate, (100) oriented n-type crystalline silicon (2 x 1018 cm-3), around 300 mm thickness, and 1-5 W·cm electrical resistivity. The reflectance of the samples was measured in the range from 200 to 1100 nm with an FS5 Edinburg spectrofluorometer equipped with an SC-30 integrating sphere. A scanning electron microscope (SEM) from Jeol, model JSM-6390LV was used in the morphological characterization. The porosity percentage was determined by gravimetry using an analytical balance Schuler Scientific SAS-225R. The microstructural analysis shows three distinct regions, as it was expected: a thin microporous layer on top of the sample, a macroporous layer with a columnar structure, and the crystalline silicon substrate. The percentage of porosity changes significantly with the anodization time, with an approximately linear increase as a function of the thickness fraction of the porous layer. The reflectance decreases notably for the PSi samples, even for low anodization times. From the reflectance results, the solar absorptance of each sample was obtained, showing a significant dependence on the percentage porosity.

Keywords
Porous silicon, solar absortance, thermal diffusivity, thermal conductivity, porosity.

Reference

I. Fernández-Peña, A. Alvarado-Palacios, E. Barrera-Calva, J. Calderón-Arenas, M. García, C. Falcony, R. Fragoso, G. Alarcon-Flores, C. Paredes-Sánchez, and M. Aguilar-Frutis, Spray-pyrolyzed Al2O3-Ag Nano-Cermets coatings for solar absorbers, Rev. Mex. Fis. 64 (2018) 392-398.

This work was supported by

Secretaria de Investigación y Posgrado del Instituto Politécnico Nacional, México; Comisión de Fomento de Actividades Académicas del Instituto Politécnico Nacional, México; Consejo Nacional de Humanidades, Ciencias y Tecnologías, México.

[CHM-157] COMMERCIAL UV-C LED CHARACTERIZATION FOR LAMP DESIGN

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Ultraviolet-C (UV-C) AlGaN light-emitting diodes (LEDs) have revolutionized disinfection systems due to their compact size, efficiency, and long lifespan. This work provides a characterization methodology focused on the wavelength range, operation temperature, heat dissipation, wavelength shift, optical power, and its effectiveness for E. coli bacteria. Therefore, this work presents a UV-C-LED lamp design for water disinfection, taking into consideration the integrity of the semiconductor device for heat generation, through several power regulation and heat dissipation techniques. So, we described the UV-C LED-based lamp effect in E. coli bacteria inoculated in eosin methylene blue agar.

Keywords
Ultraviolet light-emitting diodes; disinfection; AlGaN

Reference

Francisco A. Juarez-Leon et al.. (2020), “Design and Implementation of a Germicidal UVC-LED Lamp”, IEEE Access, DOI: 10.1109/ACCESS.2020.3034436

This work was supported by

Funding: This research was funding by TecNM/ITTG project number 18685.23-P.

[CHM-189] EFFECT OF LOW PRECIPITATION TEMPERATURE ON THE STRUCTURAL, MORPHOLOGICAL AND OPTICAL PROPERTIES OF MoO_3 POWDERS

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Molybdenum trioxide (MoO_3) has been widely investigated for applications in semiconductor devices due to its structural, morphological and optical properties. In this regard, different techniques have been reported to obtain MoO_3, but these involve a thermal stage above 200°C or high vacuum conditions (<4mPa). Although solvothermal synthesis of MoO_3 has been reported, it is not clear how the thermal precipitation process at low temperature (<200°C) can influence the physical properties of the MoO_3. In this work, molybdenum oxide was synthesized from a dilution of metallic molybdenum powder in ethanol and hydrogen peroxide, which was stirred by more than a half day. Subsequently, four different processes of thermal precipitation were performed at a temperature ≤ 150°C. Each of them produced a particular morphology, structure, and bandgap energy in the synthesized molybdenum oxide. The obtained powders exhibited blue-purple, intense yellow or yellow-orange, and intense green coloration, which may be associated with the Mo^{6+}, Mo^{5+}, and Mo^{4+} oxidation states, respectively. Phase confirmation and crystalline structure, vibrational behavior of chemical bonds, morphology, and energy bandgap were determined by XRD, FTIR, SEM, and UV-Vis characterization techniques, respectively. Through the synthesis process and precipitation temperature variation, different morphologies are observed as sheets, spheres, anhedral forms and agglomerated. Also, the presence of vibrational modes of metal-oxygen bonds in the region of 500 to 1000 cm-1. The other hand, the energy gap estimated by the Tauc method is found between 2.81 and 3.24 eV. As a result, the proprieties MoO_3 previously reported can inhibit the recombination of electron-hole pairs due to their different electronic states that influence charge transport. In addition, the present study provides a useful and convenient strategy for the fabrication of semiconductor materials.

Keywords

$MMoO_3$ Powder, low temperatures, electronic gap, charge transport.

Reference

Shi, J., Kuwahara, Y., Wen, M., Navlani-García, M., Mori, K., An, T., & Yamashita, H. (2016). Room-temperature and aqueous-phase synthesis of plasmonic molybdenum oxide nanoparticles for visible-light-Enhanced hydrogen generation. Chemistry–An Asian Journal, 11(17), 2377-2381.

This work was supported by

By CONAHCyT for the study scholarship and the PhD program in Materials Sciences-00044192.

[CHM-297] BISMUTH-BASED NANOPARTICLES SYNTHESIZED BY THE LASER ABLATION OF SOLIDS IN LIQUIDS TECHNIQUE: INFLUENCE OF LIQUID MEDIA

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In our research group, we synthesized bismuth-based colloidal nanoparticles (NPs) by using laser ablation of solids in liquids. A bismuth disk and three liquid media were used such as deionized water, hydrogen peroxide (H_2O_2, 3%), and sodium hypochlorite (NaClO, 12%). A pulsed laser Nd:YAG (1064 nm, 7 ns) was used to ablate during 20 min the Bi target at 6.32 J/cm^2 per pulse laser fluence. Depending on the liquid medium used, different colloidal dispersions were obtained initially. Colloids were deposited on monocrystalline silicon substrates (100) to be characterized by X-ray diffraction and Raman micro-spectroscopy. Results confirmed that Bi/Bi_2O_3 and $(BiO)_2CO_3$ were obtained for the synthesis with deionized water, Bi/β-Bi_2O_3 with H_2O_2, and δ-Bi_2O_3 phase with NaClO. UV-Vis spectroscopy was used to obtain their absorption spectra and then calculate the bandgap energy corresponding to each colloid. Additionally, nanoparticle average size distribution, lattice interplanar distance, and selected area electron diffraction were determined using high-resolution transmission electron microscopy (HR-TEM). These materials have potential applications in areas such as medical physics, photocatalysis, solid oxide fuel cells, and fabrication of optoelectronic devices, among others.

Keywords
Laser ablation of solids in liquids, Bismuth nanoparticles, Bismuth Oxide

Reference

C. B. Morales Ramos, M. Camacho López, M. A. Camacho López, A. R. Vilchis Néstor, M. Flores Castañeda, and S. Camacho López, δ-Bi_2O_3 nanoparticles obtained by laser ablation of solids in liquids, Mat. Lett., 309 (2022) 131415. https://doi.org/10.1016/j.matlet.2021.131415

This work was supported by

CBMR acknowledges to CONAHCYT and COMECYT (México) for the financing granted in the research program “Investigadoras e Investigadores-COMECYT” (EESP2022-005).

[CHM-305] DETECTION OF INTERNAL FLAWS IN METALLIC MATERIALS BY LASER-INDUCED ULTRASOUND TWO-DIMENSIONAL IMAGES

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This work reports on the generation of two-dimensional (2D) images using laser-induced ultrasound (LIU) to identify internal defects in metals. An aluminum sample with four artificial cavities of known geometry and different dimensions was used as an experimental model. A Nd: YAG laser with a pulse intensity of 26mJ was employed to generate the LIU signal. Ultrasound needle-type sensors were fabricated and used for LIU detection. Measurements were performed in water to couple acoustic impedances effectively. In this study, our focus lies on the analysis of longitudinal waves generated through LIU exclusively. By analyzing the flight times of the LIU signal in both front and back incidence modes, the precise location and size of the internal defects in the aluminum sample were determined. The results, obtained using the time of flight (TOF) equations, exhibited accurate calculations of the size and location of the internal defects, with a discrepancy smaller than 6%. This demonstrates the reliability and effectiveness of the LIU technique in detecting and characterizing internal defects in metals. Furthermore, representative 2D images of the areas associated with the artificial cavities were obtained through the analysis. These images provide visual evidence of the internal defect locations and dimensions, aiding in their identification and characterization.

Keywords
Laser-induced-ultrasound, internal defects, time of flight, Non-destructive testing, longitudinal waves.

Reference

1.Choi, S., & Jhang, K. Y. (2018). Internal defect detection using laser-generated longitudinal waves in ablation regime. Journal of Mechanical Science and Technology, 32(9), 4191–4200. https://doi.org/10.1007/s12206-018-0817-1

This work was supported by

The Fronteras de la Ciencia-CONAHCyT-México (Grant No. 2016-2-2029 and 376135), DAIP-UG CIIC (Grant No. 222/2023) and Tec NM Project 2023.

[CHM-335] FABRICATION AND MEASUREMENT OF DIRECTIONALITY OF NEEDLE-LIKE PHOTOACOUSTIC SENSORS

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The present work describes a method for fabricating and measuring the directivity of a needle-like photoacoustic sensor with a diameter of approximately 1mm, made of PZT ceramic. The fabrication method presented utilizes PZT ceramic as the sensitive element, enabling the production of needle sensors with dimensions of a few centimeters. On the other hand, the directivity measurement method employs a custom-designed laser ultrasonic source that generates a flat wave. This flat wave exhibits high uniformity in both amplitude and phase. To measure the directivity, the needle sensor under test is rotated around the source. The measurements demonstrated high repeatability, with a typical estimated repeatability of less than 5%. In conclusion, the characterization results of the needle-like photoacoustic sensors fabricated with PZT ceramic indicate their suitability for photoacoustic imaging reconstruction.

Keywords
Photoacoustic, Needle-Sensor, PZT Ceramic, Fabrication, Directivity Map.

Reference

[1] James A. Guggenheim et al, A Method for Measuring the Directional Response of Ultrasound Receivers in the Range 0.3-80 MHz Using a Laser-Generated Ultrasound Source. IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, Vol. 64 No. 12. 2017.

This work was supported by
CONAHCYT

[CHM-68] PHYSICOCHEMICAL CHARACTERIZATION OF MAGNESIUM BORATES DOPED WITH DYSPROSIUM FOR THE DETECTION OF IONIZING RADIATION

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Radiation is a form of energy and, being ionizing, it is unstable, with atoms or molecules acquiring an electrical charge. The detection and measurement of ionizing radiation is essential when using it. Thermoluminescence is a well-studied technique for this purpose. Magnesium Borates, as TL materials, have physical and chemical properties that can contribute in the area of personal and medical dosimetry. The characterization of TL materials is necessary, characterization techniques such as TEM and FTIR, help to discern and analyze the properties obtained in the materials for the specific application. The materils TL materials were previously synthesized to be characterized by HR-TEM and FITR with adequate preparation of material samples. The aim this work is to characterize Magnesium Borate TL materials for applications in ionizing radiation and with the results obtained were the degree of crystallinity, the phases present in the material (morphology) as well as the chemical bonds according to the absorption in the infrared for its structural identification.

Keywords
Physicochemical Characterization, Magnesium Borates, Thermoluminescence, Detection Ionizing Radiation

Reference

Torres-Cortes et. al. (2019), Synthesis and thermoluminescent response to γ-rays and neutrons of MgB4O7:Dy and MgB4O7:Dy,Na. Applied Radiation and Isotopes, 147,159-164.

This work was supported by
CONACyT

[CHM-270] DETECTION OF METHYELENE BLUE BY SERS EFFECT IN GOLD NANO-ISLAND DEPOSITS

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For the study and detection of molecules, metallic nanostructures supported on a surface have been used with the help of Raman spectroscopy it has been possible to detect them and take them to different applocations. In this work we study some variables that influence the study of the SERS effect of a 10-5 M solution of Methylene Blue. The excitation wavelength and the influence of the energy density on the Raman signals were studied, allowing the selection of the support where the gold nano islands will be deposited. The study analyzed the influence of the morphology of the Au nano-island deposits for the detection of Methylene Blue and the volume of the analyte for the SERS effect. For the analysis, 2 µl of the solution, a wavelength of 785 nm and a power of 1% were used.

Keywords
SERS, gold nano-islands, methyelene blue

Reference

A. Purwidyantri, C.-H. Hsu, C.-M. Yang, B. A. Prabowo, Y.-C. Tian, and C.-S. Lai, Plasmonic nanomaterial structuring for SERS, R. Soc. Chem., 9(2019) 4982–4992. doi: 10.1039/C8RA10656H.

This work was supported by
This work was carried out through the CONACyT project **A1-S-33899**

[CHM-328] EFFECTS OF NH_4SCN ADDITIVE IN THE $FAPbI_3$ PEROVSKITE FILMS IN A SEQUENTIAL DEPOSITION METHOD

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This study determined the effect of introducing the NH_4SCN additive in the precursor solution of $PbI_2$2 of a sequential deposition method in an open atmosphere to form $FAPbI_3$ perovskite over a glass substrate. Adding NH_4SCN leads to different intermediate layers according to the concentration of the additive. From an adequate concentration, an ionic substitution between I^- and SCN^- is promoted, providing a unique path for nucleation and growth of $FAPbI_3$ due to significant changes in morphology. The intermediate layer with a proper amount of NH_4SCN enhanced the physical properties of $FAPbI_3$. It contributed to understanding the crystallinity and morphological conditions for favorable growth of $FAPbI_3$ directly over a glass substrate. A concentration of 40% gave rise to the biggest grain size, homogeneous morphology, higher absorption, and prevalence of black phase in the α/δ phase coexistence. As a result, the perovskite with the NH_4SCN additive showed a positive effect on the growth mechanisms and enhanced stability due to the mixed α/δ-phase and grain size ~1350 nm. The preceding makes $FAPbI_3$ film with a concentration of 40% a good option for application as stable perovskite in solar cells.

Keywords
perovskite, FAPbI3, sequential deposition, ammonium thiocyanate, open atmosphere
Reference
https://doi.org/10.3390/cryst13050795
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Sesión Oral

[CHM-212] THE RELATION BETWEEN THE SHIRLEY BACKGROUND AND AUGER PEAKS IN PHOTOEMISSION SPECTRA: THE INTERCHANNEL COUPLING WITH VALENCE BAND LOSES MECHANISM

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The physical mechanism proposed in our 2017 paper about the origin of the Shirley background in photoemission spectra[1] es based on interchannel coupling[2] but with the important addition of energy losses in the valence band.[3] Besides the Shirley background, it is possible to derive other predictions of the interchannel Coupling with Valence Band Losses (ICL) mechanism. Two of them are discussed in this paper: 1) the quantitative relation between Auger peaks and the Shirley background and 2) the conduction-band-like structure of the extended region of the Shirley background.

Keywords
Interchannel coupling, Shirley background, XPS, Tougaard background, Auger peaks

Reference

"Intensity modulation of the Shirley background of the Cr 3p spectra with photon energies around the Cr 2p edge." Alberto Herrera-Gomez, et al. Rapid Communication. Surf Interface Anal. 50(2), p. 246-252 (2018). DOI: 10.1002/sia.6364. ISSN 1096-9918.

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[CHM-227] THE IVL BACKGROUND OF Ti 2p PHOTOEMISSION SPECTRA NEAR THE Ti 1s IONIZATION THRESHOLD

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In this work, we present further evidence supporting the role of an interchannel-coupling with valence-band losses (IVL) process as the primary mechanism responsible for the Shirley background observed in photoemission spectra. Our analysis focuses on Ti 2*p* photoemission spectra obtained from a metallic titanium film using Synchrotron light at Beamline 7-ID-2 at the Brookhaven National Laboratory, specifically in the vicinity of the 1*s* ionization threshold.

Significantly, we observe that the step-shaped background in Ti 2*p* photoemission spectra, referred to as the IVL background, exhibits both intensity and shape variations across the Ti 1*s* ionization threshold, providing support for the interchannel-coupling process. Through simultaneous fitting of Ti 2*p* photoemission spectra obtained at excitation energies lower and higher than the Ti 1*s* ionization threshold, we successfully replicate the step-shaped background using peaks termed IVL peaks, which exhibit a direct correlation with X-ray absorption spectra. The relative intensities of these IVL peaks enable quantification of the intensity modulation of the step-shaped background across the Ti 1*s* threshold. This finding validates the involvement of electronic transitions from the valence band to the conduction band in mediating the IVL peak structure.

Moreover, this study highlights that the intensities of the photoemission peaks remain approximately the same when utilizing an IVL background compared to a Shirley-type background, which holds practical importance for quantitative chemical composition analysis.

Keywords
IVL background, metallic Ti 2*p* photoemission spectra, Ti 1*s* threshold,

Reference

A. Herrera-Gomez, et al., Intensity modulation of the Shirley background of the Cr 3p spectra with photon energies around the Cr 2p edge, Surf. Interface Anal. 50 (2018) 246–252. https://doi.org/10.1002/sia.6364.

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[CHM-133] DESIGN, SYNTHESIS, AND OPTICAL ANALYSIS OF HOMOGENEOUS AND INHOMOGENEOUS OPTICAL FILTERS, GROWN BY REACTIVE SPUTTERING WITH MAGNETRON

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Thin films have been applied in the development of novel devices that can combine mechanical flexibility with optical transparency, but also in sustainable development when applied as a coating on the glass of buildings and cars. One of the problems in the synthesis of these filters made with the sputtering technique with DC magnetron is to control their growth with the appropriate optical properties and to ensure that it is repeatable. The work carried out in the Laboratory of Synthesis and Optical Analysis of Materials (SAOM-Lab) at the CNyN-UNAM is presented, on the design and manufacture of optical filters in the form of discrete multilayers and variable refractive index (inhomogeneous films), for optical applications such as anti-reflective films, low emissivity filters, protective layers, among others; grown by reactive sputtering technique. In addition to implementing real-time monitoring of the plasma, for the control and growth of the film, being a non-invasive technique that is directly related to the optical properties of the film, by the technique of spectro-Ellipsometry.

Keywords
Sputtering, Optical Filters, inhomogeneous films, ellipsometry, plasma

Reference

R Rodríguez-López, G Soto-Valle, R Sanginés, N Abundiz-Cisneros, J Águila-Muñoz, J Cruz, R Machorro-Mejía, Study of deposition parameters of reactive-sputtered Si3N4 thin films by optical emission spectroscopy, Thin Solid Films, 754, pp. 139313, (2022)

This work was supported by

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[CHM-327] DETAILED ANALYSIS OF THE Ti 2s PHOTOELECTRON SPECTRA OBTAINED WITH HARD X-RAY PHOTOEMISSION SPECTROSCOPY NEAR THE Ti 1s IONIZATION THRESHOLD

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Over the complete history of quantitative analysis of X-ray photoelectron spectra, the conspicuous step-like nature of the spectra has been the subject of intense debate. Since the early '70s, D. Shirley proposed a function that enabled quantitative analysis of experimental data, but, even today, no precise theoretical formalism for the latter exists. Efforts to explain diverse background features have been proposed, most notably by Tougaard since the '80s, but the theoretical framework still cannot explain the shape of the spectra and the quantitative exactitude required for chemical composition analysis. The present work presents efforts to provide evidence for an alternative explanation suggesting that valence-band excitations are the ones mainly influencing the step-like shape of the background as the photoelectron leaves the atom caused by different interchannel-coupling mechanisms [1]. The work seeks to precisely measure the background intensity using hard X-ray radiation from Beamline7-1 at the Brookhaven National Laboratory, of the Ti 2s core level. The results are intriguing, because a clear modulation of the background intensity is observed, plus, there is evidence suggesting that the step-like nature of the background has a detailed structure that can be modeled via a set of several peaks, which opens the possibility for a new understanding of how intraatomic phenomena as the photoelectron escapes the atom, influences the intensity of the integrated photoelectron signal; critical for precise quantitative analysis using this technique. We find that the intensity modulation of the Shirley background or step-like nature of the photoelectron background around the Ti 1s ionization threshold of the Ti 2s is the largest recorded for any core level reported to date.

Keywords
Shirley background, quantitative XPS, peak-fitting

Reference

[1] A. Herrera-Gomez, et.al., Intensity modulation of the Shirley background of the Cr 3 p spectra with photon energies around the Cr 2 p edge, Surface and Interface Analysis. 50 (2018) 246–252. https://doi.org/10.1002/sia.6364.

This work was supported by

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[CHM-304] HAFNIUM OXYNITRIDE ($HfO_{1-x}N_x$) AND SILICON HAFNIUM OXYNITRIDE ($SiHfO_{1-x}N_x$) COMPONENTS IN Hf 4f XPS SPECTRA

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Hafnium oxide on InGaAs is widely studied for its application in CMOS devices. However, there are still challenges to overcome, such as species migration and the growth of an interfacial layer. Nitridation is an alternative to reduce this problem. ARXPS provides non-destructive depth profiling information, offering valuable insights to understand and overcome these challenges. Nevertheless, there is a wealth of knowledge to be gained regarding the technique and its accurate application in analyzing these structures and their procedures.

Using angle-resolved X-ray photoelectron spectroscopy, we characterized and explored the limits on hafnia nitridation through remote plasma. Hf 4*f*, Si 2*p*, O 1*s*, C1*s*, and N 1*s* spectra were acquired before and after nitridation with various plasma power levels (500W-2500W). We identified the peak components using advanced tools for spectral analysis such as the Active Background Approach and Simultaneous Fitting Approach, both encompassed in the fitting software AAnalyzer®.

The Si 2*p* spectrum before nitridation shows a signal at 102.47eV attributed to $Si_{1-w}Hf_wO_2$ with a high hafnium content (*w*). The nitridation process also causes oxidation, giving rise to a peak related to SiON at 102.65eV. It was interesting to find out that the Si 2*p* peak in $Si_{1-w}Hf_wO_2$ shifts to lower binding energies with increasing power, suggesting dipole effects due to changes in the surface charges caused by the plasma. Silicon content increases in the $Si_{1-w}Hf_wO_2$ and one overlapped contribution related to $Si_{1-w}Hf_wO_{2-z}N_z$ appears. Moreover, in the Hf 4*f* spectrum before nitriding, we observed the HfO_2 (17.3eV) and $Si_{1-w}Hf_wO_2$ (17.8eV) contributions. After nitriding, the fitting revealed two extra signals at 16.8 and 16.38eV which were attributed to $SiHfO_{1-z}N_z$ and $HfO_{1-x}N_x$.

Additionally, using the multi-layer and the covariant matrix methods, we computed the structure and composition parameters, together with the associated uncertainties, for each sample. We found that the optimal power for nitridation is 2500W.

Keywords
XPS, Nitridation, HfO_2

Reference

A. Herrera-Gomez, F.S. Aguirre-Tostado, M.A. Quevedo-Lopez, P.D. Kirsch, M.J. Kim, and R.M. Wallace, "Thermal stability of nitrogen in nitrided $HfSiO_2$ / SiO_2 /Si (001) ultrathin films," J Appl Phys, (2008).

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[CHM-72] STUDY OF THE PLASMA EMISSION AND ELECTRICAL PARAMETERS OF PULSED-DIRECT CURRENT REACTIVE MAGNETRON SPUTTERING OF A SI TARGET

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Films of silicon dioxide are an essential element in optical coatings because of their low refractive index, high transparency, and mechanical properties. A reliable process is required to deposit compact thin films with high deposition rate, good substrate adhesion and minimum stress. Magnetron sputtering is an excellent technique for thin film deposition and easy to scale up in the industry. However, reactive magnetron sputtering to deposit metal oxides can generate arcing and plasma instability, especially for the silicon dioxide which is an insulator with high dielectric constant. On the other hand, pulsed-DC sputtering can overcome this problem, this system eliminates or diminish, the positive charge accumulation produced around the target. In this work, we studied the effects of the different parameters of the power supply (power, frequency, duty cycle) on the characteristics of the voltage and current waveforms. In addition, Optical emission spectroscopy (OES) is employed to study the behavior of the spectral lines of the plasma under all those parameters. Selected conditions were chosen to perform characterization curves. These curves consisted of stepwise O2 flow increments until reaching a 1:1 ratio, keeping the system pressure constant at 5 mTorr. The poisoning pattern was studied to identify the optimal regions for the SiO2 thin films deposition.

Keywords
sputtering, plasma, Emission Spectroscopy, silicon dioxide, pulsed-DC, waveform.

Reference

Rodríguez-López, R., Soto-Valle, G., Sanginés, R., Abundiz-Cisneros, N., Águila-Muñoz, J., Cruz, J., & Machorro-Mejía, R. (2022). Study of deposition parameters of reactive-sputtered Si3N4 thin films by optical emission spectroscopy. Thin Solid Films, 754, 139313.

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National Council for the Humanities, Science and Technology (CONAHCyT) Cátedras [grant number 1081] project, PAPIIT-UNAM [grant number IG101220] project, PAPIIT-UNAM [grant number IG101123] project, CONAHCyT [grant number CF-2023-I-704] project .

[CHM-271] ELLIPSOMETRY STUDY OF THE DIELECTRIC FUNCTION OF Cu_3Se_2 THIN FILMS DEPOSITED BY ELECTRODEPOSITION

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Cu_3Se_2 films have great attention as an absorber layer to substitute the CIGS in solar cells due to their optical and electrical properties[1]. However, their optical properties have been not studied in deep yet. In this work, the optical properties of Cu_3Se_2 thin films deposited by the electrodeposition method on FTO substrate are modeled by calculating the complex pseudo-dielectric function $\langle\varepsilon\rangle$. A multilayered model composed of Glass/FTO/Cu_3Se_2/roughness was used to fit the ellipsometry parameters Ψ and Δ. The pseudo-dielectric function of the Cu_3Se_2 layer was fitted using a general oscillator + Drude + Tauc-Lorentz model. The roughness of the system was fitted using the effective medium approximation model with 50% voids and 50% of Cu_3Se_2. Morphological parameters obtained by atomic force microscopy and energy band gap obtained from UV-Vis spectra were also used in the calculations and kept fixed. The thickness of the layers, and the real and imaginary parts of the dielectric function were obtained.

Keywords
Cu_3Se_2, Ellipsometry, Solar cells, absorber layer, dielectric function

Reference

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This work was supported by
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[CHM-124] STUDY OF Ni- AND Co-BASED COATINGS: MICROSTRUCTURE AND ELECTROCHEMICAL BEHAVIOR

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In the metal coating industry, corrosion protection is a crucial factor to ensuring the durability and performance of different surfaces. Coatings are typically deposited on structural components to offer protection from corrosive environments, as well as to improve wear performance and durability. In this context, electrochemical studies are extremely important when evaluating the suitability of the coating material for a certain corrosive environment. In addition, these studies are a tool to assess the influence of post-treatments, i.e., their ability to provide further protection. In this work, a detailed investigation of the corrosion resistance of CoCrW, NiCoCrAlTaY, and NiWCrSi coatings with two surface conditions: as-sprayed and pre-oxidized is presented. Prior to the corrosion test, a pre-oxidation treatment was carried out in a controlled nitrogen atmosphere to evaluate its effect on the corrosion response of the coatings. The corrosion rate was examined in a NaCl solution at room temperature using electrochemical techniques including, potentiodynamic polarization, polarization resistance, and electrochemical impedance measurements. Results showed that the pre-oxidation treatment favored the growth and formation of a homogeneous Cr2O3 layer on the surface of the Co-based coatings. On the contrary, oxide mixtures and spinels were developed on the Ni-based coatings. Electrochemical evaluation demonstrated that pre-oxidized CoCrW and NiCoCrAlYTa coatings performed better under the aqueous solution than the as-sprayed counterpart. This behavior indicates that the thermally grown oxide is capable of providing protection against the NaCl solution. An opposite behavior was found in case of NiWCrSi coatings. The pre-oxidation caused a change from amorphous to crystalline phases resulting in a detriment in the corrosion resistance of the coating regardless of the formation of an oxide layer. Under the corrosion conditions tested, the cobalt-based is the best option to protect components against aqueous environments.

Keywords
Surfaces, coatings, electrochemical corrosion, pre-oxidizing treatments

Reference

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This work was supported by

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[CHM-136] STUDY OF AB(OS)3 PEROVSKITES FOR APPLICATIONS IN SOLAR CELLS

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Perovskite solar cells (PSCs) are presented as one of the most viable options for the commercialization of solar cells in the coming years. The type of perovskite that has been postulated with the highest percentage of efficiency so far are the organic-inorganic halide hybrids, but they have presented various problems in terms of their properties and characteristics. Recently, chalcogenide perovskites are considered as a promising candidate to eventually replace halide perovskites in PSCs, using a transition metal instead of lead, an alkali metal instead of the organic part, and a chalcogen (S or Se) instead of the anion. . However, there are few reports on these materials. In this context, the BaTiS3 compound has been predicted to have exceptional properties for use in solar cells, except for its 0.7 eV bandgap; however, using a suitable combination of oxygen and sulfur, this value can be adjusted to values close to the ideal of 1.3 eV. BaTi(OS)3 perovskite was synthesized by a sulfidation process at 800 °C for four different sulfidation times, maintaining a sulfur-rich atmosphere, using carbon disulfide as reactive gas and barium titanate as precursor. From the analysis of the results, the EDX-RF spectrometry revealed that the incorporation of sulfur in the samples was achieved, resulting in a sulfur concentration higher than 23 % for the samples with 4 and 7 hours of synthesis processing. Structural analysis by XRD showed that the material presents two crystalline phases for processes of shorter duration, the hexagonal perovskite phase predominating after three hours of processing, the forbidden band was reduced from 3.04 to 1.9 eV depending on the sulfur concentration and it is estimated that with a percentage of 29% sulfur in the sample the ideal bandgap of 1.3 eV would be achieved.

Keywords

Perovskite solar cells chalcogenide transition alkali metal material analysis

Reference

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[CHM-62] THERMAL PROPERTIES OF POROUS SILICON ELABORATED WITH LOW ANODIZATION TIMES

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The photoacoustic (PA) technique is a method that has proved to be powerful in studying the optical, electronic, and thermal properties of several types of samples in a noncontact and nondestructive way with minimal sample treatment, and since its presentation has been very useful in the characterization of materials, principally for thin materials. The frequency domain photoacoustic technique (FDPAT) is a configuration for thermal properties determination. In porous materials, like porous silicon samples, thermal properties depend, in addition to the substrate characteristics and anodization conditions, on the porous structure and porosity degree. Here, FDPAT in a heat transmission configuration was used in order to obtain the values of the effective thermal diffusivity of porous silicon samples elaborated for electrochemical etching times from 0.5 to 5 min. The two-layer model, based on the concept of effective thermal resistance, was used to obtain the thermal diffusivity, thermal conductivity, and heat capacity of the porous layer as a function of porosity percentage, adjusting this model to the graph of effective thermal diffusivity for each sample as a function of porous fraction layer to the full sample.

Keywords
Porous silicon, photoacoustic technique, thermal diffusivity, thermal conductivity, heat capacity.

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This work was supported by
Secretaria de Investigación y Posgrado del Instituto Politécnico Nacional, México; Comisión de Fomento de Actividades Académicas del Instituto Politécnico Nacional, México; Consejo Nacional de Humanidades, Ciencias y Tecnologías, México.

[CHM-93] DEVELOPMENT OF AN XYZ MOTION SYSTEM FOR THE LIBS TECHNIQUE USING ARDUINO

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In the present work, an XYZ motion system was developed for the LIBS technique using an Arduino processor. The LIBS system was composed of a pulsed Nd:YAG laser (1064 nm), maximum operating energy of 215 mJ; a spectrometer Ocean optics model USB4000 with a spectral range of 200 to 900 nm, a Thorlabs brand optical fiber with a diameter of 50 μm, a Thorlabs photodetector, and a Sepradel DG-301L-17 delay capture device. CNC model 2417 equipment was used to control three stepper motors through Nema drivers for the positioning system. The XYZ motion system can be controlled manually or through a computer interface developed with C++ and C# code. The Arduino processor allows control through digital and analogue inputs and outputs, three stepper motors and the laser shot. For reproducibility purposes, the operating conditions, such as the focal length and the optical fiber position for capture, were fixed during the LIBS analyses. LIBS spectra were taken from solid samples (Cu, Al, Mg, Pb and W) in this work. The NIST database was used to identify the spectral emission lines. The control interface with Arduino allows one to carry out a dot matrix routine and multiple laser shots at a single point. Also, the system has a webcam which helps observe the laser trace on the ablated material.

Keywords
Instrumentation, LIBS, Arduino

Reference

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[CHM-355] OPTICAL ABSORPTION SPECTRUM OF URINE IN AN ANIMAL MODEL OF SEPTIC SHOCK

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The optical absorption spectra obtained by Photoacoustic Spectroscopy (PAS) have specific shapes and characteristics that are directly related to the physical properties of a sample, such as chemical composition and molecular structure, among others. In this work, PAS was used to analyze urine samples from male Wistar rats (n=21) subjected to septic shock through the administration of a lipopolysaccharide (LPS, 7mg/Kg of weight). Samples were taken before and six hours after LPS administration (high severity period in the experimental model). Optical absorption spectra showed characteristics consistent with urine components such as protein, urea, creatinine, uric acid, electrolytes, and glucose. For samples from hour six, in addition to the features related to the mentioned components, absorption of hemoglobin at around 420 nm was more intense. Organ failure, including renal failure, is known to occur in the late stages of septic shock, in addition to hemolysis in which hemoglobin is released from the erythrocyte. Kidney damage is manifested by impaired filtration of blood components. The presence of hemoglobin in urine indicates kidney damage. It is concluded that PAS is a technique that can detect changes in urine compatible with kidney damage in septic shock, which opens possibilities of using this technology in the follow-up of this pathology, which is the main cause of death in patients in critical state.

Keywords
Optical Absorption Spectra, urine, Photoacoustic Spectroscopy, Septic Shock, Physical Properties

Reference

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LUMINESCENCE PHENOMENA: MATERIALS AND APPLICATIONS

CHAIRMEN

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

The scope of the conference will cover the following areas:

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

[LPM-29] GREEN PHOTOLUMINESCENCE SIGNAL OF THE [TB-DPA] COMPLEX: A PROMISING LUMINESCENT THERMOMETER

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Temperature measurement plays an important role in various fields, from laboratory research to safety in industrial plants. Materials that exhibit changes in their luminescent properties with temperature hold promise in temperature measurement applications. Among lanthanides, Tb3+ stands out as the most popular ion with its green emission, which is very sensitive to the human eye. Moreover, the use of organic ligands as antennas can enhance the green color through energy transfer mechanisms1. In this study, we present the luminescence properties of the Tb-DPA complex excited at 330 nm, which shows the typical emission bands of Tb3+ (5D4→7F6-0).). At room temperature, the [Tb-DPA] complex exhibits a quantum yield (Φ) of 48%, a luminescence lifetime (t) of 1.5 ms at the 5D4level, and color coordinates of 0.26 and 0.72, which are very similar to those (0.29, 0.60) of the European Broadcasting Union green illuminant. We also analyze the temperature-dependent luminescence properties of the [Tb-DPA] complex in the range of 30-150 °C. Our results show that the luminescence intensity decreases with increasing temperature and finally approaches zero signal at 150 °C. We observe a linear dependence of the luminescence emission on the temperature in the range from 30 to 90 °C. The [Tb-DPA] complex exhibits an absolute sensitivity (Sa) and relative sensitivity (Sr) of 1.42 %C-1 and 6.4 %C-1, respectively, demonstrating its potential as a highly sensitive luminescence thermometer.

Keywords
Optical thermometer, Lanthanide complex, Tb ion

Reference

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This work was supported by
We thank the projects SIP 20231057 and No. 2258 of the National Polytechnic Institute IPN.

[LPM-55] SYNTHESIS OF HYDROXYAPATITE ENRICHED WITH ER (III) AND YB (III) IONS FOCUSED ON DETECTION IN ORGANIC MEDIA

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The synthesis and characterization of $Ca_5(PO_4)_3(OH)$ (hydroxyapatite or HAp) enriched with Er (III) and Yb (III) ions was carried out by means of the solvent evaporation technique using calcium chloride and monobasic ammonium phosphate supplied by Sigma Aldrich as reagents. An adequate solution of both reagents was made using deionized water as solvent, which was heated and stirred simultaneously at an approximate temperature of 90 °C for 45 minutes until the solvent evaporated, leaving a precipitate of $Ca_5(PO_4)_3(OH)$, which was placed in a muffle furnace at 700 °C for 3 hours. In this same methodology, Er (III) and Yb (III) ions were added as dopants by including Er and Yb nitrates in adequate concentrations to the solution to provide luminescent properties.
The luminescent properties of HAp:Er(III)/Yb(III) are activated by means of a continuous 980 nm laser producing two types of emissions, Stokes and Anti-Stokes, Stokes emissions occur in the near infrared area. 1520 nm due to the interelectronic transition $^4I_{13/2} \rightarrow {}^4I_{15/2}$ of the Er (III) ions, for its part, Anti-Stokes emissions occur in two regions of the visible area of the electromagnetic spectrum, the first in the region from 515 to 565 nm due to the transitions $^2H_{11/2} \rightarrow {}^4I_{15/2}$ and $^2S_{3/2} \rightarrow {}^4I_{15/2}$ of the Er (III) ions while the second region comprising from 640 to 680 nm corresponds to the transition $^4F_{9/2} \rightarrow {}^4I_{15/2}$ of the Er(III) ions

These types of materials could be used in the area of detection of cancer cells as long as an adequate functionalization is carried out with proteins that present affinity with them. This paper shows the synthesis and optical, structural and luminescent characterization of HAp:Er(III)/Yb(III) as well as a toxicological study of this type of material.

Keywords
hydroxyapatite, Er(III), Yb(III), luminescent properties, synthesis.

Reference

[1] Enhanced 1520 nm Photoluminescence from Er3+ Ions in Di-erbium-carbide Metallofullerenes (Er2C2)@C82 (Isomers I, II, and III), Yasuhiro Ito, Toshiya Okazaki, Shingo Okubo, Masahiro Akachi, Yutaka Ohno, Takashi Mizutani and other authors, ACS Nano 1, 5, (2007), 456–462

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Advanced materials synthesis laboratory, Benemérita Universidad Autónoma de Puebla.

[LPM-191] GREEN SYNTHESIS AND LUMINESCENT PROPERTIES OF CsVO3:Mn PEROVSKITE

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This work studied the structural and luminescent properties of CsVO3:Mn perovskite crystals synthetised by the Solvent Evaporation. The solvent evaporation is a versatile and eco-friendly technique potentially applicable in the industry. The X-Ray Diffraction patterns shows that the crystalline structure is the characteristic of the CsVO3 perovskite. The downshift luminescent spectra presented the characteristic emission peaks for the electronic energy levels transitions of the CsVO3:Mn perovskite crystals. The CsVO3 perovskite showed a maximum emission peak in the visible region at 527 nm, when being excited with 362 nm. The photoluminescent spectra show that the intensity of the excitation and emission spectra depends of the incorporation to manganese ions.

Keywords
Perovskite, Photoluminescent spectra, Solvent Evaporation, Emission peaks, CsVO3:Mn.
This work was supported by
Porras Sanchez María Leonor,Soriano Romero Omar, Meza Rocha Abraham Nehemias, Lozada Morales Rosendo Leovigildo, Vargas Garcia Vicente.

[LPM-166] STUDY OF QUANTUM YIELD AND PHOTOTHERMAL MEASUREMENTS OF POLYACRYLONITRILE (PAN)-BASED GRAPHENE OXIDE SEMICONDUCTOR QUANTUM DOTS

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The following work presents the results obtained from the synthesis, optical and photothermal characterization of graphene oxide semiconductor quantum dots (GOQDs) based on polyacrylonitrile (PAN), these nanoparticles are manufactured by the carbonization and exfoliation method of electrospun PAN fibers. The absorption spectra of the GOQDs were found to be between 265 and 325 nm and are the same for the different samples at different spin wash speeds. In the photoluminescence (PL) spectra of the GOQDs, two emission lines were obtained for the samples of different spin speeds, 464 nm and 417 nm for one of the samples and 444 nm and 488 nm for the other. with an excitation line at a wavelength of 370 nm. Additionally, the photothermal properties of the GOQDs were studied, for the determination of luminescent quantum efficiency (η), and the experimental variable parameter q of the thermal lens, as well as the measures to determine the variation of the refractive index with temperature dn/dT with a value of -8.02x10-4 and -9.19x10-4 respectively; With these measurements, the highest value of the quantum efficiency η was calculated, obtaining a value of 0.97 ± 0.02.

Keywords
Quantum dots, quantum efficiency, thermal lens spectroscopy.

Reference

C. Jacinto, A. A. Andrade, T. Catunda, S. M. Lima, and M. L. Baesso, Thermal lens spectroscopy of Nd: YAG, Appl. Phys. Lett. 86(3) 034104. https://doi.org/10.1063/1.1852084.

This work was supported by

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[LPM-258] PHOTOLUMINESCENCE STUDY OF CARBON QUANTUM DOTS OBTAINED FROM BANANA PEEL BY A DEHYDRATION PROCESS.

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Synthesis of carbon quantum dots from organic biowaste has attracted attention in the recent decades due to the vast variety of application fields, being the biomedical and optoelectronic applications two of the most popular owing to the excellent fotoluminescence properties of the carbon dots.
Among the fabrication techniques, one of the most used is the hydrothermal method, in which different ranges of temperatures are applied usually during long times.
In the present work a simple dehydration method followed by relative low temperature calcination was used to obtain carbon quantum dots using banana peel as the carbon source.
Banana peels were dehydrated at 56 °C for 6 hours followed by a calcination treatment at 150°C. The calcinated peels were milled in an agate mortar to produce a fine powder which was sieved in a 50-micron pore filter. The unfiltered powder was poured in bidistilled water at a concentration of 300 µg/ml and the resulting suspension was sonicated for 20 minutes in an ultrasonic bath. The suspension was filtered in a 20 micron pore filter paper and stored at room temperature.
Different concentrations of suspensions were obtained by diluting the original suspension in different volumes of water. The obtained samples were optically characterized by UV-Vis and photoluminescence (PL) spectroscopies. The PL emissions were recorded by using excitation sources of 370 and 405 nm where different components were found on the spectra. The deconvoluted signals intensity and wavelength positions were analyzed as a function of concentration.

Keywords
Carbon quantum dots, banana peel, photoluminescence
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[LPM-272] EFFECT OF TEA CONCENTRATION ON ZNO QDS STABILITY

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The rising global energy demand drives exploration of alternative, environmentally friendly, and renewable sources like solar energy. Silicon-based solar cells, known as first-generation cells, have been widely used, but advancements have led to the development of third-generation solar cells using accessible alternatives and low-impact materials. Dye-sensitized solar cells (DSSC) belong to this generation, with lower production costs and efficiencies of up to 14% [1]. These innovative cells aim to meet energy demands while minimizing environmental consequences. Despite their continuous evolution, DSSC solar cells face challenges such as high carrier recombination, dye-electrolyte system degradation, and long-term stability issues. To address the carrier recombination issue, strategies have been established, including the modification of the solar cell's photoanode. This latter can be sensitized by integrating semiconductor materials such as quantum dots (QDs), improving solar cell efficiency due to increased absorption, to the phenomena of energy down-conversion and multiple exciton generation. For this reason, quantum dots have garnered significant interest as sensitizers for the photoanode. In this work, ZnO QDs were synthesized by a wet chemical method. The effect of triethanolamine (TEA) on the optoelectronic properties was analyzed in order to assess the stability of ZnO QDs. The experiments showed that for a 37 mM TEA concentration, the ZnO QDs were stabilized for a longer time without precipitates. UV-Vis absorption spectra evidenced an absorption edge around 320 to 380 nm related to the typical electronic transition of electrons from the valence band to the conduction band in ZnO QDs. The analysis of absorbance spectra showed that the band gap energy of ZnO QDS was ~ 3.46 eV. Photoluminescence spectra evidenced different peaks associated with the presence of structural defects as a function of time and TEA concentration, which can improve light absorption capacity for the generation of charge carrier generation on solar cells.

Keywords
ZnO QDs, triethanolamine, PL spectra.

Reference

[1] Best research cell efficiencies from National Renewable Energy Laboratory (NREL) available at: https://www.nrel.gov/pv/assets/pdfs/best-research-cell-efficiencies.pdf

This work was supported by
Universidad de Guadalajara (PROSNI 2022-2023) and CONACyT Mexico (CF2021-316883). David thanks to CONACyT Mexico for the Master scholarship No. 829984.

[LPM-350] GDALO3:DY COMO CONVERSOR DE ENERGÍA

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En la actualidad el estudio de los materiales conversores de energía presenta un desafío para las instituciones dedicadas a la conversión de energía. En el presente trabajo se presenta la técnica de termoluminiscencia como una herramienta versátil para una evaluación de la impartición de la energía a un material inorgánico. Una gran variedad de materiales cerámicos y sus diferentes formas físicas permiten una determinación de la cantidad de radiación que incide en un espacio. Unas de las mejores ventajas de los cerámicos son sus pequeñas dimensiones y no necesitan empaque especial ni equipos auxiliares durante la cuantificación de la energía depositada. Como consecuencia de eso, estos son adecuados para un gran número de aplicaciones principalmente en Física Medica. Bajo este esquema en el presente trabajo tiene como objetivo estudiar las propiedades conversores de alta energía como la radiación ionizante que en este caso a las radiaciones beta en energía visible, mediante la técnica de termoluminiscencia.

Keywords
Luminescence, GdAlO3:Dy, Thermoluminescence, Beta radiation, Ionizing radiation

Reference

T. Rivera, Thermoluminescence in medical dosimetry, Appl. Radiat. Isot. 71 (2012) 30–34. https://doi.org/10.1016/j.apradiso.2012.04.018.

This work was supported by
CONAHCYT

[LPM-354] EMISIÓN LUMINISCENTE EN PELÍCULAS DELGADAS ZNO:RE (TM+3/EU+3) OBTENIDAS POR LA TÉCNICA DE ROCIÓ PROLÍTICO ULTRASÓNICO

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Rare-earth doped ZnO systems are particularly attractive for potential applications in high power lasers, visible light emitting phosphors, displays, and other optoelectronic devices. In particular, Eu+3, Tm+3 ions exhibit luminescence in the visible spectrum range. This work is focused on the determination of the conditions to obtain ZnO thin films doped with RE= Eu+3, Tm+3, Eu+3/Tm+3 looking for the concentration of impurities that favor the increase in luminescence. The films were prepared using the Ultrasonic Pyrolytic Spray technique studying the influence on the variation of the concentration of europium and thulium from 0.5 to 3% at separately. Subsequently a co-doping (Eu+3:Tm+3) was performed choosing the concentrations that presented the highest luminescent intensity.

The samples under went characterization via X-ray diffraction (XRD), UV/Vis and photoluminescence (PL). The X-ray patterns show a Wurzite structure obtained in the films. The UV/Vis spectroscopy results indicate that the GAP value varies from 3.03 to 3.3 eV according to different %Eu+3 and in the case of Tm+3 % from 2.95 to 3.2 eV. The photoluminescence emission bands in the prepared films are also analyzed in the range of 300 to 1100 nm using an excitation wavelength of 285 and 365 nm showing the transitions of the excited levels for both Eu+3 and Tm+3 ions.

Keywords
Luminiscence, Rare Earths, Thin films, ZnO, Spry Pyrolysis

Reference

D. Clake, On the optical Band GAP of Zinc Oxide, J. Appl. Phys. 83 (10), 5447, (1998).
S.Mauricio, Luminescence dynamics and enhancement of the UV and visible emissions of Tm+3 in LiYF4:Tb+3, Tm+3 upconverting nanoparticles, Nanoscale Adv. 1, 4492 (2019).

This work was supported by
Universidad Autónoma de Zacatecas
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Sesión Oral

[LPM-13] STRUCTURAL AND LUMINESCENT PROPERTIES OF BaZrO3:Er3+ NANOPARTICLES

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In this work the structural and photoluminescent properties of Barium Zirconate ($BaZrO_3$) doped with erbium trivalent ions (Er^{3+}) are reported. The synthesis was carried out by the hydrothermal route using a reaction time of 120 minutes at a temperature of 200 °C. How precursor elements were used chlorides at a concentration 0.4 molar. The pH of the solution was adjusted to 12, using a 2M solution of sodium hydroxide (NaOH), obtaining NaCl as residue of the reaction, making this a friendly process with the environment; subsequently the material was subjected to a heat treatment of 800°C for 8 hours. The material obtained was characterized by X-ray diffraction (XRD). The XRD pattern showed broad and well-defined peaks that correspond to a $BaZrO_3$ cubic perovskite-type structure, according to diffraction chart 00-089-2486. Morphology and particle size were obtained using a High-Resolution Scanning Electron Microscopy (HRSEM). The SEM micrographs shows particles larger than 50 nm. The structural analysis included the study by high resolution transmission electron microscopy (HRTEM), being able to observe particles larger than 200 nm with crystals around 40 nm. The luminescent properties were obtained by the photoluminescent emission spectra as a function of erbium concentration, exciting with a wavelength of λexc= 376 nm. The emission spectra showed the $^2H_{11/2} \rightarrow {}^4I_{15/2}$; $^4S_{3/2} \rightarrow {}^4I_{15/2}$ transitions, characteristic of the trivalent erbium ion. The highest emission was obtained in the impurified sample with 0.01% Er, that correspond to the quenching concentration.

Keywords
Luminescence, Barium Zirconate, Erbium, Hydrothermal.

Reference

Transient Adsorption Behavior of Single Fluorophores on an Electrode-Supported Nanobubble.
Wes R. Leininger, Zhuoyu Peng, and Bo Zhang
Chemical & Biomedical Imaging
https://doi.org/10.1021/cbmi.3c00020

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[LPM-10] ADVANCEMENTS IN [EU2DPA3]N MOF AS A HIGHLY EFFICIENT RED-EMITTING PHOSPHOR WITH THERMAL STABLE LUMINESCENCE

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Lanthanide Metal-Organic Framework (La-MOF) are materials that have attracted the attention of science and technology due to their high luminescence [1]. Their luminescent properties are due to the phenomenon of energy transfer between the organic ligand and the lanthanide ions. In particular, the Eu^{3+} ion is widely used because of its narrow emissions in the visible spectrum, especially for the $^5D_0 \rightarrow {}^7F_2$ (615 nm) transition, which is in the red region of the visible spectrum. Red-emitting luminescent materials are proposed for technological applications such as light-emitting diodes (LED), red components in white LEDs, plant growth, and lighting. The luminescent properties of the $[Eu_2DPA_3]_n$ MOF were obtained by exciting it at 300 and 395 nm with the typical emission bands of Eu^{3+} ($^5D_0 \rightarrow {}^7F_{0,1,2,3,4}$). The photometric study of the $[Eu_2DPA_3]$n MOF indicates that the excitation at 300 and 395 nm is practically identical, with high purity color >98%, and a chromatic coordinate of 0.65, 0.35, which is very close to the ideal red-emitting phosphor used by the National Television Standard Committee (0.67, 0.33). The temperature-dependent luminescence properties of the MOF were analyzed in the 30-150 °C range, revealing a stable luminescent signal when the temperature increased up to 150 °C with a 3% signal loss and an energy quenching (ΔE) of 0.21 eV.

Keywords
Europium, MOF, Red Phosphor, Thermal Stable Luminescence

Reference

1. Wei, C.et al. Advances in luminescent lanthanide complexes and applications. Sci. China Technol. Sci. 61, 1265–1285 (2018).

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[LPM-70] REDOX EFFECT ON POWDER LUMINESCENT OF CA2ALO4 CODOPED WITH EU AND DY

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Calcium aluminate codoped with earth rare (Ca2Al4: Eu2+; Dy3+) present very interesting structural, optical, and luminescence characteristics. The luminescence role of Eu ions in the Ca2Al4: Eu2+; Dy3+ matrix is really interesting, due to its prominent application over unconventional light technologies, displays, OLEDs, and solar cells, among others. The important role of Eu ions can be present in sundry emissions in blue, yellow, and IR spectra regions.
These materials have been synthesized by combustion method using nitrides of precursors and carbohydrazide of fuel to promote the exothermal reaction. The combustion method is characterized by an inexpensive procedure, fast and expansive to an industrial level.
This project is focused on the study of the effect of Eu ions concentration on Ca2Al4: Eu2+; Dy3+ powders, modifying Eu (NO3)3 precursor quantities on the reaction, and the Redox effect of Eu ions by thermal treatment in NH3 and O2 atmosphere. The samples were characterized by SEM, TEM, EDS, XRD, and CL techniques.

Keywords
Luminescence, calcium aluminate, Redox effect, Eu ions.

Reference

Patel, K., Blair,V., Douglas,J., Dai,Q., Liu, Y., Brennan, R.,Ren, S., (2017) Structural Effcts of Lanthanide Dopants on Alumina. ScientificReports s | 7:39946 | DOI: 10.1038/srep39946.

This work was supported by

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[LPM-74] UPCONVERSION LUMINESCENCE OF CaLaAlO4: Tm3+, Yb3+ PHOSPHOR SYNTHESIZED VIA SOLUTION COMBUSTION METHOD FOR SOLID-STATE LIGHTING APPLICATIONS

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CaLaAlO4:Tm3+,Yb3+ upconversion phosphors were prepared via combustion method. The Tm3+ dopant concentration was constant (Tm=0.5mol%), while the concentration of Yb3+ dopant was varied (Yb= 1-10mol%). The X-ray diffraction studies show that the phosphors present a mixed crystalline phase (tetragonal and hexagonal of CaLaAlO4 and LaAlO3). The optical absorption spectra of the upconversion phosphors samples exhibited two bands centred at 253 nm and 440 nm. The band at 253 nm was attributed to the charge transfer band of Yb3+, while the broad band located at 440 nm was ascribed to defect states in the lattice. The optical band gap and refractive index of the optimized samples were 4.73 eV and 1.76 respectively. The upconversion emission peaks centred at 478 nm, 654 nm and 801 nm are ascribed to the 1G4 → 3H6, 1G4 → 3F4, and 3H4 → 3H6 electronic transitions of Tm3+ ions, respectively (Etafo et al., 2023). As the Yb concentration increases, the colour emission is tuned from bluish-white to blue light. The CCT and CIE coordinate of (0.2419, 0.2463) showed that the phosphor doped with 3mol% of Yb3+ produces a bluish-white and its colour purity was 80%. Thus, the strong bluish-white light emission produced by the CaLaAlO4:Tm3+, Yb3+ phosphors could be used for solid-state lighting or in multicolour displays.

Keywords
Photoluminescence; Upconversion; bluish-white; Phosphor; Combustion synthesis.

Reference

N. O. Etafo, C. R. Garcia, T. A. Esquivel-Castro, M. I. León-Madrid, A. Santibañez, and J. Oliva, The Effect of a Yb Co-Dopant on the Blue Upconversion and Thermoluminescent Emission of SrLaAlO4:Yb3+,Tm3+ Phosphors, Coatings, 13 (2023), 1003. https://doi.org/10.3390/coatings13061003.

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[LPM-240] SYNTHESIS OF Al2(WO4)3:Eu3+ PHOSPHORS USING EVAPORATION METHOD

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In this work, Europium-doped Aluminum Tungstate powders were synthesized via evaporation method using DI water as solvent, Aluminum Chloride ($AlCl_3$) Europium Chloride ($EuCl_3$) and Sodium Tungstate (Na_2WO_4) as precursors; then it was submitted to heat treatment at 400°C for 2 hours. Evaporation is a procedure characterized by simple steps and low amounts of toxic byproducts. Its optical properties were studied by ultraviolet-visible Photoluminescence (PL) spectrometry. Characteristic Eu^{3+} emission peaks were observed; host presented photoluminescence emission peak at 393nm. Future Raman spectroscopy and X-ray studies will be performed.

Keywords
Aluminum tungstate, Europium, Luminiscence, Evaporation method

Reference

Macalik, L., Hanuza, J., Hermanowicz, K., Godlewska, P., & Sidorov, N. V. (2004). Luminescence properties of Eu3+-doped Al2 (WO4) 3. Mater. Sci. Poland, 22, 145-1152.

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Benemérita Universidad Autónoma de Puebla.

[LPM-173] CDO-B2O3-PR (III) INVERTED GLASSES, A BRIEF LUMINESCENCE STUDY

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The $CdO-B_2O_3$ system has been previously reported, however, its chemical stability is limited due to moisture absorption. To address this issue, stabilizer oxides like Bi_2O_3 or PbO are often added. Boron in the $CdO-B_2O_3$ system can function as a network former or modifier, leading to the formation of inverted glasses without the need for stabilizers. On the other hand, Trivalent rare-earth ions, such as Pr (III), are known for their optical properties, this work aims to investigate the structural and photoluminescence properties of Pr (III)-activated $CdO-B_2O_3$ inverted glasses.
The inverted glasses were prepared using the melting method, and their composition consisted of 90 mol% CdO, 10 mol% B_2O_3, and varying concentrations of Pr (III). Characterization techniques such as X-ray diffraction, Fourier transform infrared spectroscopy, optical absorption spectroscopy, and photoluminescent measurements were employed.
The present work provides insights into the structural and photoluminescence properties of Pr (III)-activated $CdO-B_2O_3$ inverted glasses. The findings contribute to the understanding of inverted glasses and their potential applications in laser and WLED technologies.

Keywords
Inverted glasses; Pr (III), infrared emission luminescence, laser applications.

Reference

Spectroscopic analysis of Nd3+-doped cadmium-vanadate invert glasses for near-infrared laser applications, O. Soriano-Romero, et. al., Journal of Non-Crystalline Solids, 572, (2021), 121085.

This work was supported by

Authors thank Consejo Nacional de Humanidades, Ciencias y Tecnologías (Mexico) for its financial support through A-1-S 22057 grant.

[LPM-111] FORMATION AND CHARACTERIZATION OF CALCIUM TUNGRAMATE ACTIVATED WITH TERBIUM SYNTHESIZED BY THE MICROWAVE-ASSISTED SOLVOTHERMAL TECHNIQUE

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Terbium-doped calcium tungstate nanophosphors were obtained by the microwave-assisted solvothermal method.
Calcium tungstate acts as a host for a variety of rare earth ions, the structural units of the tungstate ion absorb light in the short- and medium-wave UV range through charge transfer from oxygen ions to tungsten ions and the absorbed energy is transferred to rare earth ions, which subsequently undergo f-f transitions and produce sharp emission peaks.
To characterize the structure and morphology of the nanophosphors, transmittance analysis, X-ray diffraction (XRD), scanning electron spectroscopy (SEM) were performed, and their optical properties were determined by FTIR methods.
The nanophosphors present emission peaks when excited with a wavelength of 265 nm and 378 nm, which correspond to the emissions of the matrix and terbium, the emission wavelength of the matrix is between 350 nm and 500 nm, peaks are also observed at wavelengths of 487 nm, 545 nm, 587nm, 622 nm and 657 nm, which are transitions associated with terbium ions ranging from $^5D_4$ to $^7F_1$, $^7F_3$, $^7F_4$, $^7F_5$ and $^7F_6$ respectively, where the most intense emission is at 545 nm, which corresponds to to the transition from $^5D_4$-$^7F_5$.

Keywords
Calcium tungstate, Terbium, doped, lanthanides

Reference

K. Gayatri Sharma, N. Shanta Singh, Y. Rangeela Devi, N. Rajmuhon Singh, Sh Dorendrajit Singh, Effects of annealing on luminescence of CaWO4:Eu3+ nanoparticles and its thermoluminescence study, J. Alloys Compd. 556 (2013) 94–101.

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[LPM-172] COMMERCIAL 3D RESIN BLENDED WITH CAWO4 BASED PHOSPHORS, A SHORT LUMINESCENCE STUDY

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Synthesis and characterization of calcium tungstate-based micro-nanophosphors are reported in the present abstract. These materials were synthesized by spray pyrolysis technique. According to Scanning Electron Microscopy measurements, $CaWO_4$ and $CaWO_4$:Eu (III) have quasi-spherical shape. $CaWO_4$ presents blue luminescence whose origin is an electron transition within unperturbed WO_4^{2-} complexes, while $CaWO_4$:Eu (III) luminescent properties are generated by the presence of Eu (III) ions, which produced light emissions at 591, 615, 655, and 702 nm. Such emissions are due to radiative transitions from the excited state $^5D_0$ to ^7F_j (j = 1, 4) inter-level transitions within Eu (III) electronic energy states. These phosphors were blended with a commercial 3D print photocurable resin (Sain Smart 101-90-840TS) and their luminescent properties were transferred to resin. Besides in this case, blended 3D resin has an intrinsic blue luminescence due to its π and π* bonds which is activated under 380 nm excitation wavelength, however blended 3D resin can be also activated under 465 nm excitation which only activates Eu (III) ions producing a red emission 3D luminescent photocurable resin.

Keywords
CaWO4 phosphors; Eu (III), red emission luminescence, Commercial 3D resin.

Reference

Commercial 3D resin blended with TTA functionalized CaWO4:Eu (III), synthesis route and a luminescence study, K.B. García-López, et. al., Optical Materials, 142, (2023), 114008.

This work was supported by

Investigadores por México CONAHCyT program, Grant No. 572 (2018).

[LPM-329] LUMINESCENT AND BIOCOMPATIBILITY STUDY OF THE ERBIUM-BASED MOF

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In this investigation, the synthesis of an organic metal framework formed by the organic ligand 1,4-benzenedicarboxylic (BDC) and the Er3+ ion as metal center was carried out. The MOF was obtained by stirring the precursors at room temperature. In the optical properties, the excitation and emission spectra, chromaticity diagram and decay time of the MOF will be shown, as well as the absorption spectra of the MOF in the different culture media to test its stability. The culture media used were Aqueous, PBS, DMEM and DMEM +10% FS and by means of Alamar blue assays it was determined that MOF does not inhibit the proliferation of HaCaT cells, which indicates that MOF can be used in biological applications given its low toxicity.

Keywords
Er-Lanthanide, MOF, Luminescence, Biocompatibility.

Reference

Room temperature synthesis of nanometric and luminescent silver-MOFs. Vanessa Celis-Arias, Ismael A. Garduño-Wilchis, Gilberto Alarcón, Fernando González Chávez,Efrain Garrido Guerrero, Hiram I. Beltrán and Sandra Loera-Serna. Frontiers-Frontiers in Chemistry (2022), China.
https://doi.org/10.3389/fchem.2022.1065622.

This work was supported by

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MICROELECTRONICS AND MEMS

CHAIRMEN

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Dr. Israel Mejía Silva (CIDESI), israel.mejia@cidesi.edu.mx

Internet of Things (IoT) is providing several stand-alone internet-connected sensors that can be monitored and/or controlled from a remote location, this is an example of how silicon-related technology is changing the world for human benefit.
In this regard the mission of this Microelectronics and MEMS (MicroSystems) Symposium is to bring together scientists and technologists interested in these two interrelated fields. The program will highlight recent advances in the design and fabrication of integrated circuits (IC´s), Microelectronics Technology, Materials Science for Micro and Nanoelectromechanical devices and systems (NEMS), as well as the different strategies for the integration and packaging of MEMS and NEMS.
Microelectronics; which in its widest conception includes the design, fabrication, characterization, and modeling of micro- and nano- devices, and circuits, has emerged as the fundamental technology for the fabrication of Microsystems. In this field, it is interesting to analyze the scaling laws and size regimes in which macro theories start requiring further non-linear analysis. The purpose is to obtain a deeper understanding of the physical consequences of downscaling electrostatic, electromagnetic, fluidic, optical, thermal, chemical devices, and some combinations of them. It is of great importance to study the non-linear behavior of miniaturized devices and systems, which apart from reason involving economics, volume and weight, can lead to new operating principles and even to increase the system performance. All of them is the basis for current technology trend.

Main Topics:
The Microelectronics and MEMS Symposium is focused on the integration of materials and processes for developing MEMS/NEMS devices. Invited Talks, Oral and Poster 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-309] IMPLEMENTATION OF NMOS LOGIC GATES WITH IN-GA-ZN-O THIN FILM TRANSISTORS

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In-Ga-Zn-O (IGZO) thin film transistors (TFTs) are now commercially used as backplane drivers of flat-panel displays, and now there is a pursuit of applications beyond this. To build electronic circuits based on oxide semiconductors TFTs, the basic logic gates are necessary to implement. In this work, the logic gates like inverters (NOT), NOR, NAND, and XOR were designed and fabricated with a TFT technology of channel length of 5um. The TFTs were fabricated with the bottom gate top contact structure using gold as the gate, Al2O3 as dielectric, IGZO as semiconductor, molybdenum as source/drain electrodes, and PMMA as the passivation layer. All the fabrication process was carried out with a maximum temperature of 150^{o}C. All the fabricated logic gates exhibit correct logic functions, according to their truth tables, in a VDD range of 3 to 9 V, and a frequency range of 50 Hz to 1 kHz. For a VDD equal to 6 V at 1 kHz the rise and fall times were: 55/4 us for a NOT, 56/7 us for a NAND, 67/2 us for a NOR, and 58/13 us for a XOR. These results are very attractive for the implementation of complex circuits such as adders, flip flops, and multiplexers.

Keywords
TFT, IGZO, logic gates.
This work was supported by
This work was supported by: SIP-IPN under grant 20230982.

[MEM-311] SELF-ALIGNED IN-GA-ZN-O THIN FILM TRANSISTORS

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In-Ga-Zn-O thin film transistors (TFTs) are very promising for flexible electronics including applications in wearables devices and the Internet of things. In this work, the TFTs were fabricated with the bottom gate top contact structure using chromium/gold as the gate, Al_2O_3 as dielectric, IGZO as semiconductor, aluminum as source/drain electrodes, and PMMA as the passivation layer. In the self-aligned structure, the sour/drain electrodes are self-aligned with respect to the gate contact which reduces the parasitic capacitance by eliminating the overlap between these electrodes. The reduction of parasitic capacitance is related to an increment in the operating frequency of the circuits. The electrical parameters of TFTs, with a fixed channel width of 40 um and a variable channel length (5, 8, 10, 15, and 20 um), were mobility of around 10 cm^2/V-s, a threshold voltage of 1.1 V, a subthreshold slope of 100 mV/dec, and an Ion/Ioff ratio of seven orders of magnitude. An inverter gain of around 7 was obtained with a saturation load configuration (pull-up W10/L40 and pull-down W1000/L10, units in microns). Further optimization of the inverter is necessary to fabricate more elaborated digital circuits for TFT applications beyond displays.

Keywords
TFT, IGZO, pseudo-CMOS.
This work was supported by
This work was supported by: SIP-IPN under grant 20230982.

[MEM-321] TEOS MATRIX FUNCTIONALIZED WITH GALLIUM OXIDE

Alessandra Yadira Escobar Vera Estudiante[1], Rogers García Domínguez Estudiante[1], Cristian Mitchel Pérez López Estudiante[1], Francisco Ramírez González Doctor[1], Jorge Evaristo Conde Díaz Doctor[2], Héber Vilchis Bravo Doctor[1]

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Gallium oxide is a semiconductor material that can be obtained with different electrical and optical properties based on the synthesis methods because gallium oxide presents polymorphs highlighted in thin films, nanostructures, and bulk gallium oxide[1]; with application in CO_2 detection due to different adsorption energies and changes in the electronic structures on the material surface. Tetraethyl orthosilicate (TEOS) has been reported as a precursor to silicon dioxide in the semiconductor industry, as a silica source for the synthesis of some zeolites, and as a coating to protect stones and metals [2]. In this work, structural andmorphological properties of TEOS modified with gallium oxide is presented, with the aim to evaluate this application as a material sensor of CO_2. TEOS was prepared using 3.3 ml tetraethyl orthosilicate mixed with 3.28 ml Ethyl alcohol stirring at 650 RPM for 20 min. On the other hand, gallium oxide was obtained by thermal conversion of gallium arsenide (1 1 1) samples at 800 °C [3]. The obtained Ga_2O_3 was milled andprocessed through the same thermal treatment for a second time. Then, the Ga_2O_3 powder was dispersed in 30 ml ethyl alcohol stirring at 650 RPM for 10 min, four concentrations were made(0.1, 0.2, 0.3, and 0.4 gr). TEOS synthesis was modified by changing the EtOH for the Ga_2O_3 colloidal suspension. Finally, the solution was deposited on glass substrates by drooping the solution to form layers. The samples were characterized by X-Ray diffraction patterns, Raman and Force Atom Microscopy to study the incorporation of Ga_2O_3 into the TEOS matrix. The aim is to develop a composite Ga_2O_3/TEOS applicable on CO_2 detection.

Keywords
Carbon dioxide, Gallium oxide, Tetraethyl Orthosilicate.

Reference

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[MEM-280] DESIGN OF A PHOTODETECTOR IN THE INFRARED REGION TO BE APPLIED IN THE DETECTION OF NUTRIENTS DURING THE DRYING OF AGRICULTURAL PRODUCTS IN SITU

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The agricultural industry related to the dehydrated process of fruits and other agricultural products lacks official and recognized standards that guarantee that dehydrated products have the nutrients required for human consumption. This is due to the fact that current practices for monitoring the loss of moisture and volatile nutrients require processes that do not guarantee adequate monitoring, since when the drying chambers are opened, control of the drying conditions is lost. In this work it is proposed to design the first part of an optical system that is placed inside the dehydrators to monitor in real time the dehydration curve of any agricultural product. For the design of the photodetector, the L-edit software will be used to optimize the manufacturing steps of the device using photolithography. The required wavelength is 1040 nm, since around 900 to 1000 nm it is possible to detect C-O bonds attributed to organic compounds related to carbohydrates and carotenoids. So n-type silicon is used as the substrate and gold contacts. As results, different optimized schemes of the photodetector are presented. Considering a matrix of different diodes connected in different series-parallel arrangements, increase the current generated as a result of excitation of light. The electrical simulations indicate that it is possible to use the proposed design to respond to the spatial signal that is reflected from an organic sample.

Keywords
Photodetector, dehydrated products, moisture, electrical simulations.

Reference

Detection of moisture ratio and carotenoid compounds in mamey (pouteria sapota) fruit during dehydration process using spectroscopic techniques. López G., López-Paz M.F., López P., Carriles R., Vilchis H.; Journal of Food Science and Technology 60 (2023) DOI: 10.1007/s13197-023-05728-w.

This work was supported by
Universidad de Ciencias y Artes de Chiapas.

[MEM-292] A COMPARATIVE STUDY ON A-IGZO THIN-FILM TRANSISTORS FABRICATED ON RIGID OR FLEXIBLE SUBSTRATE

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Flexible electronics has been of interest due to the generation of innovative devices and the exploration of new lines of technological research. Thin-film electronics based on amorphous oxide semiconductor (AOS) are growing since they share characteristics with flexible substrates. In this work, thin-film transistors based on indium-gallium-zinc oxide (a-IGZO) were fabricated as a semiconductor material deposited at room temperature and Al_2O_3 as a dielectric material. A comparative study with these AOSTFTs is carried out with two different substrates, rigid and flexible, to point out the scalability of the device in large area systems and flexible electronics. TFTs on rigid substrate shows slightly higher initial characteristics compared to TFTs on flexible substrate, with a threshold voltage V_{TH}≈0.84 V and a field effect mobility μ_{FET}≈11cm^2/Vs. Degradation in flexible devices is attributed to constant mechanical stress and roughness of the flexible substrate. Flexible devices under conditions of mechanical stress with a radius of curvature of 4 mm, present a combined behavior of a flexible device without mechanical stress towards a device fabricated on a rigid substrate. The amorphous structure of the active layer makes it possible to maintain similar properties in devices made even over large areas. Through a suitable design of the device structure, it is possible to reduce the effect of mechanical deformation on the active layer, which allows the realization of highly deformable transistors.

Keywords
Thin-film transistors, flexible substrate, amorphous oxide semiconductor, IGZO, Al_2O_3

Reference

Pablo Toledo et al 2022 Flex. Print. Electron. 7 025015, DOI 10.1088/2058-8585/ac7186.

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[MEM-308] CO GAS SENSORS APPLICATION OF ZNO THIN FILMS DEPOSITED BY SILAR

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Carbon monoxide (CO) is a colorless and non-irritating gas which is formed by burning fuel in industry, household applications, and automobiles. A CO exposure higher than 35 ppm produces headache and dizziness; if it exceeds 1600 ppm, the CO is dangerous to our health. In this work, zinc oxide (ZnO) thin films were obtained by the Successive Ionic Layer Absorption and Reaction method (SILAR). The SILAR sequence is described in 4 steps, the first one is zinc chloride complexed with ammonium as a cationic solution, the second one is a rinsing with just deionized water, then the third step is deionized water at 90°C as cationic solution and finally the fourth step is another rinsing with deionized water. After the thin film deposition, a final rinsing of the thin film in ethanol and hydrogen peroxide was performed along with an air annealing to complete the ZnO thin film formation. A gas sensor structure was fabricated with the e-beam evaporation of Ti/Au 30/70nm contacts in an interdigitated design. The minimum finger separation was 20um defined by photolithography and wet etch. The CO sensitivity was tested at gas concentrations of 0, 5, 10, 50, 100, 200, 300, 400, and 500 ppm. The operating temperature was analyzed at 100, 200 and 300°C.

Keywords
ZnO, SILAR, gas sensor.

Reference

Pineda-Reyes, A. M., Herrera-Rivera, R., Rojas-Chávez, H., Cruz-Martínez, H., & Medina, D. I. (2021). Recent advances in ZNO-Based Carbon Monoxide sensors: role of doping. Sensors, 21(13), 4425. https://doi.org/10.3390/s21134425.

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[MEM-310] PSEUDO-CMOS INVERTERS FABRICATED WITH IN-GA-ZN-O THIN FILM TRANSISTORS

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Oxide semiconductors such as In-Ga-Zn-O are very promising for thin film transistors in flexible electronics including wearables and internet of things. However, there is still a challenge in the implementation of reliable NMOS and PMOS fabrication processes towards complementary circuits. The pseudo-CMOS logic circuits is an alternative to improve the NMOS circuits (i.e. resistive load, active-load or saturation-load). The pseudo-CMOS inverter consists of four transistors with two-stage structure and three power rails. The TFTs were fabricated with the bottom gate top contact structure using gold as gate, Al_2O_3 as dielectric, IGZO as semiconductor, molybdenum as source/drain electrodes and PMMA as passivation layer. All the fabrication process was carried out with a maximum temperature of 150^{o}C. The preliminary results demonstrated working logic gates of the pseudo-CMOS inverter, NAND and NOR with rise time and fall times at 1kHz of 62/49, 62/100, and 121/26 microseconds, respectively. The inverter gain turned out to be around 7 which is necessary to improve by properly selecting the transistor dimensions. One advantage of the pseudo-CMOS structure is that the output voltage did not drop. Further improvements in the design is necessary to surpass the performance of non pseudo-CMOS structures.

Keywords
TFT, IGZO, pseudo-CMOS, NMOS circuits
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[MEM-316] GRAPHITE INCORPORATION TO TEOS FOR CO_2 SENSORS

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Graphite is an allotrope of carbon with excellent conductors of electricity and heat properties. Nanomaterials based on carbon as carbon dots, carbon nanotubes, graphene, graphite, and carbon composites have been reported as materials for electrodes for batteries, catalysis, coatings, and sensors, among other applications because the material properties such as high active surface area, electric and thermal conductivity, high chemical stability, and easy production. On the other hand, tetraethyl orthosilicate (TEOS) is used in the semiconductor industry as a silica source for silicone polymers and as a precursor to silicon dioxide (SiO2) production. TEOS hydrolyzation produces nanoparticles of silica, which have sensor applications due to the reactivity of the Si-OR bonds. In this work, TEOS is obtained by sol-gel deposition technique adding graphite powder to incorporate the carbon allotrope. First, colloidal suspensions of 30 ml ethyl alcohol were prepared with 0.1, 0.2, 0.3, and 0.4 gr of graphite powder. The samples were obtained using 3.3 ml tetraethyl orthosilicate mixed with 3.28 ml colloidal suspension, stirring at 650 RPM for 20 min. Then, 0.53 ml distilled water and 0.001 ml hydrochloric acid were added, stirring at 650 RPM for 45 min. Finally, the solution was deposited on glass substrates by drooping the solution, forming layers. X-Ray diffraction patterns (XRD) show graphite peaks at 26.48° (002) and 54.5° (004) regarding the incorporation of graphite into the TEOS matrix. The topography of the samples was obtained by Force Atom Microscopy (AFM). The experimental conditions, to incorporate graphite into TEOS, were determined by XRD, these conditions were reproduced to coat an optic fiber, which is going to be used to detect CO2.

Keywords
Grafito, tetraethyl orthosilicate, sensors and material.

Reference

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Sesión Oral

[MEM-48] FLUID TURBULENCE EFFECT MITIGATION IN A HOT WIRE MICRO ANEMOMETER AND ITS IMPLEMENTATION IN A MECHANICAL VENTILATOR

Iker Rodrigo Chavez Urbiola Dr.[1], Pablo Alfonso Tirado Cantu Dr.[1], Jesus Javier Alcantar Peña Dr.[1], Gilberto De León Muñoz Ms[1], Noe Amir Rodriguez Dr.[1], Luciano Nava Balanzar Dr.[1], Francisco Rodriguez Oronia Ms[1], Daniela Díaz Alonso Dr.[2]

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This work is presented the design process of flow sensors according to the needs of mechanical ventilation and its normative regulation. The employed principle for the micro anemometer was a calorimetric flow or hot-wire. The calorimetric flow sensor is done by two main components, a micro heater, and a resistive temperature detector. Both components were designed by analytical methods and finite element simulations as the first stage. The anemometer design is a micro heater surrounded by resistive temperature detectors. The mechanical ventilator needs a fast response at least 500 microseconds and a monitoring range between +/- 120 liters per minute. To check these requirements, especially the flow range is necessary to realize a transducer container with specific dimensions. But transducer container design implies following ISO normative for specific materials and connections, ISO 5356 and ISO 10993. A calorimetric flow sensor depends on the generated heat, as the higher heat produced higher the sensibility achieve. The produced heat on the membrane bridge produces thermal expansion that is transformed into mechanical stress. We implemented a mechanical micro damper that absolves the thermal stress produced by the membrane bridge. Flow sensibility and direction were improved by the implementation of mechanical bridges for the resistive temperature detectors. We analyze the distance between the micro heater and the temperature sensors by sequential simulations where the desired distance was obtained. As well it depends on the relation between the microsensor and airflow regimen, it was designed structural case that reduce Reynold's number over the sensor, and as a result noise level was mitigated. As well we present an alternative solution to resolve a traditional problem of accuracy due to the pressure effect in the flow line, which has a relation with flow density. The presented design covers the requirements for a mechanical ventilator for a human adult.

Keywords
MEMS, Microanemometer, mechanical ventilator.

Reference

ISO 5356
ISO 10993

This work was supported by
CONACYT project No. 319037, Escuela Mexicana De Ventilación (EMV).

[MEM-81] SIMULATION OF MEMS LOW-PRESSURE SENSORS WITH POLYETHYLENE TEREPHTHALATE DIAPHRAGM 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 polyethylene terephthalate (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. The flexible pressure sensor could be used for medical applications in this pressure range.

Keywords
Piezoresistive effect, nichrome gauge, pressure sensors, flexible diaphragm, polyethylene terephthalate.

Reference

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[MEM-294] DEPLETION-MODE IN-HF-ZN-O THIN FILM TRANSISTORS

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Continuous research on thin-film transistors (TFTs) based on amorphous oxide semiconductors (AOS) remains active due to their relatively high mobility and stability, thus these devices have attracted great attention for integrated circuit (IC) applications, in portable electronic devices, flexible display drivers and among others. Semiconductor oxides based on Zinc oxide (ZnO), such as Hafnium-Indium-Zinc Oxide (HIZO), are presented as an alternative of use in the study of AOSTFTs. Thin-film transistors based on HIZO by room temperature sputtering and Al2O3 as high-k dielectric by atomic layer deposition were designed and fabricated. The transistors have a threshold voltage (Vth)≈ -2.5V, field effect mobility μFET ≈14 cm2/Vs and a suthreshold slope of SS ≈ 300 mV/dec. Due to the type of characteristics obtained, a negative voltage is necessary to turn off the transistor, as a result the transistor can work in depletion mode in the design of IC. Inverter circuits are shown using these devices. The characteristics of the semiconductor layer depend on the deposition methods used, high-k dielectric is essential to reduce the operating range of the TFTs, and the use of low temperature fabrication makes it compatible with lost cost processes.

Keywords
AOS-TFTs, Hafnium-Indium-Zinc Oxide, high-k dielectric, depletion-mode, low temperature fabrication.

Reference

J. Zhang et al., "Enhancement-/Depletion-Mode TiO2 Thin-Film Transistors via O2/N2 Preannealing," in IEEE Transactions on Electron Devices, vol. 67, no. 6, pp. 2346-2351, June 2020, doi: 10.1109/TED.2020.2988861.

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[MEM-314] IMPLEMENTATION OF A 5UM NODE WITH NMOS TECHNOLOGY BASED ON IN-GA-ZN-O THIN FILM TRANSISTORS

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Nowadays, In-Ga-Zn-O (IGZO) thin film transistors (TFTs) are commercially used as backplane drivers of flat-panel displays. Besides, there is a pursuit of applications in wearable devices and internet of things. To build electronic circuits with certain complexity based on oxide semiconductors TFTs, the basic logic gates are first necessary to implement. In this work, the logic gates like inverters (NOT),OR, AND, NOR, NAND, and XOR were designed and fabricated with a TFT NMOS technology of channel length of 5um. The TFTs were fabricated on glass substrates with the bottom gate top contact structure using chromium/gold as gate electrode, Al_2O_3 as gate dielectric, IGZO as semiconductor, molybdenum as source/drain electrodes and PMMA as passivation layer. All the fabrication process was carried out with a maximum temperature of 150oC. After fabrication, all logic gates exhibit correct logic functions, according to their truth tables, in a VDD range of 3 to 9 V, and a frequency range of 50 Hz to 1 kHz. As an example, for a VDD equal to 6 V at 1 kHz the rise and fall times were: 55/4 us for a NOT, 56/7 us for a NAND, 67/2 us for a NOR, and 58/13 us for a XOR. These results are very attractive for the implementation of a multi-project wafer dedicated to the academia for the development of electronic circuits made of TFT technology compatible with flexible substrates.

Keywords
TFT, IGZO, circuits
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[MEM-358] DESIGN PLATFORM FOR RADIATION-HARDENED DIGITAL CMOS INTEGRATED CIRCUITS

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Integrated circuits (ICs) used in environments exposed to ionizing radiation, such as outer space, requires the implementation of design and process variations to reduce degradation in performance, reliability, and lifetime. A cost-effective strategy is the Radiation Hardening by Design (RHBD), which integrates special considerations in the system architecture, circuit design or physical layouts of an IC fabricated without changing a standard fabrication process. For the CMOS process, Enclosed Layout Transistors (ELT) with guard rings has been proven to reduce the effects of Total Ionizing Dose on its I-V characteristics. However, the ELTs are not usually compatible with the design rules defined for a CMOS process node. In semi-custom designs using hardware description languages, there is also a lack of verified standard cells based in ELTs.This work presents the current advances in developing a Process Design Kit (PDK) for a CMOS process that includes a radiation-hardened standard cell library. The standard cells are designed using scalable design rules for a CMOS technology being developed at CIDESI that could be accessed through a multi project wafer scheme. The PDK is compatible with a design flow based on Open Source Electronic Automation Design (EDA) tools and can be used to synthesize radiation-hardened digital integrated circuits.

Keywords
Integrated circuit, RHBD, CMOS, ELT, PDK
This work was supported by
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MULTIFUNCTIONAL AND MAGNETICS MATERIALS

CHAIRMEN

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

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

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

Sesión Oral

[MUL-348] EXPLORING DNA IN SUSPENSION BY ELECTRICAL IMPEDANCE SPECTROSCOPY

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Impedance spectroscopy is one of the least invasive of the non-destructive techniques, it is capable of electrically characterizing the physicochemical properties in liquids, solids and gases, composite materials, and also in biological materials in suspension. The power of this technique resides in the possibility of collecting micro information of the system through measurements of macro samples. Biological media in suspension in liquids can be characterized by the application of an electric field at different frequencies. Biological cells exposed to variable frequency electric fields are polarized, and are characterized by the relaxation time; detailed data of a given sample may be collected. Applying a mixed model, based on the Maxwell electromagnetic theory, it is possible to characterize the biological material of these cells, and specific results of its biological properties may be analyzed. Our hypothesis asserts that it is possible to differentiate the electrical characteristics of DNA from a healthy person from that of a person affected by a pathology, such as cancer of different types, through a detailed analysis of the dielectric response acquired through Electrical Impedance Spectroscopy measurements. It is expected to have very significant implications to be used by the pharmaceutical industry and, of great importance, in successful therapeutic practice. We are betting on a fast, reliable, reproducible, and economical diagnostic technique that should have a formidable impact on modern medical practices. This work will present and thoroughly discuss a general view of the technique, a detailed description of the construction of a plastic (and a quartz) cell for sample handling, and the preliminary calibration results.
Keywords: Electrochemical Impedance Spectroscopy, DNA, biomedicine, nanoparticle in medical applications
Reference: Li Wang, Sonpei Hu, Kai Liu, Bai Chen, Hongtao Wu, Jiabin Jia, Jiafeng Yao, A hybrid Genetic Algorithm and Levenberg Marquardt (GA-LM) method for cell suspension measurement with electrical impedance spectroscopy, Rev. of Sci. Instr., 91, 12410 (2020) https://doi.org/10.1063/5.0029491.
This work was supported by: funds provided by Coordinación de la Investigación Científica, Secretaria Académica y Secretaría Técnica de Intercambio Académico, and by Centro de Nanociencias y Nanotecnología, both of Universidad Nacional Autónoma de México.

[MUL-153] POSITIVE EXCHANGE BIAS IN COFEB/D019-MN3GE NONCOLLINEAR ANTIFERROMAGNETIC POLYCRYSTALLINE THIN FILMS AT ROOM TEMPERATURE FOR SPINTRONICS APPLICATION

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Single crystal and polycrystalline antiferromagnetic D019-Mn3Ge thin films were grown on cubic Pt (111) and hexagonal GaN (0001) template layers using varied substrate temperatures. Subsequently, to induce a spin coupling, an ultrathin film of ferromagnetic CoFeB layer was grown like a stack on top of the D019-Mn3Ge films at room temperature. An increase in the coercivity of the CoFeB ultrathin films was observed due to the high surface roughness of induced single crystal D019-Mn3Ge thin films, meanwhile a relatively low surface roughness and uniaxial texture were observed on polycrystalline D019-Mn3Ge thin films, which induced positive exchange bias at room temperature by cooling the sample under a magnetic field of 2 T. There was no presence of exchange bias with samples measured at lower cooling applied magnetic fields. Despite the magnetic disorder at grain boundaries, the lower surface roughness of the polycrystalline antiferromagnetic thin films plays a major role in the formation of positive exchange bias.

Keywords
Positive exchange bias; D019-Mn3Ge; CoFeB; substrate temperature; polycrystalline thin films.

Reference

Nogués, C. Leighton, I.K. Schuller, Correlation between antiferromagnetic interface coupling and positive exchange bias, Phys. Rev. B 61 (2000) 1315–1317, https://doi.org/10.1103/PhysRevB.61.1315.

This work was supported by

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[MUL-25] MAGNETIC PROPERTIES AND COERCIVITY MECHANISM OF COZR ALLOYS RARE EARTH FREE PERMANENT MAGNETS

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The remarkable characteristic of permanent magnets (PM) is their independence from a continuous supply of electrical power or other energy sources to maintain their magnetic field. PMs are used in a wide variety of devices. In recent decades, there has been significant research on rare earth (RE)-containing alloys to develop advanced permanent magnetic materials due to their outstanding intrinsic magnetic properties. However, the escalating demand for RE permanent magnets has resulted in scarcity and increasing prices of RE elements. Therefore, there is a growing need to explore RE-free permanent magnetic materials that can be applied in industrial settings. One potential candidate for such materials is Co-Zr alloys, which demonstrate excellent performance in terms of hard magnetic properties. This study focuses on optimizing the annealing conditions and investigating the hard magnetic behavior of rare earth-free CoZr alloys, aiming to enhance the magnetic properties of these materials. The alloys were obtained using the melt spinning technique.

For development of the work the alloys of $Co_{74}Zr_{16}Mo_4Si_3B_3$ were process under different annealing conditions and were comparative respect the as cast conditions. The optimal results were achieved when the alloys were annealed at 903 K for 180 minutes, leading to the formation of predominantly rhombohedral Co_5Zr phase with a small amount of cubic Co_6Zr_{23}. This increase in the hard magnetic phase resulted in notable enhancements in various magnetic properties. Specifically, the coercive field (H_c) increased from 6kOe to 7.3kOe, saturation magnetization (M_s) rose from 18 to 29 emu/g, remanence magnetization (M_r) increased from 10 to 17 emu/g, and the grain size decreased from 55 to 47nm. Moreover, this enabled the investigation of the coercivity mechanism, which is a crucial aspect in studying and characterizing hard magnetic materials. The coercivity mechanism in these alloys predominantly revolves around the nucleation process of reverse domains.

Keywords

Positive exchange bias; D019-Mn3Ge; CoFeB; substrate temperature; polycrystalline thin films.

Reference

R. Madugundo, N. Venkata, R. Rao, D. Salazar, A.A. El-gendy, Recent Developments in Nanostructured Permanent Magnet Materials and Their Processing Methods, (2018) 74-77. https://doi.org/10.1016/B978-0-12-813904-2.00006-1.

This work was supported by

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[MUL-337] OPTICAL AND MAGNETIC CHARACTERIZATION OF LiCoO2 AND LiNiO2 NANOPARTICLES

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$LiCoO_2$ and $LiNiO_2$ [1] are important compounds in battery technology since they can be used as cathodes in rechargeable lithium batteries, due to their high energy density and good cyclability. These parameters are strongly influenced by the microstructure of the materials. In particular, the tortuosity factor, which determines the diffusion of lithium ions within the electrode and, therefore, the efficiency of these devices. efficiency of these devices. Tortousity, in turn, depends directly on the microstructure, specifically on the porosity. On the other hand, it is well known that the synthesis method plays a determining role in the microstructure of materials. This work presents the synthesis of LiCoO2 and LiNiO2 compounds by the coprecipitation method and their structural and microstructural characterization by powder X-ray diffraction and scanning electron microscopy. XRD analysis show different pure phases of LiCoO2 and LiNiO2 under the same synthesis conditions. Measurements of diffuse reflectance were done in order to obtain the values of the energy of the forbidden gap. Measurements of the magnetization as a function of the applied magnetic field are also presented.

Keywords
Lithium oxides, Lithium batteries, Nanoparticles of $LiCoO_2$, Nanoparticles of $LiNiO_2$.

Reference

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This work was supported by
CONACYT México. 1843 Jóvenes Investigadores por México 2021.

[MUL-14] EFFECTIVE PROPERTIES OF MULTI-LAMINATED COSSERAT ELASTIC COMPOSITES WITH QUASI-PERIODIC STRUCTURE

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Micromechanical models have been efficient tools for the study of multiphase composite materials. They allow the understanding of the characterization mechanisms of composite materials, of their structure-property relationships, as well as contribute to the design and optimization of manufacturing processes for new materials. In practical applications, many heterogeneous composite materials have non-periodic, quasi-periodic, or even random structures. Restrictions to periodic geometric microstructures in composite materials imply limitations and are not frequent in real engineering applications [1]. In this sense, knowing the effects of the micro-structure, the constituent phase materials, and their volume percentages, among others, on the composite effective properties can help to manipulate and to obtain appropriate properties for better composite functionality.
In this contribution, a study of the effective moduli of multi-laminated elastic micropolar composites with quasi-periodic structures is developed through the two-scale asymptotic homogenization method (AHM), following the ideas of [2]. Here, the constituents are assumed centro-symmetric and isotropic materials, and perfect contact conditions are considered at the interface. The quasi-periodic arrangements follow the Fibonacci sequence. From AHM, the local problems over the representative cell Y and the corresponding non-null effective stiffness and torque properties are presented. Numerical results are illustrated and discussed. The effect of the quasi-periodic structure is noteworthy on the overall effective behavior of the micropolar elastic composite.

Keywords
Asymptotic homogenization method, Cosserat composite, Quasi-periodic structures, Multi-laminated composite.

Reference

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NANOSTRUCTURES

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Dear Friends and Colleagues,

We take pleasure to invite you to participate in the Nanostructures symposium of the XVI international conference on surfaces, materials and vacuum. Participants interested in presenting an oral or poster contribution are invited to submit an abstract.

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

We look forward to welcoming you.

[NSN-51] STUDYING THE INTERACTION OF GRAPHENIC SUBSTRATES WITH HUMAN INTERLEUKIN-6 AND ITS MONOCLONAL ANTIBODY BY RAMAN IMAGES

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Interleukin-6 (IL-6) is a cytokine with wide-ranging biological effects, playing an important role on the immune system and inflammatory responses. Therefore, it is important to develop alternative, highly sensitive and reliable analytical methodologies for the accurate detection of this biomarker in biological fluids. Graphene substrates (GS), such as pristine graphene (G), graphene oxide (GO), and reduced graphene oxide (rGO), have shown great benefits for biosensing and in the development of novel biosensor devices. In this work, we present a proof of concept for the development of a new analytical platform for the specific recognition of human interleukin-6, that is based on the coffeering formation of monoclonal antibodies of interleukin-6 (mabIL-6) onto amine functionalized GS.The prepared GS/mabIL-6/IL-6 systems were successfully used to show that IL-6 was specifically and selectively adsorbed onto the area of the mabIL-6 coffee-ring. Raman imaging was confirmed as a versatile tool to investigate different antigen-antibody interactions and their surface distribution. This experimental approach can be used to develop a wide variety of substrates for antigen-antibody interaction allowing the specific detection of an analyte in acomplex matrix.

Keywords
Interleukin-6, Nanomaterials of graphene substrates, Biosensors.

Reference

de la O-Cuevas, E., et al. Modulating the interaction of graphenic substrates with human interleukin-6 and its monoclonal antibody: a study by Raman images, RSC Advances. 13 (2023) 15114-15120. https://doi.org/10.1039/D3RA01627G

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[NSN-67] GREEN SYNTHESIS OF STABLE GOLD AND SILVER NANOPARTICLES USING AQUEOUS EXTRACT OF SARGASSUM SPP. AND THEIR APPLICATION IN CATALYSIS

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The present work reports an eco-friendly approach for the synthesis of stable gold (Au) and silver (Ag) nanoparticles using the aqueous extract of *Sargassum spp*. collected from caribbean beaches in Yucatan, Mexico. The aqueous Sargassum extract contains active biomolecules, which act as reducing and capping agents during the synthesis and posterior stability of the resulting metal nanoparticles. The formation of Au and Ag NPs was detected by their characteristics surface plasmon resonance band in the visible region of UV-vis absorption spectra. The stability of metal nanoparticles was studied by monitoring the position of plasmon band over several weeks. The XRD patterns revealed the formation of FCC crystalline structure of metal nanoparticles. The formation of spherical Au and Ag NPs with average sizes in the range of 15 to 20 nm was observed in TEM micrographs. FTIR spectrum of Sargassum extract exhibited the presence of -OH and -NH2 functional groups, which are possibly responsible for metal ion reduction. The colloidal suspension of Au and Ag were employed as catalysts for p-nitrophenol reduction, where Ag nanoparticles exhibited higher catalytic performance than Au nanoparticles under similar experimental conditions.

Keywords
Green synthesis, nanoparticles of Au and Ag, Sargassum spp., Catalysis.

Reference

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[NSN-71] MORPHOLOGY, COMPOSITION, AND STRUCTURE IMPACT ON OPTICAL RESPONSE IN NANOSTRUCTURED HEMATITE THIN FILMS

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This work focuses on the investigation of nanostructured hematite films for their potential applications as photoactive materials. The challenge lies in understanding the intricate behavior of their optical properties influenced by the nanostructure. Through the study by AFM, XRD, and XPS we presented a comprehensive ellipsometric analysis of the optical response of nanostructured hematite films synthesized using chemical bath deposition. We demonstrate a remarkable agreement between the measured and calculated Δ and Ψ angles, achieved through rigorous fitting procedures, providing compelling evidence of the reliability of the constructed ellipsometric model. Furthermore, the study establishes a strong correlation between the thicknesses obtained from ellipsometry and those determined using AFM and profilometry, thereby further validating the analytical approach. By analyzing the parameters derived from the fitted model, we distinct two porosity contributions in the films, named gross and fine porosities, which derive from the microscopic and nanometric morphological features of the hematite films. Collectively, these results expose an intricate relationship between morphology and optical response, shedding light on essential aspects of nanostructured hematite films such as density and porosity. Exploiting these findings may cover the way for enhancing their performance in potential applications as photoactive materials.

Keywords
hematite thin films, nanostructured morphology, ellipsometry.

Reference

D. A. Mazón-Montijo, D. Cabrera-German, A. S. Sánchez-Ovando, O. Y. Ramírez Esquivel and Z. Montiel-González, Role of morphology, composition, and structure on the optical response of nanostructured hematite thin films, Optical Materials. 110 (2020) 110496. https://doi.org/10.1016/j.optmat.2020.110496.

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CONAHCYT

[NSN-79] ELECTRONIC AND OPTICAL PROPERTIES OF BLACK-PHOSPHORENE/MoS2 BILAYER WITH VACANCIES

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The two dimensional materials and their vertical stacking, called van der Waals (vdW) heterostructure, have novel and interesting properties. Black phoshorene (BP) and molybdenum disulfide (MoS_2) are recognized two dimensional materials because they have emerged as candidates in different applications, due to their direct bandgap, as well as, the high charge mobility and broader spectrum range of absorption in phosphorene monolayer, and the high refractive index in MoS_2 monolayer. Also, researches have reported that the vertical stacking conformed for black phosphorene and MoS_2 has high absorption coefficient in visible zone and the reduction of bandgap in comparison with the single monolayers bandgap. On other hand, the presence of vacancies in two bidimensional materials and their vertical stacking allows the study of possible experimental effects in the obtaining of these materials, and the modulation of their properties. In this work we systematical calculate the electronic and optical properties within density functional theory (DFT) methodology of BP/MoS_2 van der Waals heterostructure with different number of phosphorus atoms vacancies. The results indicate interesting modifications in the heterostructure of BP/MoS_2 as the semiconductor to metal transition with one and three phosphorus atom vacancies and the reduction of bandgap with two and four phosphorus atoms vacancies.

Keywords
vdW heterostructure, Black Phosphorene, MoS2, vacancy, DFT.

Reference

R. Kochar and S. Choudhary, MoS2/Phosphorene Heterostructure for Optical Absorption in Visible Region, IEEE J. Quantum Elect. 54 (2018) 1-6.
https://doi.org/10.1109/JQE.2018.2850450.

This work was supported by

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[NSN-85] ACTIVATED CARBON FROM MORINGA OLEIFERA SHELLS FOR REMOVAL OF ATRAZINE

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Currently, emerging water pollutants such as herbicides have received more attention and require sustainable remediation technologies. One of the most commonly used methodologies for the remediation of contaminated aqueous systems is based on adsorption, which is advantageous over other methods because of its simple operation and facile extraction of the adsorbent from solutions. Using activated carbon for water treatment can be particularly expensive in developing countries, where it is usually imported. Thus, it is desirable to produce activated carbon from agricultural and industrial wastes to be used as an adsorbent of herbicides. Atrazine (ATZ) is an herbicide widely used all over the globe to control weeds, and it is essential in agricultural development. However, the widespread use of the ATZ can have serious hazardous effects on aquatic organisms and humans because its residues end up on the surfaces and water sources, causing stress within aquatic organisms and damaging ecological systems. In this study, the shells of the Moringa Oleifera (MO) were used as precursors to the production of carbon. Furthermore, it is utilized as a superior adsorbent for the removal of ATZ, owing to its cost-effectiveness. Agricultural precursor MO shells were collected, grinded, and pyrolyzed at a temperature range between 750–950 °C. The characterization of activated carbon includes scanning electron microscopy (SEM), powder X-ray diffraction (XRD), Fourier-transform infrared (FTIR) and Raman spectroscopy, and gas adsorption. Adsorption studies of atrazine (ATZ) from aqueous solutions with granular activated carbon were monitored by UV-vis spectroscopy and the adsorbent dosage varied in the range from 10–150 mg. The sample displayed an atrazine removal capacity of 52% when 150 mg of material was used.

Keywords
Moringa Oleifera, activated carbon, atrazine, adsorption.

Reference

L.F. Cusioli, C.O. Bezerra, H.B. Quesada, A.T. Alves, L. Nishi, M.F. Vieira and R. Bergamasco, Modified Moringa Oleifera Lam. Seed husks as low-cost biosorbent for atrazine removal, Environmental Technology, 42:7, 1092-1103, https://doi.org/10.1080/09593330.2019.1653381.

[NSN-89] TUNING OF THE CAVITY STATES AND RELATED ELECTRIC FIELD IN A ONE-DIMENSIONAL DIELECTRIC-GRAPHENE PHOTONIC CRYSTAL WITH A CAVITY INCORPORATED

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In this work, an analytical deduction of the structure of photonic bands, the dispersion relation, as well as the macroscopic spectra of transmission and reflection for a one-dimensional dielectric-graphene photonic crystal of a bi-periodic unit cell in the chemical potential is made. The unit cell consists of two graphene sheets separated by an isotropic dielectric medium, where the chemical potential for the first graphene sheet is μa and for the second sheet is μb. The analytic equations to photonic bands, the dispersion relation, and the transmission and reflection spectra of incident electromagnetic waves are deduced by using the transfer matrix formalism; In addition, the optical conductivity of graphene is implemented taking into account both intra and interband contributions. We found that this bi-periodic photonic structure of chemical potential shows the formation of new photonic gaps in comparison with the conventional one-dimensional graphene dielectric photonic crystal, moreover, these non-propagation regions can be seen directly from the transmission and reflection spectra that are calculated from the expressions that are found. Finally, we showed that the new photonic gaps formed can modulate their thickness in frequency through the values of the chemical potential in the graphene sheets of the unit cell.

Keywords
photonic crystal, graphene, dielectric, cavity, allowed states.

Reference

R. Kochar and S. Choudhary, MoS2/Phosphorene Heterostructure for Optical Absorption in Visible Region, IEEE J. Quantum Elect. 54 (2018) 1-6.
https://doi.org/10.1109/JQE.2018.2850450.

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[NSN-99] PHOTOCATALYTIC MATERIALS BASED ON SiNWs TESTED UNDER DIFFERENT LIGHT INTENSITIES FOR THE DEGRADATION OF CONTAMINANTS

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This study focuses on the photocatalytic activity of materials based on Si nanowires decorated with Cu. The Si nanowires were fabricated using the metal-assisted chemical etching technique and subsequently decorated via electroless deposition. Surface tests were conducted under different illumination conditions, revealing the influence of light intensity on the percentage reduction of pollutant concentration and reaction rate values. A direct relationship between increased light intensity and enhanced reaction rate was observed. The activity improvement is also dependent on the material configuration, as demonstrated in the case of CuO-decorated Si nanowires, where light intensity positively contributes to their performance. However, this effect is not reflected in the same manner on the surfaces of undecorated Si nanowires or those with other tested types of decoration.

Keywords
Photocatalysis, Nanostructures, Silicon nanowires, Degradating contaminants, Metal-assisted chemical etching, MACE.

Reference

O. A. Cárdenas Cortez, J. J. Pérez Bueno, Y. Casados Mexicano, M. L. Mendoza López, et al., CoO, Cu, and Ag Nanoparticles on Silicon Nanowires with Photocatalytic Activity for the Degradation of Dyes, Sustainability 14 (2022) 13361. https://doi.org/10.3390/su142013361.

This work was supported by

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[NSN-137] EVALUATION OF TiO_2 NANOTUBE Ag-DOPED BY ANODIZATION AS ELECTRODE FOR THE DETECTION OF ASCORBIC ACID

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Titanium oxide nanotubes (TiO_2-NTs) offer important functional properties with environmental, clinical, and agroalimentary applications. Among their characteristics, biocompatibility, non-toxicity, low cost, and chemical, physical, and mechanical stability stand out. Thanks to its electrical and catalytic properties, it is one of the best materials for the development of electroanalytical devices for redox compounds called nanosensors. Its highly ordered morphology obtained by the electrochemical anodization synthesis method provides greater surface area than the bulk material or other morphology, moreover, the incorporation of a dopant element reduces electron-hole recombination, these improve the electronic charge transport in the TiO_2-NTs electrode, which is key for sensing mechanism [1]. This work presents the developed acid ascorbic nanosensor based on a silver-doped titanium nanotube electrode (Ag-TiO_2NTs). The synthesis was carried out by electrochemical anodization in a single step, starting from a sheet of metallic titanium (1.5x2cm) subjected to mechanical and chemical cleaning followed by the anodizing process at a constant voltage of 30 volts for 45 minutes, using an electrolyte of ethylene-glycol and deionized water, ammonium fluoride and silver nitrate. Finally, a heat treatment was applied at 500 °C for 2 h. The morphology was analyzed by SEM and FTIR. The results showed the obtaining of a highly ordered TiO_2 nanotube array with an average diameter of 80 nm and the presence of Ag in an atomic percentage of 0.29. The analytical response to ascorbic acid (AA) was investigated with the cyclic voltammetry (CV) technique. Evidenced the irreversible nature of the system and confirmed the response of the Ag-TiNTs electrode to AA with a sensitivity of 148.15 $\mu A/mM \cdot cm^2$ and a detection limit of 213 µM.

Keywords
TiO2NT´s, sensitivity.

Reference

[1] S, Sharma, S.K. Ganeshan, S. Kundu and N. Chappanda. Effect of doping on TiO2 nanotubes based electrochemical sensors: Glucose sensing as a case study. IEEE Transactions on nanotechnology. 20 (2021). https://doi:10.1109/TNANO.2021.3060786.

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[NSN-139] LOW-DIMENSIONAL THERMOELECTRICITY IN FIBONACCI BILAYER GRAPHENE SUPERLATTICES

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We investigate numerically the transport and thermoelectric properties of Fibonacci bilayer graphene superlattices generated by applying an external electric field. We present an analysis of the impact of aperiodic order on transmittance, conductance and thermoelectric properties such as Seebeck coefficient, power factor and figure of merit. For the calculations we implement the hybrid matrix method, the Landauer-Bütikker formalism and the thermoelectric transport coefficients. We present whether the Fibonacci sequence improves the thermoelectric properties of the bilayer graphene.

Keywords
Transport, Thermoelectricity, Bilayer-graphene, Fibonacci, Superlattices.

Reference

J. A. Briones-Torres, R. Pérez-Álvarez, S. Molina-Valdovinos, and I. Rodríguez-Vargas, Thermoelectricity in bilayer graphene superlattices, Phys. Scr. 98, (2023) 035713. https://doi.org/10.1088/1402-4896/acbbaf.

[NSN-143] EFFECT OF THE APERIODICITY ON SPIN-VALLEY TRANSPORT PROPERTIES IN COMPLEX MAGNETIC SILICENE STRUCTURES

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Complex structures are characterized by having a certain type of order know as aperiodic order, which is used to study physical properties with fundamental characteristics such as fractality, self-similarity, and fragmentation. In this work, we show that self-similar aperiodicity optimizes simultaneously the spin-valley polarization and tunneling magnetoresistance in complex magnetic silicene structures following the substitutional rules of the Cantor sequence giving rise to versatile structures [1]. The transport properties are calculated with the transfer matrix method and the Landauer-Büttiker formalism. Our findings show that the complex arrangement of the magnetic barriers along with structural asymmetry reduce the conductance oscillations, typical of magnetic superlattices in silicene [2]. Furthermore, it is possible to have two well-defined spin-valley polarization states by simply reversing the direction of magnetization. In this case, the magnetoresistance is not as prominent as in silicene magnetic superlattices, however, it is better than in simple magnetic junctions. The optimization of the spin-valley dependent transport properties caused by the complex structures is superior to the one found in aperiodic structures such as Fibonacci and Thue-Morse [3]. Thus, self-similar aperiodicity is a useful tool to create versatile structures.

Keywords
Silicene, Complex Structures, Transport Properties, Aperiodicity.

Reference

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[2] J. G. Rojas-Briseño et al., Phys. Rev. B 103 (2021) 155431.
[3] P. Villasana-Mercado et al., J. Phys.: Condens. Matter 35 (2022) 085302.

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CONACYT-SEP Mexico through grant A1-S-11655.

[NSN-147] STUDY OF THE EFFECT ON THE TEXTURAL PROPERTIES OF ZnTe NANOSTRUCTURED FUNCTIONALIZED WITH ETHYLENDIAMINE THROUGH A HYDROTHERMAL METHOD

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Zinc telluride (ZnTe) is one of the II-VI interesting semiconducting compounds widely used in various optoelectronic applications.
In this work, ZnTe nanomaterials were synthesized by the hydrothermal method at 180 °C, using elemental zinc and tellurium precursors. The functionalization of the ZnTe materials was carried out using an In-situ method, adding the necessary amounts of ethylenediamine to the precursors in different percentages by weight (1, 3 and 5%). The structural, morphological and textural properties of pure and functionalized ZnTe nanomaterials were studied. The ZnTe nanomaterials were structurally characterized by powder X-ray diffraction where it was observed that they have a zincblende-type cubic structure with crystal sizes ranging from 25-46 nm, morphologically by scanning electron microscopy (SEM) particles with spherical morphology were observed, with an average particle size range of 40 to 80nm. Additionally, the materials were analyzed by infrared spectroscopy where the characteristic signals of ethylenediamine in the ZnTe materials were observed. On the other hand, for the determination of the textural properties of the materials, these materials were analyzed by physisorption of N_2, it was observed that by increasing the percentage of the amine on the ZnTe, the specific area tends to increase.
The characterization results of the synthesized ZnTe nanomaterials showed promising properties for their potential application in the field of photocatalysis and gas sensors, which we are interested in for future work.

Keywords
Hydrothermal method, ZnTe, Nanomaterials, organic functionalization.

Reference

J. J. Rodriguez and M. de la L. Olvera, "Photocatalytic degradation of Malachite Green dye from ZnTe powders under visible light," 2022 19th International Conference on Electrical Engineering, Computing Science and Automatic Control (CCE), 2022, pp. 1-7, doi: 10.1109/CCE56709.2022.9975882.

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[NSN-151] EXTENDED STATES IN DISORDERED DIMER SUPERLATTICES IN GRAPHENE

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Ordered and disordered semiconductor superlattices represent structures with completely opposed properties. For instance, ordered superlattices exhibit extended Bloch-like states, while disordered superlattices present localized states. These characteristics lead to higher conductance in ordered superlattices compared to disordered ones. Surprisingly, disordered dimer superlattices, which consist of two types of quantum wells where one type always appears in pairs, exhibit extended states [1,2]. The percentage of dissimilar wells does not need to be large to have extended states. Furthermore, the conductance is intermediate between ordered and disordered superlattices. In this work, we explore disordered dimer superlattices in graphene. To achieve this, we calculate the transmission and transport properties applying the transfer matrix method and the Landauer-Büttiker formalism, respectively. We identify and discuss the main energy regions where the conductance of disordered dimer superlattices in graphene is intermediate to that of ordered and disordered superlattices. Additionally, we analyze the transmission coefficient within these particular regions.

Keywords
Superlattices, Graphene, Random Dimer Wells, Conductance.

Reference

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CONACYT-SEP Mexico through grant A1-S-11655.

[NSN-161] BIOSYNTHESIS OF Ag AND Au NPs AND THEIR INTERACTION WITH BACTERIAL SPORES OF BACILLUS SUBTILIS SPECIES

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The study of metallic nanoparticles is an area of research that is currently gaining importance within the scientific community, due to its wide field of applications in medicine, optics, electronics, biochemistry, agriculture, among others, in addition to its essential use for the development of new technologies. The biological synthesis of metal nanoparticles using metabolites from plants, bacteria and fungi is considered an economical and environmentally sustainable method. One of the main applications of gold and silver nanoparticles is their use as effective antimicrobials, however, their antimicrobial effect against highly resistant biological structures such as bacterial endospores has been few studied. In this work, the interaction of Au and Ag nanoparticles obtained by fungal biosynthesis with Bacillus subtilis bacterial endospores was analyzed using the Fourier Transform Infrared Spectroscopy technique. The nanoparticles obtined by biological synthesis usig fungal metabolites was characterized by spectroscopic methods (UV-Vis, EDX-RF, XRD, FTIR).

The results obtained show that the synthesis process was successful since a high performance of the biosynthesis process was obtained. UV-Vis spectroscopy it was demonstrated the presence of an absorption band between 500 and 550 nanometers indicative of the formation of a surface resonance plasmon associated to the formation of the gold nanoparticles. Using the EDX-RF method, the elemental composition of the samples was determined and their crystalline structure was demonstrated by X-ray diffraction. Finally, FTIR spectroscopy analysis revealed the presence of bands characteristic of bacterial endospores in the range of 1000 to 1800 cm^{-1}.

Keywords
Nanoparticles, Spectroscopy, Endospore, Synthesis, Bacteria.

Reference

Tikariha, S., Singh, S., Banerjee, S., & Vidyarthi, A. S. (2012). International Journal of Pharmaceutical Sciences and Research, 3(6), 1603. http://dx.doi.org/10.13040/IJPSR.0975-8232.3(6).1603-15.

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[NSN-185] A FIRST PRINCIPLES STUDY OF HYDROGEN ADSORPTION ON DOPED (Li, Ca, K) γ-GRAPHYNE

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One of the biggest challenges for the development of the hydrogen economy is the search for materials for its storage. The storage of hydrogen in solid-state materials is an area of great interest for current research with the potential to overcome this obstacle. Considering the effect of Van der Waals interactions, the behavior of hydrogen storage in different metal-doped γ-graphynes was investigated using first-principles plane-wave calculations with DFT-D3 correction. Results show that most desirable adsorption site for Li, Ca and K atoms is the triangular hollow site of 12 atoms on the γ-graphyne with a hydrogen adsorption energy range of -171 and -46 meV/H2. The polarization caused by the electrostatic field of metal atoms on γ-graphyne and the hybridization between the metal atoms and hydrogen molecules were mostly attributed to the physisorption mechanism. This study shows that (Li, Ca, K) doped γ-graphyne may be a promising candidate for hydrogen storage applications at ambient conditions.

Keywords
γ-Graphyne, physisorption, doped, DFT, hydrogen storage.

Reference

Wang, Y., Xu, G., Deng, S., Wu, Q., Meng, Z., Huang, X., Bi, L., & Lu, R. (2020). Lithium and sodium decorated graphdiyne as a candidate for hydrogen storage: First-principles and grand canonical Monte Carlo study. Applied Surface Science, 509. https://doi.org/10.1016/j.apsusc.2019.144855

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[NSN-201] QUANTUM TUNNELING IN 2D NANOWIRE SUPERLATTICES: A THEORETICAL STUDY

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Semiconductor superlattices consists of alternating layers of two or more different semiconductors with thicknesses of just a few nanometers each. In such systems, only certain quantized energy states for electrons and holes are allowed. If, instead of abrupt interfaces between the layers, nano-corrugated interfaces are induced in the epitaxial growth process, then a 2D array of semiconductor nanowires (NWs) is obtained. Experimentally, one of the methods to obtain such corrugation is the use of self-assembly on high index substrates by Molecular Beam Epitaxy, which can produce periodic crystalline nanostructures of high uniformity. By controlling the thickness and composition of such layers it is possible to tune the energy levels of the electrons and holes and create a variety of interesting physical phenomena.

In this work, we present a theoretical study of 2D systems of M×N-NW superlattices, with M and N the number of NWs along the x and y axis, ranging from 1 to 12. By solving the one-electron Schrödinger equation and following the transfer procedure and the Kronig-Penney model we calculate the transmission coefficient, the probability densities and the electronic densities in GaAs-NW arrays embedded into an AlGaAs matrix. Our results suggest that these systems can be interesting candidates for information storage applications in nanoelectronics or quantum computation.

Keywords
Nanowires, semiconductors, superlattice, tunneling.
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[NSN-207] OPTICAL CHARACTERIZATION OF SELF-ASSEMBLED SEMICONDUCTOR QUANTUM WIRES WITH A SYMMETRICAL SILICON-DELTA-DOPING GROWN BY MBE

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The synthesis of one-dimensional (1D) arrays, such as GaAs quantum wires (QWRs) is an essential topic of study due to the unique quantum effects predicted for 1D systems and by the numerous potential new applications of these nanostructures in electronic and optoelectronic and improve existing devices. In this work, a study was carried out on the effects of silicon delta doping on the optical properties of the samples. The synthesis of the GaAs/AlGaAs heterostructure was carried out by Molecular Beam Epitaxy (MBE) using GaAs (631) substrates. The QWR arrays were studied by atomic force microscopy (AFM). The optical properties were studied by photoluminescence (PL), micro-photoluminescence (μ-PL), and photoreflectance (PR) techniques. Strong emission was obtained from PL and μ-PL even at room temperature. In addition, a signal associated with delta-type doping was observed and studied as a function of the temperature. Good agreement was obtained between the experimental observation and a theoretical model for quantum wire transitions. In conclusion, samples with the right characteristics to produce a multi-channel QWR high electron mobility transistor (HEMT) were obtained, where each QWR works as one independent channel.

Keywords
Quantum Wire, MBE, GaAs.

Reference

E. Cruz-Hernández, S. Shimomura, and V. H. Méndez-García, Highly ordered self-assembled nanoscale periodic faceting in GaAs(631) homoepitaxial growth, Appl. Phys. Lett. 101 (2012) 073112. https://doi.org/10.1063/1.4746423

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Conahcyt

[NSN-211] CRYSTALLINE PHASE TRANSFORMATION OF ELECTROSPUN ZnO NANOFIBERS CARRIED OUT BY HEAT TREATMENT

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In this work, the controlled synthesis of ZnO nanofibers obtained by the electrospinning technique is presented. By varying the distance between the tip of the needle and the collector it was possible to control the diameter and formation of the fibers within the nanometer scale. By means of scanning electron microscopy (SEM) it was possible to corroborate the formation of nanofibers with an elongated cylindrical shape without the presence of defects called "rosaries"[1]. The fibers with the smallest diameter were obtained at a working distance of 20 cm. The functional groups of the ZnO nanofibers were obtained by infrared spectroscopy (FTIR) and by energy dispersive spectroscopy (EDS) and chemical stoichiometry. The structure and crystalline phase of the ZnO nanofibers were controlled through annealing in a range from 0 to 1000 °C in an air atmosphere. The results of the characterization by X-ray diffraction and Raman scattering of the fibers obtained with different heat treatments are presented. The transformation of the crystalline phase varied as a function of the temperature of the heat treatment. By X-ray diffraction it was found that at annealing temperatures lower than 200 °C the fibers are amorphous, the hexagonal wurtzite phase occurs from 300 °C, and finally at annealing temperatures higher than 700 °C more crystalline fibers were obtained.

Keywords
electrospinning, heat treatment, crystalline phase.

Reference

[1] Secundino-Sánchez, O., Sánchez-Ramírez, J. F., & Diaz-Reyes, J. (2021). Systematic Structural and Optical Characterization of TiO2 Nanofibres Synthesised by Electrospinning. WSEAS Transactions on Electronics, 12, 106-115.

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[NSN-217] STUDY OF TiO2@BiOBr HETEROJUNCTION IN PHOTOCATALYTIC ACTIVITY UNDER VISIBLE LIGHT IRRADIATION

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The photocatalysis mechanism is an important method that helps remove organic compounds from dyes in contaminated water. A potential material is TiO2 titanium dioxide. But this material has a major limitation, the band gap is in the ultraviolet region. A compound that shows good photocatalytic activity is bismuth oxide bromide (BiOBr) and bonded with other materials has a good performance in that field. For this reason the main objective of this work is to test the TiO2@ BiOBr Heterojunction in different molar ratios 1:1, 2:1 and 1:2. The photocatalytic activity was measured using rhodamine ratio 30 ppm at 1 g/L photocatalyst and using only visible light irradiation. The results suggest that heterojunction works better than materials in pristine mode, and also works in visible light radiation. The study shows us perspectives for more photocatalytic applications.

Keywords
Heterojunction, Visible irradiation, rhodamine, nanostructures, Titanium dioxide.

Reference

1. Wang, X., Yang, W., Li, F., Zhao, J., Liu, R., Liu, S., & Li, B. (2015). Construction of amorphous TiO2/BiOBr heterojunctions via facets coupling for enhanced photocatalytic activity. Journal of Hazardous Materials, 292, 126–136. doi:10.1016/j.jhazmat.2015.03.03.

[NSN-221] OBTENTION OF MoS2 USING LIQUID PHASE EXFOLIATION OF MOLYBDENITE RESIDUES FROM THE WUZHOU MINE

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The exponential growth of technology has its foundations in the research and development of new materials whose application in various fields benefit the population. In this sense, 2D materials are a new alternative, due to their improved mechanical, optical, electrical, thermal, and elastic properties. Molybdenum disulfide has unique properties such as, a large bandgap (~1.8 eV) that changes from an indirect to a direct gap in thin structures, its properties also change depending on its structure, it can be semiconductor, metallic or superconducting; therefore, it can be applied in fields like electronics, especially as optical sensors and biosensors. This work focuses on obtaining sheets of molybdenum disulfide (MoS_2) from molybdenite residues obtained in the Wuzhou mine, located in the Guanxi province of China. The liquid phase exfoliation method assisted by intercalating molecules was used. Potassium cetyl phosphate (PCP) and N-(N-butyl) thiophosphoric triamide (NBPT) are used as intercalating molecules, these stabilizing agents allow the separation of the sheets and facilitate the Mos_2 dispersion in an aqueous medium. The properties of the obtained sheets are characterized by means of Raman spectroscopy, UV-vis spectroscopy, and transmission electron microscopy (TEM). The MoS_2 sheets obtained from molybdenite mineral residues are compared with MoS2 sheets obtained from commercial molybdenite from the company ALDRICH Chemistry. It is expected that the quality of the MoS_2 obtained from mineral residues will be comparable with commercial MoS_2 and thus, demonstrate that nanomaterials can be obtained economically and taking advantage of mineral resources, favoring the industry, and thereby generating new ways of obtaining novel nanomaterials.

Keywords
2D materials, MoS2, liquid phase exfoliation.

Reference

J. Wu, J. Feng, B. Yang et al. The anisotropic adsorption of potassium cetyl phosphate on molybdenite surface and its implication for improving the flotation of molybdenite fines. Journal of Molecular Liquids 378 (2023) 121616.

This work was supported by

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[NSN-237] STUDY OF InAs QDs SEMICONDUCTOR DEVICES IN ASYMMETRIC (Al)GaAs MATRICES FROM THE MANIPULATION OF GROWTH PARAMETERS IN THE PROCESS BY MBE

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Semiconductor quantum dots (QDs) possess interesting physical and optical properties that have allowed for the design of the so-called next-generation semiconductor devices, and also have released new research areas like quantum photonics, spintronics, quantum computing, quantum communication, among others. For some of these applications the vertical stacking of QDs layers is necessary and thus several interrelated effects like the adatoms diffusion, segregation, intermixing of the alloys and stress effects are required to be accounted. In this work, we present a study of the elastic and electronic properties of self-assembled InAs QDs embedded within AlGaAs alloys with different Al content (%Al), leading to asymmetrical potential barriers. The changes of the %Al in the QDs layers conduced to several variations in the island's distribution, their geometry, size and density. The effects of the strain fields distribution around the QDs as well as in the nucleation zones were studied, which gave us information about the vertical correlation probability. As expected, the electronic structure of the multistacked QDs heterostructures were modified. Besides of the self-assembly process, the covering of QDs leads to additional variations on the QDs size and geometry depending on %Al. The intermixing and strain change the overall aspect of the QDs. Therefore, we studied the biaxial strain and electronic structure for different models, such as pyramidal, dome tip, and truncated pyramidal. It was found that compressive strain in the center of truncated pyramids increases up to 20% compared to the other geometries of QDs, pulling out the electronic confinement states [1]. We studied the vertical correlation probability and found that it doesn't depend solely of the spacer layer, but the strain fields surrounding the particular tip shape of the QDs [1].

Keywords

Asymmetrical matrixes, Quantum dots, biaxial strain (εxx).

Reference

J. P. Olvera Enríquez, et al. Band structure and strain distribution of InAs quantum dots encapsulated in (Al)GaAs asymmetric matrixes. J. Vac. Sci. Technol. A 41 (2023) 042714. https://doi.org/10.1116/6.0002674

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[NSN-291] MODELING OF AN SPR BIOSENSOR BASED ON 2D MATERIALS FOR SENSING DIFFERENT GLUCOSE CONCENTRATIONS

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Modern life demands the development of high technology aimed at providing human beings with devices that allow them to improve their quality of life through real-time information that allows them to make decisions in their daily lives, as well as in industrial life. A technology that allows us to achieve this is based on sensors of different types and uses, such as chemical, mechanical, pressure, acoustic and optical, among others. Surface plasmon resonance (SPR) sensors have been used for the detection of a wide range of compounds, from ions, proteins, viruses, and even small molecules; this allows them to be applied in environmental monitoring, water quality analysis, food quality, industrial safety, clinical diagnosis, etc. With the synthesis of graphene, and a wide range of 2D (atomic order thickness) materials, which have extraordinary optical properties, it has been possible to improve the quality of traditional SPR sensors. In this project, we seek to improve the performance parameters of SPR sensors applied to the detection of different glucose concentrations. These parameters quantify the quality of the sensor, its feasibility, and its detection capability. The SPR sensors to be analyzed are prism-coupled sensors in Kretschmann configuration, formed by different heterostructures based on 2D materials, metals and dielectrics. Among the 2D materials to be considered are graphene, transition metal dichalcogenides, black phosphorene, MXenes, among others. The study is performed by attenuated total reflection (ATR), calculated through the transfer matrix method. The theoretical results we have obtained improve the sensitivity by 30% and the quality factor and detection accuracy by approximately 40%.

Keywords
2D materials, SPR biosensor, glucose concentrations.

Reference

Lei, Z. L., & Guo, B. (2022). 2D Material-Based Optical Biosensor: Status and Prospect. In Advanced Science (Vol. 9, Issue 4). John Wiley and Sons Inc. https://doi.org/10.1002/advs.202102924.

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[NSN-343] EFFECT OF DRY OXIDATION ON THE OPTICAL RESPONSE AND MORPHOLOGY OF FIBONACCI STRUCTURES WITH ASYMMETRIC MIRRORS

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In this study, we designed and produced Fibonacci structures positioned between two asymmetric mirrors utilizing porous silicon and porous Si-SiO_2. These structures were crafted via electrochemical etching on p-type silicon wafers with (100) orientation, possessing resistivity values of 0.01-0.02 and 0.001-0.005. Subsequently, a two-stage dry oxidation process was employed, creating porous Si-SiO_2 structures exhibiting two defect modes within the visible spectrum.Upon undergoing dry oxidation, we observed that the defect modes of porous silicon structures produced on silicon wafers with 0.001-0.005 resistivity experienced a wavelength shift towards the lower end compared to those produced on silicon wafers with 0.01-0.02 resistivity. However, the two defect modes present in porous Si-SiO_2 structures originating from silicon wafers with 0.001-0.005 resistivity displayed reduced visibility compared to their counterparts in porous Si-SO_2 structures with 0.01-0.02 resistivity. Scanning Electron Microscopy (SEM), analysis revealed that porous Si-SiO_2 structures formed on silicon wafers with 0.001-0.005 resistivity exhibited a spherical shape with surface porosity, whereas those generated on silicon wafers with 0.01-0.02 resistivity displayed a flat surface with porosity. Notably, both types of structures maintained their porous characteristics even after undergoing the dry oxidation process.The optical characterization of Fibonacci structures with asymmetric mirrors was performed using UV-VIS-NIR techniques. Additionally, morphological and structural insights were obtained using a JOEL FE-SEM JSM-7800.

Keywords
Fibonacci structures, Dry oxidation, Morphology, asymmetric mirrors.

Reference

Vivanco MRJ, Becerra RH, Solano MT, Misaghian K, Lugo J. Optical and Structural Study of a Fibonacci Structure Manufactured by Porous Silicon and Porous SiO2. International Conference on Trends in Electronics and Health Informatics: Springer; 2022. p. 311-20.

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[NSN-345] INFLUENCE OF As CONTENT ON STRUCTURAL AND SURFACE PROPERTIES OF InGaAsSb EPILAYERS

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This study explores the impact of varying As content on the structural and surface characteristics of InxGa1-xAsySb1-y films grown using liquid phase epitaxy on GaSb (100) substrates. The films maintained a constant of x=0.145 while altering the As content. X-ray ωθ-2θ scans were employed to visualize the crystalline quality and lattice parameter of the quaternary epilayer, revealing a decrease in lattice parameter as As content increased. Strain analysis at the In10.145Ga0.855AsySb1-y/GaSb interface provided a comprehensive insight into lateral strain in relation to As content. Quaternary alloys with y<0.126 exhibited a positive lattice mismatch, leading to compressive strain, uniform and homogeneous epilayer formation, and high quality due to supercooling-mediated avoidance of substrate dissolution. Conversely, exceeding y = 0.126 resulted in a negative lattice mismatch, inducing tensile stress and the emergence of structural defects like 3D step-like corrugations on the surface. Photoluminescence spectra revealed a bound exciton transition in InxGa1-xAsySb1-y films, with an additional peak in samples under tensile strain attributed to native defect centers. This investigation deepens our understanding of how As content influences the crystalline and surface attributes of quaternary alloys, thereby expanding their potential for innovative optoelectronic applications.

Keywords
III-V semiconductors, InGaAsSb, Crystalline, Epilayer.

Reference

González-Morales, M. A., Cruz-Bueno, J. J., Villa-Martínez, G., Ramírez-López, M., Flores-Ramírez, D., Rodríguez-Fragoso, P., ... & Mendoza-Álvarez, J. G. (2022). Importance of liquid phase epitaxy on achieving near-lattice-matched growth of In0. 145Ga0. 855As0. 132Sb0. 868 layers on GaSb (100) substrates. SuperficiesyVacío, 35.

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[NSN-351] SYNTHESIS OF NANOSTRUCTURES FROM ELECTRONIC WASTE

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Electronic waste (e-waste) is produced from the electronic devices that are discarted every day, and e-waste generation has increased considerably in the last decades becoming a serious problem of global dimensions. Therefore, finding a strategy that helps solving that problem is fundamental for the sake of society, and the goal of this job is to contribute on dealing with the waste by transforming it into useful materials. Which can be achieved by extracting valuable resources from the e-waste to then, turn those resources into materials with unique properties that can be used for interesting applications. In this work, we synthesized gold nanoparticles from RAM memories that were extracted from old computers. To extract the gold from the RAM memories we used a process known as lixiviation, that consists in digesting the gold contained into the printed circuits with aqua regia. Later, the obtained liquor is diluted at a rate of 1 to 10 in deionized water and mixed with a concentrated dilution of NaOH in deionized water (~ 10 M). This gives as result gold nanoparticles with the shape of clusters of about 40 nm.

Keywords
e-waste, AuNPs, nanoclusters, aqua regia, NaOH.

Reference

[1]. Josias do Rocio Vitor do Nascimento, Karen Wohnrath , and Jarem Raul Garcia.
Synthesis of Gold Nanoparticles Using Recovered Gold from Electronic Waste
Orbital: Electron. J. Chem. 2021, 13(2), 153-159

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[NSN-359] ELECTROCHEMICAL SYNTHESIS OF GRAPHITE NANOPARTICLES AND ITS RELATIONSHIP WITH QUANTUM CONFINEMENT

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Graphite nanoparticles (GNs) are materials of reduced dimension in 0D and their optical properties until today have been poorly understood for their use in coupling applications. There are some characteristic optical phenomena of CDs, such as up conversion photoluminescence (UCPL) and excitation photoluminescence (PLE). The PLE shows some characteristics of the material, showing in the spectra a displacement to the infrared or as well called red shift accompanied by a decrease in the intensity of photoluminescence, giving two main reasons for the origin of PL:

1. PL related to carbon nucleus.

2. PL related to functional groups that surround the nanoparticle.

In this speaking audience, the obtaining of carbon dots(CDs) synthesized through a top-down process, defragmenting the graphite extracted from a pencil by an electrochemical synthesis method with current densities ranging from 10 to 200 mA/cm2, will be shown. obtaining a difference of the carbon core and associating its forbidden band depending on the size.

Keywords
Carbon dots, electrochemical, photoluminiscence, carbon nucleus, functional groups.

Reference

Li, H., et al., Water-soluble fluorescent carbon quantum dots and photocatalyst design. Angew Chem Int Ed Engl, 2010. 49(26): p. 4430-4.

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[NSN-361] MANIPULATION OF ELECTRONIC PROPERTIES IN GaN BILAYERS WITH TWO STACKING CONFIGURATIONS VIA EXTERNAL ELECTRIC FIELD

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The materials composed of two-dimensional (2D) gallium nitride (GaN) have been studied due to their promising optoelectronic properties, chemical stability, and mechanical strength, which are attractive for many technological applications, in particular for optoelectronic devices, photonics, sensors, and lightning. It has also been shown that the optoelectronic properties of 2D GaN can be modulated with changes in its configurations, such as different stacking, doping, the presence of electric and magnetic fields, and so on. In this work, using first-principles calculations based on density functional theory (DFT), we report the electronic properties for two different stacking of GaN Bilayers, with AA and AB configurations, in the presence of an external electric field, by considering two exchange-correlation functionals, PBE and GLLB-SC. We investigated and reported the evolution of band structure and the bandgap energy for the two stacking in the presence of an external electric field, and we can conclude that is possible to modulate the bandgap energy, depending on the electric field intensity, around 0.20 eV for the AA configuration and 0.60 eV for the AB configuration.

Keywords
Gallium Nitride, Bilayer, Density functional theory, Electric Field, AA, AB.

Reference

S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov. Electric Field Effect in Atomically Thin Carbon Films. Science, 306(5696):666–669, 2004.

[NSN-8] FABRICATION OF A ZnO NANOSTRUCTURES-BASED MIS DIODE THROUGH CHEMICAL ROUTES

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Because its physical properties, ZnO is considered a potential semiconductor compound for fabricating electronic and optoelectronic functional devices. In this regard, several growth techniques have been developed in order to meet the requirements of commercial devices based in this material. On the pathway for improving the performance of the current devices, low-dimensional ZnO structures seem 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 (Al2O3/Al). While the semiconductor layer was obtained through a low-temperature hydrothermal route, the insulator-metal interface was fabricated by anodizing the surface of an aluminum foil (previously electropolished). Finally, the MIS structure was annealed at 300 °C in order to ensure solid-contact at the interfaces. The obtained MIS architecture was characterized by scanning electron microscopy/focus ion beam (SEM/FIB), energy dispersive spectroscopy X-ray (EDS), x-ray diffraction (XRD), micro-Raman spectroscopy (μRS), cathodoluminescence (CL) and electrical measurements (I-V, C-V). The formation of a sandwich-like structure was confirmed by SEM/FIB techniques. The EDS analysis suggests formation of three different phases: ZnO, Al2O3 and Al phase; the XRD results confirms the latter. It is shown that the obtained semiconductor layer is constituted by interconnected leaf-like ZnO nanostructures with average thickness of ~ 50-100 nm. According with the Raman spectrum, these ZnO nanostructures are crystalline, although native defects are present as the broad visible-band centered at 533 nm in CL spectrum reveals. Finally, the characteristic response of a metal-oxide-semiconductor junction is observed in the acquired I-V and C-V curves, demonstrating that it is possible to fabricate a ZnO nanostructures-based MIS diode using chemical routes.

Keywords
MIS diode, ZnO nanostructures, Chemical synthesis routes

Reference

W. Li, F. Reisdorffer, T.P. Nguyen, and H.L. Kwok, Structural, electrical, and optical properties of p-type ZnO thin films with Ag dopant, Sci. Mater. Electron. 24, (2013), 3788-3792.

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[NSN-26] SURFACE MORPHOLOGY OF AMORPHOUS SiO2 SUBSTRATES IMPLANTED WITH 1.8 MeV Au ION

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Although ion implantation was known primarily for the fabrication of semiconductors, this technique can be used for surface texturization with applications in nanofluidics, tissue bioengineering and the fabrication of more efficient solar cells. In ion implantation, high-energy incident ions (200 keV-several MeV) penetrate substrates to depths of a few micrometers and surface modification occurs primarily by energy deposition of the implanted ion, instead than surface erosion (sputtering) observed at lower energies (0.1-200 keV), where the atoms near the surface are ejected directly by collisions with the incident ions. Currently, there are few studies of surface nanopatterning induced by ion beam irradiation where the implantation process dominates over direct surface erosion. In this work, the surface morphology of amorphous SiO_2 substrates implanted with 1.8 MeV Au ions at an incidence angle of 45^o is studied. The topography surface evolution was observed with optical microscopy, scanning electron microscopy (SEM) and atomic force microscopy (AFM). Elemental surface composition was measured by SEM-EDS and AFM-Raman. At the first stages, faint wavy patterns and isolated micrometer wave packed formations or bug-like structures (BLS) are observed. Recently, these BLS have captured attention because their formation is not predicted by theoretical models for surface growth. As the ion fluences increase, the wavy background amplitudes become greater and surround the BLS to be progressively hidden by the ripple structure. The SEM-EDS and AFM-Raman studies showed that Au ions were preferentially implanted at the beam exposed slopes of BLS. For the highest fluences applied the formation of nonlinear patterns is observed. Quantitative analysis of the surface roughness, as well as the BLS density and size distribution, was performed. An estimate for the contribution of possible pattern formation effects, as sputtering, mass transport and implanted ions is made.

Keywords
ion implantation,surface modification, surface morphology evolution, surface nanopatterning.
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[NSN-30] SURFACE PLASMON RESONANCE BIOSENSOR BASED ON GRAPHENE-METAL-GRAPHENE STRUCTURES: RECURRENCE RELATION THEORY

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The last years, graphene has opened exciting new fields in graphene plasmonics, due to the graphene´s unique optoelectronic properties such as long-lived collective excitation, extreme optical confinement in graphene plasmonics and extraordinary light-matter interactions in metamaterials. Therefore, these excellent properties make graphene a favorable candidate for novel plasmonic devices and potential applications in photonics, optoelectronics and sensor technologies. In this work, theoretical investigations are carried out to in Graphene-Metal-Graphene structure for enhanced surface plasmon resonance sensitivity based on the recurrence relations' method. We find that the graphene-metal-graphene structure supports both high-energy optical plasmon oscillations and out-of-phase low energy acoustic charge density excitations. Since a high performance of surface plasmon resonance biosensor should exhibit a large depth of dip (small reflectivity), the minimum of reflectivity in the hybrid structure can be manipulated dynamically by changing the thickness of the metallic film, the number of the graphene layers and the dielectric proprieties of the surrounding dielectric materials, which is an efficient method to realize highly sensitive biosensor devices.

Keywords
Graphene plasmonics, plasmons, reflectance.

Reference

G. González de la Cruz, Revista Mexicana de Física (2023), Surface Plasmon based on Graphene-Metal-Graphene structures: Recurrence Relation Theory, 69 0316031-6.

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[NSN-36] ZINC OXIDE ELECTROSPUN NANOFIBERS: ADVANCEMENTS IN PHOTOVOLTAIC DEVICE APPLICATIONS

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Zinc oxide (ZnO) electrospun nanofibers have gained significant attention in recent years for their potential application in photovoltaic devices. ZnO is an important material due to its unique properties, including wide bandgap, high electron mobility, and excellent optical transparency. These characteristics make ZnO an ideal candidate for various optoelectronic applications, particularly in solar cells.

Keywords
Zinc oxide, electrospun nanofibers, photovoltaic devices, energy conversion.

Reference

Mohtaram, F., Borhani, S., Ahmadpour, M., Fojan, P., Behjat, A., Rubahn, H. G., & Madsen, M. (2020). Electrospun ZnO nanofiber interlayers for enhanced performance of organic photovoltaic devices. Solar Energy, 197(December 2019), 311–316. https://doi.org/10.1016/j.solener.2019.12.079.

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[NSN-46] STUDY DFT OF ELECTRONIC STRUCTURE AND OPTICAL PROPERTIES FOR 2D GaAs WITH AMPHOTERIC Si, Ge, AND Sn DOPANTS

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In the last two decades, there has been a significant surge in activity within the field of two-dimensional systems. While the theoretical existence of these systems was first proposed by P.R. Wallace in 1947 (1), it was the groundbreaking experiments conducted by Andre Geim and Konstantin Novoselov in 2004, where they mechanically exfoliated graphene, that earned them the Nobel Prize in 2010 (2). This discovery had a profound impact on both theoretical and experimental investigations into other two-dimensional materials, such as silicene, borophene, arsenene, and phosphorene.
In this study, our focus is on the imaginary part of the dielectric function and absorption coefficient in a 2D GaAs system, considering both pristine and amphoteric substitutional impurities. These impurities, namely silicon (Si), tin (Sn), and germanium (Ge), can function as either n-type or p-type impurities, depending on the atom being substituted. Our findings reveal that the introduction of n-type (or p-type) impurities, specifically Si and Ge atoms, leads to the emergence of energy levels near the conduction band (or valence band). However, such energy levels do not appear in the case of Sn atoms. Moreover, we observed that the energy level for n-type impurities is situated at the Fermi level, while the energy level for p-type impurities is in close proximity to the valence band maximum.
Additionally, we examined the impact of these impurities on the absorption coefficient of the system. Our results indicate a slight modification in the visible region of the electromagnetic spectrum due to the presence of impurities. These findings provide valuable insights for future studies and applications of 2D systems.

Keywords
2D GaAs system, impurity, absorption coefficient, silicon, tin, germanium.

Reference

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This work was supported by

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[NSN-64] WATER TREATMENT SUPERVISION TROUGH THERMAL WAVE RESONANT CAVITY, AN EFFICIENT TOOL TO EVALUATE PHOTOCATALYTIC ACTIVITY

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Being water the most appreciated liquid due to its importance to life, depolluting is mandatory. Nowadays wastewater treatments face many challenges, including high cost, high energy demand, and the generation of secondary pollution during the treatment process. Such problems have focused the scientific community on the implementation of innovative oxidation processes; photocatalytic degradation has resulted to be a more sustainable and efficient alternative. In this research, TWRC (thermal-wave resonant cavity) analytical technique was used to evaluate the photocatalytic activity of AgTiO2 y Ag2CrO4 in the degradation process of chemical dyes methylene blue and rhodamine 6G. The nanoparticles were synthesized to evaluate their activity against the dyes when irradiated by sunlight. The degradation process was also followed by UV-Vis Spectroscopy, Transmission Electron Microscopy (TEM) was used to elucidate its morphology, X-ray Diffraction (XRD) was used to determine its crystalline nature and X-ray photon spectroscopy (XPS) were used to determine its chemical composition. It was demonstrated that tracking thermal conductivity and optical absorption are reliable and unexpensive techniques to monitor the conversion degree of the process. The synthesized catalytic materials presented similar kinetic behavior when irradiated with sun light to degrade methylene blue and rhodamine 6G.

Keywords
water treatment, photocatalytic activity, TWRC, chemical dyes.

Reference

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[NSN-76] EVALUATION OF SIO2-TIO2 COATING FOR WATER-REPELLENT COTTON TEXTILE

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Self-cleaning surfaces have garnered significant interest for their properties to repel dirt, water, and other contaminants, reducing maintenance and enhancing durability. A key attribute to create them is hydrophobicity, that enables water to form droplets and roll off the surface, carrying away any contaminant. This investigation evaluates cotton textiles coated with SiO_2-TiO_2 composite synthesized by sol-gel method coupled with sonochemistry. The composite exhibits synergy of these two properties, aiming to achieve enhanced hydrophobicity, durability, and self-cleaning properties. The SiO_2-TiO_2 coating was applied to samples of cotton fabric through spray method, employing two concentrations; 100% composite (SP100) and diluted 1:1 with ethanol (SP1-1). FTIR-ATR analysis successfully characterized the chemical composition of the coating's functional groups and surface curing process through cross-linking The hydrophobicity evaluation was carried out with determination of contact angle (CA), demonstrating a difference, the SP100 method exhibited a CA of 147° before AATCC 61 accelerated washing norm, which decreased to 137°. On the other hand, the SP1-1 method exhibits a CA of 151° with a slight reduction of CA of 144°. In the AATCC 22: 'Water repellency: Spray test' norm, water repellency for 30 seconds, was assessed on the samples. SP100 sample achieved a repellency rating of ISO 3 indicating partial repellency, while SP1-1 exhibited complete wetting ISO 5. Regarding the chemical resistance evaluation, SP1-1 sample demonstrated qualitatively better resistance to corrosion effects avoiding spreading and maintained higher contact angles for longer periods compared to SP100 sample. Spray methods were determined to be effective improving hydrophobic characteristics, and each concentration offers advantages.

Keywords
Silicon dioxide, Titanium dioxide, Sonochemistry, Hydrophobic, Intelligent textiles.

Reference

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[NSN-78] SYNTHESIS AND CHARACTERIZATION OF SILVER NANOPARTICLES FOR THEIR APPLICATION AS A FUNGICIDE

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Metrics based on process mass intensity have significant advantages, and it is the starting point to measure the ecological impact of an experimental methodology. Our interest is to improve the historical Faradaic method for noble metal nanoparticle synthesis, particularly silver, with the aim of sonochemistry, and using sodium citrate as a reductant agent. Also, we look for an agricultural application against crop fungus with the silver nanoparticles synthesized. The importance of the reagents concentration ratio, metallic precursor, and reductant agent has been analyzed. To achieve silver nanoparticles (AgNPs) synthesis we used high-power ultrasonic energy, replacing conventional stirring and heating of the reagents in aqueous solution. Reagents used were silver nitrate ($AgNO_3$ ACS reagent, ≥99.0%, Merck), trisodium citrate dihydrate ($C_6H_5Na_3O_7 \cdot 2H_2O$, ≥99%, Merck), and deionized water (18MΩ, ≤4.3 μS/cm, Millipore). Ultrasonic Homogenizer 300VT BioLogics, Inc. was used with titanium sonotrode (diameter = 9.5 mm, length = 108 mm). An aqueous solution of $AgNO_3$ (0.25 mM), and a solution of sodium citrate (SC) and ascorbic acid (AA) were prepared. The working power was 90 W. The 10 ml solution containing the silver ions and the buffer solution was exposed to ultrasonic radiation for 5 minutes. It is important to mention that for two samples, only one of the reductant agents was used. The representative curves obtained by UV-Vis characterization facilitate us determine the optimal concentration of the reagents in the AgNPs synthesis to size and shape control. Sample with the 1:1 molar concentration ratios of SC and AA (1mM each reductant agent), showed an absorbance curve with two characteristic peaks of surface plasmon resonance.

Keywords
silver nanoparticles, sonochemistry, green chemistry, agronanotechnology, optical properties.

Reference

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[NSN-94] ELECTROMAGNETIC WAVE PROPAGATION IN 1D DIELECTRIC-GRAPHENE PHOTONIC CRYSTALS OF BI-PERIODIC UNIT CELL

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In this work, an analytical deduction of the structure of photonic bands, the dispersion relation, as well as the macroscopic spectra of transmission and reflection for a one-dimensional dielectric-graphene photonic crystal of a bi-periodic unit cell in the chemical potential is made. The unit cell consists of two graphene sheets separated by an isotropic dielectric medium, where the chemical potential for the first graphene sheet is μa and for the second sheet is μb. The analytic equations to photonic bands, the dispersion relation, and the transmission and reflection spectra of incident electromagnetic waves are deduced by using the transfer matrix formalism; In addition, the optical conductivity of graphene is implemented taking into account both intra and interband contributions. We found that this bi-periodic photonic structure of chemical potential shows the formation of new photonic gaps in comparison with the conventional one-dimensional graphene dielectric photonic crystal, moreover, these non-propagation regions can be seen directly from the transmission and reflection spectra that are calculated from the expressions that are found. Finally, we showed that the new photonic gaps formed can modulate their thickness in frequency through the values of the chemical potential in the graphene sheets of the unit cell.

Keywords
Potonic crystal, Unit cell, Photonic Bands, Transmission, Reflection

Reference

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[NSN-98] SYNTHESIS OF SI NANOPARTICLES BY LASER ABLATION OF BULK SI IN HYDROGEN PEROXIDE SOLUTIONS

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Silicon is one of the most important elements for scietific and technological research due to its semiconductor properties and its abundance in Earth's crust. For bulk silicon, optoelectronic properties are non-existent, but by reducing its size to nanometric scales, properties like photoluminecense arise. In the present work, it is shown the synthesis of silicon nanoparticles in a colloidal form making use of *Laser Ablation of Solids in Liquids* (LAL). With the objective of producing an oxidation layer in the particles surfaces, laser ablation was performed in different liquid media, those being oxigen peroxide, distilled water, and a mixture between the two (1:1 in volume). For characterization of particle structure, XRD was used; UV-vis for the BandGap value; and Raman Spectroscopy for size determination based on different mathematical models. After analyzing the data from Raman modes, particle sizes of around 3.4, 3.5 and 2.8 nm were found, depending on the solution in which ablation of silicon was held.

Keywords
Silicon, Ablation, Nanoparticles, Oxidation, Raman.

Reference

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[NSN-114] Au AND Ag NANOSTRUCTURES OBTAINED BY GALVANIC DISPLACEMENT IN LOC DEVICES FOR DYNAMIC SURFACE MODIFICATION

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Microfluidics is a growing and promising technology with wide range of applications. Microfluidic systems offer advantages in nanostructures generation, particles separation, mixers and reactors. Currently, digital light synthesis (DLS) is a fastest way to 3D print microfluidic devices with micron-scale features. In this context, 3D printed microfluidic channels can by use as chemical microreactors for shape-controlled nanoparticles formation. In this study, we describe the design and fabrication of three proof-of-concept valves (fish valve) able to reduce tetrachloroauric Acid (H[AuCl4]) and silver nitrate (AgNO3) onto different 0D, 1D, 2D nanostructures. The fish valve inner surface and channel features were design and modify to achieve different microfluidic characteristics on a same experiment. The quantity and size of microstructures (scales) inside the channels were vary in three groups with the aim of obtain and optimize process parameters. The inner walls of the microchannels were coated with a 100-400 nm thick Cu thin layer by high vacuum thermal evaporation. A solutions of 2 mM H[AuCl4] and AgNO3 were prepared and individually pushed through the fish valves at 10 µL per minute. The dynamic galvanic displacement reaction that occurs between Cu with H[AuCl4] and AgNO3 respectively, generates nanoparticles, nanowires and nanoflakes decorating the Cu surface. The flow parameters and concentration gradient were studied using COMSOL software simulations in order to find and relate the determining flow parameters linked to the formation of nanostructures. This process represents a novel method to tune the production of SERS surfaces and nanostructures for different applications with no need of electrochemical reactions.

Keywords
Microfluidics, nanostructures, galvanic displacement, dynamic surfaces modification.
Reference
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[NSN-160] PHYSICOCHEMICAL PROPERTIES OF ZnTiO3/BiOCl NANOPARTICLES AND THEIR PHOTOCATALYTIC APPLICATION

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Environmental pollution due to the indiscriminate use of hydrocarbons has caused a great impact on the quality of natural resources. For this reason, there is an intense motivation to find materials that can replace the heavy dependence on hydrocarbons. Heterogeneous photocatalysis is an alternative for wastewater treatment and sustainable energy generation. Some materials such as binary oxides (TiO2, and ZnO) have been extensively studied. However, despite the great advantages that these materials present, there are still drawbacks to overcome, such as the high recombination of charge carriers, photochemical stability, and useful life. Therefore, alternative materials have been explored to contribute to the development of nanomaterials with photocatalytic applications. The development of heterojunctions emerges as an alternative to mitigate the high recombination of charge carriers and increase the photocatalytic activity. In this work, ZnTiO3/BiOCl nanoparticles were synthesized using the molten salt (ZnTiO3) and impregnation (BiOCl) methods to form the ZnTiO3/BiOCl heterojunction. The structural, optical, morphological, chemical, and superficial properties of the ZnTiO3/BiOCl nanoparticles allowed to correlate the physicochemical properties with their photocatalytic activity for the production of hydrogen and photodegradation of RhB.

Keywords
photocatalysis, water splitting, ZnTiO3/BiOCl

Reference

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[NSN-198] EFFICIENT PHOTOCATALYTIC HETEROJUNCTION OF La2Ti2O7@BiOBr DECORATED WITH METALLIC NPs FOR RhB DEGRADATION BY VISIBLE LIGHT

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The textile industry consumes large amounts of water in different stages of the process, such as dyeing and washing, releasing significant volumes of water with dyes and their respective additives. These dyes are highly resistant to conventional water remediation processes, and their presence in water bodies hinders their use in other industries, such as agriculture, due to their bioaccumulation and high toxicity. Therefore, it is crucial to effectively remove dyes from wastewater by coupling conventional processes with new Advanced Oxidation Processes (AOPs) such as ozonolysis, radiolysis, and heterogeneous photocatalysis.
In recent years, research has focused on the development of heterojunctions using photocatalytic semiconductors with low band energy, visible/solar light activation, and low recombination rate. In this study, a novel Z-scheme heterojunction was developed, employing two-dimensional (2D) layered semiconductors La2Ti2O7@BiOBr, synthesized through a two-stage hydrothermal method. To observe the effect of ohmic contact in the 1:2 heterojunction, it was decorated using the photo-deposition technique with noble metals such as gold (Au) and silver (Ag), initially depositing La2Ti2O7 followed by the growth of BiOBr. These decorations improved the photocatalytic response in the degradation of the dye rhodamine-B (RhB) under visible light irradiation by 51.43% and 42.82%, respectively, with degradation constants of τ=4.79±0.93 min and τ=5.64±0.76 min for the heterojunction decorated with silver (Ag) and gold (Au) nanoparticles, respectively. Characterization techniques such as X-ray diffraction (XRD), transmission electron microscopy (TEM), Raman spectroscopy, Fourier-transform infrared spectroscopy, and diffuse reflectance spectroscopy were employed to confirm the formation of the junction, crystallinity, morphology, and characteristic bands of the La2Ti2O7@M@BiOBr heterojunction (where M=Au, Ag).
The significant improvement in photocatalytic activity by introducing metallic nanoparticles between the two layered semiconductors suggests a Z-scheme charge transfer mechanism that exhibits much higher photocatalytic activity than its individual components.

Keywords
La2Ti2O7@BiOBr, green-synthesis, heterojunctions, 2D nanomaterial, noble metals, photocatalysis, visible light.

Reference

Meng, F. et al. Visible light photocatalytic activity of nitrogen-doped La2Ti2O7 nanosheets originating from band gap narrowing. Nano Res 5, 213–221 (2012).

This work was supported by
CONAHCYT

[NSN-204] PHOTOCATALYTIC ACTIVITY OF HETEROUNIONS ZnO@BiOX (X=Cl. Br, I), AS PHOTOCATALYST ACTIVED WITH VISIBLE LIGHT

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

Keywords
ZnO, BiOX, photocatalysis, rhodamine-B, visible light.

Reference

L. Lin, et al., Fabrication of a three-dimensional BiOBr/BiOI photocatalyst with enhanced visible light photocatalytic performance, Ceramics International (2014), http://dx.doi.org/10.1016/j.ceramint.2014.03.039.

This work was supported by

Apoyos CONACyT 2023

[NSN-210] PROCESSING OF DIRECT COATED ZINC FERRITE (ZnXFe3-XO4) NANOPARTICLES WITH NATURAL EXTRACTS: CLOVE (SYZYGIUM AROMATICUM), STAR ANISE(ILLICIUM VERUM) AND MEXICAN OREGANO (LIPPIA GRAVEOLENS)

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The functionalization of addressable superparamagnetic nanoparticles (SPIONs) have allowed the promising development of drug delivery, diagnosis and hyperthermia cancer treatment. Zinc ferrite ($ZnFe_2O_4$) is a spinel ferrite with inverse spinel structure, Sizes below 20 nm have improved their magnetic and optical properties, which depend on $Zn_xFe_{3-x}O_4$ stoichiometry control [1]. Currently, functionalization with polyphenols of natural extracts has allowed the coating and linking of -OH over Zn_x $Fe_{3-x}O_4$ surfaces as core-shell nanoparticles. This kind of SPIONs can be stimulated from magnetic field AC and controlled by their addressable magnetic domains. This produce a local energy change and nanoparticles heating to generate local hyperthermia. In this work, Zn_x $Fe_{3-x}O_4$ nanoparticles were obtained by coprecipitation route with (a) clove (*Syzygium aromaticum*), (b) Star Anise (*Illicium verum*) and (c) Mexican Oregano (*Lippia graveolens*). The saturation pH and temperature conditions were the key to obtain SPIONs with particles sizes of (a) 13.89 nm, (b) 14.15 nm (c) 13.17 nm, respectively. Their properties were analyzed by X ray diffraction (XRD), Fourier- transform infrared spectroscopy (FTIR), energy dispersive spectroscopy (EDS), X-ray photoelectron spectroscopy (XPS) and Vibrating-sample magnetometer (VSM-SQUID). The results showed the inverse spinel structure, phenol contribution and superparamagnetic behavior. The perspective are to analyze their properties and hyperthermia responses.

Keywords
SPIONS, zinc ferrite, polyphenols, hyperthermia.

Reference

[1] M. Bohra, V. Alman and R. Arras, Nanostructured ZnFe2O4: An Exotic Energy Material. Nanomaterials 11(2021) 1286. https://doi.org/10.3390/nano11051286.

This work was supported by
Cathedra Marcos Moshinsky 2018 and CONAHCYT through PhD fellowship for Nidia Esther Moreno Cabrera. Thanks to the technical support of Eng. Marcela Guerrero (XRD, FTIR) and Dr. Marlene Gonzalez Montiel (VSM-SQUID).

[NSN-224] Bi2O3/BiOX MULTIFUNCTIONAL HETEROJUNCTIONS FOR THE DEGRADATION OF POLLUTANTS IN WATER

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Bi_2O_3 nanoparticles were synthesized by a solvothermal method and subsequently modified by a simple in situ method with halogen salts in order to obtain Bi_2O_3/BiOX heterojunctions (X= F, Cl, Br, I). The formation of the heterojunctions was confirmed by different characterization techniques such as transmission and scanning electron microscopies; X-ray diffraction; N_2 physisorption; Fourier infrarred, Raman and UV-Vis spectroscopies. These heterojunctions were evaluated for the adsorption of methylene blue and the photocatalytic degradation of caffeine in aqueous solutions. The heterojunction with the best performance in both processes was Bi_2O_3/BiOBr achieving 98% of methylene blue adsorption in 50 minutes and a 81% of caffeine photodegradation in UV-light in 5 hours. In order to improve the photocatalytic properties of this heterojunction, silver was added by a deposition-precipitation method. The Ag/Bi_2O_3/BiOBr material achieved 92% of caffeine photodegradation in UV-light in 5 hours and demonstrated to be active also when irradiated with visible light. The catalytic properties of the Ag/Bi_2O_3/BiOBr material for the reduction of nitroaromatic compounds were also evaluated. Therefore, the multifunctionality of the Bi_2O_3/BiOX heterojunctions was demonstrated by the removal and degradation of different types of pollutants by different processes.

Keywords
bismuth, heterojunctions, adsorption, photocatalysis, catalysis.

Reference

Gómez-Velázquez, L. S. (2018). The bismuth oxyhalide family: thin film synthesis and periodic properties. https://doi.org/10.1039/C8DT02642D

Ruiz-Castillo, A. L. (2022). Photocatalytic activity of Bi2O3/BiOCl heterojunctions under uv and visible light illumination for degradation of caffeine. DOI:10.1007/s11244-022-01644-z.

This work was supported by

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[NSN-236] STRAIN AND SHAPE CONNECTION IN QUANTUM DOTS SELF-ASSEMBLING

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Nanotechnology is currently one of the milestones of the frontier science and has represented a radical change in the mankind lifeway from everyday aspects to a complete revolution in the industry., Self-assembly of quantum dots (QDs) represents one of the most challenging and promising achievements in nanotechnology because these nanostructures possess outstanding optical and electronic properties that differ from larger particles. For example, semiconductor QDs give rise to the development of more efficient solar cells and optoelectronic devices and are the building blocks of new research areas like quantum photonics and quantum computing. QDs can be self-assembled with molecular beam epitaxy (MBE) which grants for high precision and control in the ordered growth of monocrystalline layers. In this work, in-situ analysis is performed during the QDs self-assembling that takes place during the growth of lattice mismatched semiconductors like InAs and GaAs. The mismatch strain is the driving force for the formation of 3D nano-islands or QDs, and so we proposed to modify the strain in order to study the related changes in QDs morphology during the self-assembling. The QDs usually assume the rhombic pyramidal geometry whose facets are crystallographic planes accounted by the reflection high-energy electron diffraction technique (RHEED). The (002) RHEED chevron spot analysis shown that the QD facets undergoes through the family planes {531}, {631} and {731} during self-assembling [1]. Throughout simulations with experimental inputs like the QDs volume and angle between facet it was possible to determine the internal strain and the surrounding strain of the islands. The results indicated that at the initial stages of self-assembling the facets are determined by the adatoms diffusion instead of local elastic interactions, while for bigger islands the ultimate geometry of the QDs results from the overall strain distribution.

Keywords
Quantum dots, self assembly, strain, InAs, nano-islands.

Reference

M. I. Favila Castañeda. Geometría y Relajación de Puntos Cuánticos de InAs/GaAs modulados por tensión. Tesis licenciatura, Benemérita Universidad Autónoma de Zacatecas (2020).

This work was supported by
This work was supported by: The Laboratorio Nacional de Análisis Físicos, Químicos y Biológicos/UASLP, CONAHCYT CF-2023-I-1300, COPOCyT Fideicomiso 23871, and Investigadoras e Investigadores por Mexico.

[NSN-244] SYNTHESIS AND CHARACTERIZATION OF Ti-Ce NANOALLOYS BY HYDROTHERMAL METHOD WITH DIFFERENT BASES FOR POTENTIAL CATALYTIC APPLICATIONS (PHOTOCATALYSIS, LITHIUM ION BATTERY AND/OR HYDROGEN GENERATION)

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The present work consists of the synthesis and characterization of titanium and cerium nanoalloys using the hydrothermal method with different alkaline bases (NaOH and KOH). The main objective is to synthesize the Ti-Ce nanoalloys and characterize the samples using analytical techniques to determine their crystalline structure, morphology, particle size and chemical composition, such as X-ray diffraction (XRD) via Rietveld Refinement, Raman spectroscopy, ultraviolet visible spectroscopy diffuse reflectance (UV-Vis) using Kubelka Munk method to determine band gap, transmission electron microscopy (TEM) and high resolution transmission electron microscopy (HRTEM) and energy dispersive elemental mapping (STEM-EDS). Some of this properties were compared to DFT simulations results. The properties of these materials show promising catalytic applications, such as photocatalysis, battery electrochemistry, and hydrogen generation.

Keywords
Alloys, Nanocompounds, Hydrothermal, Simulation, XRD.

Reference

Hernández-Arteaga, J. G. R., et al (2022). Thermal tuning of the morphology of hydrothermally synthesized CeO2 nanotubes for photocatalytic applications. In Ceramics International (Vol. 48, Issue 12, pp. 17802–17815). Elsevier BV. https://doi.org/10.1016/j.ceramint.2022.03.051.

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[NSN-276] PREPARATION OF NANOTEXTILES CONTAINING SILVER NANOPARTICLES WITH ANTIBACTERIAL ACTIVITY

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The preparation of functional cotton textiles using different concentrations the silver nanoparticles is presented in this work. The Synthesis of nanoparticles was performed by the in-situ method on the surface of cotton textiles through the pre-activation with potassium hydroxide and silver nitrate (0.02, 0.015, 0.01, 0.005 and 0.0025M). The metal reduction was carried successfully using the borohydride of sodium at room temperature. Surface energy on cotton fabric were modified using hexadecyltrimethoxysilane. Textiles with properties, superhydrophobic, antibacterial and UV protection were obtained. The results of the characterization of the samples using techniques SEM, EDS, transmittance spectroscopy and contact angle measurement are presented in this research. The results showed that modified cotton has potent antibacterial activity against Staphylococcus epidermidis bacteria. The modification of the surface composition of the textile was carried out successfully. Blocking ultraviolet light was measured by transmittance data in280-400 nm and shown ultraviolet protection factor taller than pristine cotton, also it exhibits a static water contact angle > 150° for a 5 µl droplet.

Keywords
Nanotextile, Nanoparticles, Cotton.

Reference

E. Pakdel, J. Sharp, S. Kashi, W. Bai, M. P. Gashti, y X. Wang, Antibacterial superhydrophobic cotton fabric with photothermal, self-cleaning, and ultraviolet protection functionalities, ACS Appl. Mater. Interfaces 15, 28, (2023) 34031–34043. https://doi.org/10.1021/acsami.3c04598.

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[NSN-286] RAMAN IN SITU STUDY OF TIO2-CEO2 NANOCUBE NANOALLOYS SUBJECTED TO HIGH TEMPERATURE AND THEIR PHOTOCATALYTIC APPLICATION

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Nanotechnology has garnered significant attention due to the unique properties of materials at the nanometric scale. Metal oxide nanoparticles, such as TiO_2 and CeO_2, have attracted particular interest in the field of chemical materials, as their properties make them ideal for a broad range of applications in areas such as medicine, information technology, catalysis, energy storage, and sensing. Researchers have therefore focused on developing synthetic pathways to create such nanostructures. Temperature analysis have been shown to improve properties and help find an optimal application of these materials. In this study, $Na_{0.5}Ce_{0.5}TiO_3$ nanocubes were hydrothermally synthesized and characterized by Transmission electron microscopy (TEM), Raman spectroscopy, X-Ray diffraction (XRD), UV-vis diffuse reflectance, spectroscopy and Brunauer-Emmett-Teller (BET) analysis. Additionally, we used in situ Raman spectroscopy to investigate the structural and optical properties of the nanocubes at high temperature. Finally, we compared the effect of temperature on these materials to optimize their application in solar photocatalysis, where the results showed that these nanoalloys perform better in solar photocatalysis than pristine Ti and Ce materials.

Keywords
Nanocubes, Na0.5Ce0.5TiO3, Hydrothermal synthesis,Raman in situ, photocatalysis.

Reference

J.G.R. Hernández-Arteaga, et al. Thermal tuning of the morphology of hydrothermally synthesized CeO2 nanotubes for photocatalytic applications, Ceramics International, Volume 48, Issue 12, 2022, 17802-17815.

This work was supported by
CONAHCYT

[NSN-302] INDIUM CONCENTRATION IN CUBIC InxGa1-xN/GaN QUANTUM WELLS BY XPS AND ANALYSIS OF OPTICAL PROPERTIES

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The growth of $In_xGa_{1-x}N$/GaN quantum wells in the cubic phase is a promising alternative in applications such as light-emitting diodes.it benefits from a reduced bandgap and is free of the strong polarization fields [1]. We report the growth of $In_xGa_{1-x}N$/GaN quantum wells (QWs) in cubic phase by conventional Molecular Beam Epitaxy on GaAs (001) substrate. These nanostructures are 10 nm and 30 nm thick for the GaN wells and barriers respectively. The concentration of Indium in each well was determined by X-ray photoelectron spectrometry (XPS) and through mathematical calculations (matricial method). The analysis of the optical properties of these nanostructures allowed us to study the excitonic transitions in the visible spectrum range from 495 to 570 nm by photoacoustics and photoluminescence This work can contribute to LED technology in green color of the visible spectrum.

Keywords
$In_xGa_{1-x}N$/GaN quantum wells, cubic phase.

Reference

[1] D. J. Binks, P. Dawson, R. A. Oliver, and D. J. Wallis, Cubic GaN and InGaN/GaN quantum Wells, Appl. Phys. Rev., 9, 041309 (2022). doi: 10.1063/5.0097558.

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CONACYT

[NSN-346] HEAVY SI DOPING IN n-GaN/AlN/Si (111) HETEROSTRUCTURES GROWNBY MOLECULAR BEAM EPITAXY

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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. In this work n-GaN/ AlN heterostructures on Si (1 1 1) substrates were grown by molecular beam epitaxy, the GaN films were n-type doped with silicon at different doping concentrations. We found that Si doping promotes a reduction of dislocation density [1] as revealed by x-ray data analysis and transmission electron microscopy. Furthermore, a decrease in the yellow band measured by photoluminescence spectroscopy was observed when silicon doping concentration was increased up to 1.7 × 1019 atoms cm−3. Electrical properties were obtained by Hall effect and Current vs Voltage measurements, the change in mobility is discussed in terms of doping density.

Keywords
GaN, AlN, Si, Heteroepitaxy, Heterostructures.

Reference

[1] Sánchez A M, and et al. 2000 Si doping effect on the defect structure in GaN/AlN/Si(111) heteroepitaxial systems Bol. Soc. Esp. Cerám. Vidrio 39 468–71.

This work was supported by
Conahcyt

[NSN-356] MODULATING THE SCHOTTKY BARRIER IN Au/MoO_3 HETEROJUNCTION WITH Au NANOPARTICLES

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This work aims to study the Au nanoparticle size dependance in the schottky barrier height of the Au/MoO3 heterojunction. Schottky contact is formed by a semiconductor substrate and a metalic coating; substrate is made of α-MoO3 nanorods synthesized by thermal oxidation at 500 °C, and the metalic coating was made of Au nanoparticles dispersed on substrates surface via DC-Sputtering. In order to vary the nanoparticle size, sputtered samples were subjected to a calcination process at different temperatures. Characterizations were made to the substrate and to the calcinated samples, such as XRD and SEM in order to study the samples phase, morphology and composition of the samples at all its stages. To inquire the Schottky barrier height, it is used XPS analysis, as result, different nanoparticle sizes were obtained with the proposed range of calcination temperatures, as well as diferent heights of the barrier.

Keywords
Nanostructures, Schottky Barrier, Heterostructures, XPS, Sputtering.

Reference

E. F. Vázquez Vázquez, H. Rojas Chávez, Y. M. Hernández Rodríguez, J. Morales Bautista and O. E. Cigarroa Mayorga, The role of AuNPs on the photocatalytic degradation enhancement in MoO3-based heterostructures, Materials Letters 290 (2021) 129464.https://doi.org/10.1016/j.matlet.2021.129464.

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Consejo Nacional de Humanidades, Ciencias y Tecnologías (CONAHCyT).
Intituto Politécnico Nacional (IPN).

[NSN-360] SYNTHESIS OF MOLYBDENUM DISULFIDE THROUGH THERMOCOLLOIDAL METHOD

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Two-dimensional Molybdenum disulfide, MoS_2, has been extensively studied and synthetized by different methods, including chemical vapor deposition, laser ablation, microwave synthesis, and mechanical exfoliation; however, most of these methods need specialized equipment to carry out the preparation of materials. In this work, MoS_2 was synthesized by a thermocolloidal method using MoO_3 and elemental sulphur as raw materials, and oleylamine and oleic acid as solvents. During the synthesis process, oleylamine and oleic acid were respectively taken at different volume ratios, i.e., 100:0, 75:25, 50:50, 0:75, and 0:100, and as a result different morphologies were obtained. As confirmed by XRD, XPS, Raman spectroscopy, SEM, and TEM, the semiconducting 2H-MoS_2 phase was mainly obtained for the 75:25 and 50:50 ratios. In particular, the sample fabricated at a ratio of 50:50 showed an exceptional result, as it was formed by four layers.

Keywords
Thermocolloidal synthesis, MoS2, Raman, XPS, oleylamine.

Reference

A. Castellanos-Gomez, M. Barkelid, A. M. Goossens, V. E. Calado, H. S. J. Van der Zant, G. A. Steele, Nano Lett. 2012, 12, 3187-3192.

This work was supported by

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Sesión Oral

[NSN-320] EXOTIC PHENOMENA IN PHOSPHORENE JUNCTIONS

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The quantum relativistic nature of the charge carries in graphene characterize by pseudospin, chirality and Berry phase gives rise to several exotic phenomena such as Klein tunneling, anti-Klein tunneling, electronic cloaking and Fano resonances to mention a few. In the case of phosphorene, the charge carriers are regarded as Dirac electrons in the armchair direction due to a linear term in the dispersion relation and as Schrödinger electrons in the zigzag direction due to the parabolic dispersion relation. These assumptions are not at all valid because phosphorene is a 2D material with a special pseudospin texture [1]. Here, we show that this special pseudospin texture gives rise to various exotic phenomena in phosphorene junctions along the zigzag direction. In particular, electronic cloaking, persistent electronic cloaking and Fano resonances. In the armchair direction, perfect transmission at normal incidence or Klein tunneling takes place by closing the phosphorene's band gap. The characteristics of these exotic phenomena on the transport properties are discussed and analyzed.

Keywords
Fano-resonances, phosphorene-junctions, pseudospin-texture, electronic-cloaking, Klein-tunneling.

Reference

[1] Jung, S.W., Ryu, S.H., Shin, W.J. et al. Black phosphorus as a bipolar pseudospin semiconductor. Nat. Mater. 19, 277–281 (2020). https://doi.org/10.1038/s41563-019-0590-2.

[NSN-255] Ag/TiO2 NANOPARTICLES SYNTHESIZED FROM SILVER SALT REDUCTION BY MEANS OF LASER ABLATION OF SOLID Ti IMMERSED IN AQUEOUS SILVER NITRATE SOLUTIONS

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Green synthesis of silver nanoparticles by reducing salts needs the use of reducing agents such as different kind of teas, or leaves, among others. Sometimes the reducing process is assisted by ultraviolet or microwave radiation, which energy, is high enough to induce accelerated reduction or smaller nanoparticles or even different morphologies. Irradiating with high power lasers is not common due to the fact that the increase in temperature is highly localized in small volumes for focused beams which ends up in low salt contents exposed and thus, low nanoparticle production rates. On the other hand, if the laser beam is not focused, the energy is not high enough to produce the salt reduction.

In the present work, irradiation of metallic Ti foils immersed in aqueous silver nitrate solutions with nanosecond pulses of a high power laser resulted in the reduction of the nitrate, and thus in the fabrication of silver nanoparticles. This reduction process was produced at the liquid-metal interface due to the laser heating. Additionally, Ti nanoparticles were ejected from the metallic surface into the solution and subsequently they were oxidized to form TiO2 nanoparticles together with Ag nanoparticles. Irradiation times were 20, 40, 60 and 80 seconds. It was demonstrated that even 20 s of irradiation was enough time to produce highly brown colored suspensions, indicating high concentrations of Ag nanoparticles. A Ti foil was irradiated in bidistilled water in order to corroborate the presence of TiO2 nanoparticles. Samples were optically characterized by UV-Vis spectroscopy, from which the surface plasmon resonance of silver was observed together with the band edge transition for TiO2, which confirmed the presence of Ag/TiO2 nanoparticles. Methylene blue solutions containing nanoparticles were irradiated with UV light to see the photocatalytic effect of the nanoaprticles.

Keywords

Silver nanoparticles, Laser ablation, Silver nitrate.

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[NSN-52] PHOTOELECTROCATALYTIC ACTIVITY OF SILICON NANOWIRES DECORATED WITH ELECTROLESS COPPER NANOPARTICLES, GRAPHENE OXIDE, AND g-C3N4 USING PLASMA JET FOR REMOVAL OF METHYL ORANGE UNDER VISIBLE LIGHT

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Silicon nanowires (SiNWs) have been studied due to their interesting properties, such as light trapping and catalytic activity for removing organic molecules. In this work, silicon nanowires are decorated with copper (SiNWs-CuNPs), graphene oxide (SiNWs-GO), and both copper and graphene oxide GO (SiNWs-CuNPs-GO). They were prepared and tested as photoelectrocatalyst to remove the azoic dye methyl orange (MO). The silicon nanowires were synthesized by the MACE process using HF/AgNO3 solution. The decoration with copper nanoparticles was made by galvanic displacement reaction utilizing a copper sulfate/HF solution, while decoration with GO was achieved using an atmospheric pressure plasma jet system (APPJ). The as-produced nanostructures were then characterized by SEM, XRD, XPS, and Raman spectroscopy. Cu(I) oxide was generated during the decoration with copper. Cu(II) oxide was produced when SiNWs-CuNPs were exposed to the APPJ. GO and g-C3N4 were successfully attached on the surface of silicon nanowires and silicon nanowires decorated with copper nanoparticles. The photoelectrocatalytic activity of silicon nanostructures was tested under visible light, leading to the MO removal efficiency of 96% within 175 min with SiNWs-CuNPs-GO, followed by SiNWs-CuNPs, SiNWs-GO, undecorated SiNWs, and bulk silicon.

Keywords
Graphene oxide, Silicon nanowires, g-C3N4, APPJ, CuO2, photocatalysis, photoelectrocatalysis, electrochemistry.

Reference

C. Hernández Rodríguez, J. J. Pérez Bueno, A. X. Maldonado Pérez, M. Ruiz Flores, G. Oza, Photoelectrocatalytic activity of silicon nanowires decorated with electroless copper nanoparticles and graphene oxide using a plasma jet, RSC Advances 13 (2023) 10621–10635. https://doi.org/10.1039/D3RA00932G.

This work was supported by

This work was funded by CONACYT through grant No. 320114 and CF-19/2096029; the National Laboratory of Graphene Materials and the LANIAUTO; “Fondo Sectorial CONACYT-SENER Sustentabilidad Energética” grant 207450, CEMIE-Sol project P62, The World Bank - SENER 002/2017-PRODETES-PLATA.

[NSN-275] SURFACE ENHANCED RAMAN SPECTROSCOPY OF METHYLENE BLUE DEPOSITED ON AG NANOSTRUCTURED SUBSTRATES PREPARED BY PULSED LASER DEPOSITION

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Pulsed laser deposition has proven to be a suitable technique to fabricate nanostructures of noble metals with different sizes and morphologies on glass substrates. Generally, this is done by varying the number of laser pulses impinging on the target. However, it is well known that the produced plasma plume has an inhomogeneous angular distribution and the quantity/density of material deposited on the substrate is higher in the center than in the periphery. Actually, a noble metal (silver in the present case, gold or copper) density gradient starting with a continuous region in its center and progressively evolving to complicate nanostructures and finally to nano-spherical particles is obtained. Taking advantage of this morphological variation, drops of highly diluted methylene blue were deposited radially. Furthermore, TEM grids were placed in the same way. This technique gives the possibility of directly correlate the SERS signal, the underlying noble metal morphology and the optical absorption in very similar regions. In the present work we develop this method and discuss the obtained results.

Keywords
SERS, Raman spectroscopy, Ablation laser, nanostructure Ag, Au.

Reference

A. Szaniawska and A. Kudelski, Applications of Surface-Enhanced Raman Scattering in Biochemical and Medical Analysis, Front. Chem. 9 (2021) 664134. Volume 9 - 2021 https://doi.org/10.3389/fchem.2021.664134.

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[NSN-47] RECYCLED POLYSTYRENE WITH GRAPHENE MATERIALS AS COATINGS FOR THE PROTECTION OF METAL ART PIECES

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Human-generated contaminants are a major threat to several materials. The effect of these compounds on metal parts has been studied for many years, since corrosion is an important issue in our country due to the many pieces with cultural value that are found throughout Mexico, either remembering important moments in our history or as artistic expression purposes. Coatings can be used as chemical barriers to protect this type of parts, most of them derived from methacrylate that use toxic solvents for health and are not usually very efficient in the long term. Nanomaterials such as graphene can modify the physicochemical properties of materials, thus giving very interesting applications. In this work recycled polymer is functionalized with a few layers graphene (FLG) and graphene oxide (GO) and proved as coating to protect metal pieces. The recycling of plastic waste is an alternative to reduce pollution, due to the large amount of plastic waste that is produced. An example, thousands of tons of polystyrene are generated per year creating substantial amounts of garbage since this plastic generates many empty spaces, its composition is 98% air and 2% polymer, Although the production od plastics does not represent a major problem, because the do not degrade in their environment, their elimination does, since it is cumulative. During this work, the problems of corrosion in metal pieces caused bye corrosives contaminants and plastic recycling are considered, a polystyrene coating functionalized with graphene materials is synthetized and characterized by Raman spectroscopy and contact angle. Afterwards, the functionalized polymer was used as protecting coating of pieces of bronze and iron, common materials of metal art pieces. Finally, improvements in the properties of polymer after its functionalization with graphene were observed, such as, enhanced adherence to surfaces and a better protection of metal in corrosive environments.

Keywords
graphene, coating, polystyrene.

Reference

Cui, G., Zhang, C., Hann, K., Zhou, X., Xing, X., Liu, J., Li, Z., Chen, Q., & Lu, Q. (2021). Research progress on self-healing polymer/graphene anticorrosion coatings. Progress in Organic Coatings, 155, 106231. https://doi.org/10.1016/j.porgcoat.2021.106231.

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[NSN-319] ELECTRONIC STRUCTURE FOR SPHERICAL AND ELLIPSOIDAL MULTI-SHELL GaAs/AlXGa1−XAs QUANTUM DOTS AS A FUNCTION OF ELECTRIC AND MAGNETIC FIELDS

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Electronic and optical properties of quantum dots have been a topic of great interest the basic physics point of view, but they also hold great possibilities for application in optoelectronic devices. Quantum dots are systems that has been experimentally synthesized by chemical and physical methods. The shapes of these quantum dots cover pyramidal-shaped quantum dots, quantum rings, or spherical ones, and recently, the multi-shell configurations. Among the large number of possible quantum dot heterostructures, we are interested in III-V ones, in this case, GaAs/AlxGa1−xAs/Al0.3Ga0.7As core/shell/shell quantum dots. Here, we theoretically report, by working in the effective mass approximation, the energy levels, and the corresponding wave functions as a function of electric and magnetic fields, as well as a function of geometrical parameters. We discuss that the main finding is that the structural parameters give us the possibility to propose an initial optimized core/shell/shell quantum dot structure that be tuned by electric and magnetic fields, with electrical properties for potential intraband transitions in the terahertz range of the electromagnetic spectrum.

Keywords
Semiconductors, Optoelectronic properties, Quantum dots.
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[NSN-225] FABRICATION OF ZEOLITE/POLYMERS NANOFIBERS PHOTOCATALYSTS

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One of the significant global issues facing our planet is water pollution, primarily caused by the release of harmful substances like oils, dyes, and heavy metals due to human activities. In this study, waste materials from polyethylene terephthalate (PET) and polystyrene (PS) bottles were used to fabricate nanocomposites of Zeolite/PET-fibers and Zeolite/PS-fibers, by the electrospinning technique. Conditions for electrospinning were employed, such as 12 kV voltage, 1 mL/h flow rate, and 10 cm distance between the collector and needle, with 1% and 2% of zeolite content. The objective was to evaluate the photocatalytic efficiency of these nanocomposites in degrading methylene blue, a commonly used dye. SEM, FTIR, UV-Vis, and contact angle measurements were conducted to examine the morphological, structural, and photocatalytic properties influenced by the polymers. The results of this study demonstrated the photocatalytic efficiency of methylene blue within 120 minutes, achieving an 80% degradation with the Zeolite/PET nanocomposite, which is highly applicable for the removal of organic contaminants in water treatment and environmental protection.

Keywords
Nanofiber, electrospinning, polyethylene-tereftalate, polystyrene, zeolite, photocatalysis.

Reference

González-Crisostomo, J.C.; López-Juárez, R.; Yocupicio-Gaxiola, R.I.; Villanueva, E.; Zavala-Flores, E.; Petranovskii, V. Chabazite Synthesis and Its Exchange with Ti, Zn, Cu, Ag and Au for Efficient Photocatalytic Degradation of Methylene Blue Dye. Int. J. Mol. Sci. 2022, 23, 1730. https://doi.org/10.3390/ijms23031730.

This work was supported by

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[NSN-22] ADSORPTION AND PHOTOCATALYTIC CHARACTERISTICS OF CO-FE MIXED OXIDE NANOPARTICLES SYNTHESIZED BY THE PECHINI-TYPE SOL-GEL METHOD

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This work studies the effect of crystal structure, morphology, and optical properties of Co-Fe mixed oxide nanoparticles (NPs) on the photocatalytic degradation and adsorption characteristics of methylene blue (MB). The Co-Fe mixed oxide NPs were synthesized by the Pechini-type sol-gel method using a molar ratio of 1:2 Co:Fe and sintered at 500 °C for 2 h. Adsorption and photocatalytic degradation were performed for aqueous MB solutions with 5, 3, and 1 mg/L concentrations, using 0.0025 g of Co-Fe mixed oxide NPs as a photocatalyst. FT-IR study evidenced the chelation reaction between citric acid and metal ions, the esterification reaction between citric acid and ethylene glycol, and the identification of Fe-O and Co-O bonds. X-ray diffraction (XRD) revealed that the NPs had a mix of Co_3O_4, α-Fe_2O_3, and $CoFe_2O_4$ phases, with the $CoFe_2O_4$ phase having a 60 nm crystallite size. Raman spectroscopy confirmed the phase combination observed in XRD. The morphological analysis revealed that the NPs presented spherical, disk, and octahedral morphologies corresponding to the Co_3O_4, α-Fe_2O_3, and $CoFe_2O_4$ phases. The values for the optical bandgap were 3.5 eV for $CoFe_2O_4$ and 2.86 eV for α-Fe_2O_3. The adsorption mechanism was attributed to the formation of MB monolayers on the Co-Fe mixed oxide NPs, according to the linear fit of the adsorption isotherms of the Langmuir model. The maximum adsorption capacity (q_m) and Langmuir constant (K_L) were 12.05 (mg/g) and 52.22 (L/mg), while the separation factor (*RL*) was more significant than zero, demonstrating that the adsorption was favorable. The % degradation of MB in 120 min and the kinetic constants *k* were 88.59, 83.58, 54.09 % and 0.0155, 0.0134, and 0.0053 min^{-1} for MB concentration of 1, 3, and 5 mg/L, respectively. The possible degradation mechanism was related to the heterojunction of the semiconductors Co_3O_4, α-Fe_2O_3, and $CoFe_2O_4$.

Keywords
Nanoparticles, Pechini, Bandgap, Photocatalysis, Adsorption, Phase

Reference

L.E. Caldeira, W.C. Guaglianoni, J. Venturini, S. Arcaro, C.P. Bergmann, S.R. Bragança, Sintering-dependent mechanical and magnetic properties of spinel cobalt ferrite (CoFe2O4) ceramics prepared via sol-gel synthesis, Ceram Int. 46 (2020) 2465–2472. https://doi.org/10.1016/j.ceramint.2019.09.240.

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[NSN-184] ELECTRONIC AND STRUCTURE PROPERTIES OF HYDROGEN ADSORPTION ON γ-GRAPHYNE AND γ-BNyne

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The study of two-dimensional materials expands the spectrum of properties with great potential in technological applications, that one-dimensional materials like carbon nanotubes and boron-nitrogen nanotubes have been presenting. The recent report on the synthesis of γ-graphyne (Hu et al., 2022) has sparked scientific interest in describing the properties that this material and its analog (γ-BNyne) may exhibit under different physical and chemical conditions. In this study, the effect of hydrogen molecule (adsorption on the γ-BNyne surface is presented for the first time and compared with the properties reported for γ-graphyne, this through first-principles calculations using Density Functional Theory (DFT) including DFT-D3 Grimme's correction. The results showed that the preferred site for adsorption on γ-graphyne is within the hexagon formed by the 6 atoms, in contrast to the γ-BNyne system, where adsorption was found to be more favorable within the hexagon of 12 atoms. The hydrogen bonding mechanisms were investigated by analyzing the partial density of states (PDOS) showing that the pz orbitals of the most stable atoms on the hexagon surface in each case, interacting with the *s* orbitals of , have an important contribution to the physisorption mechanism. The results presented here showed that adsorption on these two-dimensional surfaces does not significantly alter their pristine structural and electronic properties, demonstrating their stability under molecular hydrogen storage conditions. This work contributes to the promotion of these two-dimensional materials as potential candidates for technological applications such as nanosensors, nanomedicine, and hydrogen storage, among others.

Keywords
γ-Graphyne, γ-BNyne, adsorption, DFT, hydrogen storage.

Reference

Hu, Y., Wu, C., Pan, Q. et al. Synthesis of γ-graphyne using dynamic covalent chemistry. Nat. Synth 1, 449–454 (2022). https://doi.org/10.1038/s44160-022-00068-7.

This work was supported by

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[NSN-115] SYNTHESIS OF CARBONO QUANTUM DOTS WITH DIFFERENT EMISSION SPECTRA FROM CITRIC ACID FOR ITS APPLICATION AS BIOLOGICAL MARKERS

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The discovery of quantum dots (QDs) also known as nano-crystals or artificial atoms. aroused the interest of scientists for the creation of new carbon-based optoelectronic materials because they present very good optical and electronic properties and are friendly to the environment, unlike traditional inorganic semiconductors such as quantum dots that contain toxic ions heavy metals (eg, Cd, Pb, among others). The advantage of carbon quantum dots is their simple production ("green synthesis") from low-cost, earth-abundant elements (eg, carbon, nitrogen, oxygen, etc.), environmentally friendly precursors. the environment, good biocompatibility and high photo stability. The present work presents the synthesis of carbon quantum dots (CQDs) from the constant temperature calcination of Citric Acid (AC) using L-Cysteine (CYS) and Diethanolamine (DEA) as nitrogen and sulfur carrier molecules to obtain of functionalized CQDs. Different concentrations of reagents and calcination times are evaluated. The CQDs obtained are analyzed by ultraviolet-visible absorption spectroscopy (UV-VIS), transmission electron microscopy (TEM), infrared spectroscopy (IR) and X-ray emitted photoelectron spectroscopy (XPS). Finally, the optical properties of the CQDs are evaluated through their excitation and emission spectrum. Different optical properties are obtained by varying the synthesis parameters of the CQDs. Due to the functionalization of CQDs with nitrogen and sulfur groups that can interact with cell membrane proteins. It is hoped that these can be used as biological markers in specific cell lines.

Keywords
Carbon quantum dots (CQDs), Calcination, optical properties.

Reference

(Krysmann et al., 2012)Krysmann, M. J., Kelarakis, A., Dallas, P., & Giannelis, E. P. (2012). Formation mechanism of carbogenic nanoparticles with dual photoluminescence emission. Journal of the American Chemical Society, 134(2), 747–750. https://doi.org/10.1021/ja204661r

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[NSN-156] DEGRADATION ANALYSIS OF TRIPLE-CATION PEROVSKITE SOLAR CELLS BY ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY

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In this work, the electrical properties of different triple-cation compositions with the formula Cs0.05FA1−XMAXPb-(I1−XBrX)3 have been analyzed. The perovskite solar cells were subjected to ambient conditions to compare their results in terms of ambient degradation. Their morphology, optical properties, and photovoltaic performance were characterized. We analyzed the causes and effects of ambient degradation mechanisms on the devices. The MA percentage decrease in the composition of triple cation perovskites, APbX3 produces an improvement in the stability and durability of perovskite solar cells. This enhancement is due to the reduction of the amount of ion vacancies helping to reduce the degradation in the device by avoiding the accumulation of defects.

Keywords
Perovskite, Solar Cells, Degradation

Reference

Torres, J., Zarazua, I., Esparza, D., Rivas Martínez, J. M., Saliba, M., Mora-Sero, I., ... & Abate, A. (2022). Degradation Analysis of Triple-Cation Perovskite Solar Cells by Electrochemical Impedance Spectroscopy.

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[NSN-277] SYNTHESIS OF 2D NANOSHEETS OF La2Ti2O2 AND ITS MODIFICATIONS WITH Ce FOR SUBSEQUENT STUDY OF THERMAL-STRUCTURAL PROPERTIES USING RAMAN SPECTROSCOPY IN SITU RAISING TEMPERATURE

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Among the families of layered perovskites, the Brandon-Megaw family with the formula $A_2B_2O_{(3n+2)}$ can be found. One of these materials, $La_2Ti_2O_7$, has garnered attention due to its high-temperature ferroelectric property (1700 K) and photocatalytic activity. In this study, the investigation of the solid solution $La_2Ti_2O_7$ (LTO), $La_{62/32}Ce_{2/32}Ti_2O_7$ (LCTO1/32), and $La_{30/16}Ce_{2/16}Ti_2O_7$ (LCTO1/16) was carried out to observe the changes in the opto-structural properties caused by the substitution of La^{3+} with Ce^{3+}. The synthesis of the layered perovskites was performed through a hydrothermal process and subsequently characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD), diffuse reflectance spectroscopy (DRS), and in situ Raman spectroscopy with increasing temperature. The TEM results revealed that the morphology consisted of layers with average dimensions of 300×800 nm and a thickness below 100 nm. Through Rietveld refinement of the XRD data, it was determined that the composition of the samples was over 95% in the monoclinic phase with $P2_1$ space group. In DRS, it was observed that the cerium-doped samples exhibited absorption in the visible and ultraviolet regions, while only the LTO sample showed absorption in the ultraviolet region. Changes in Raman shift and broadening with respect to temperature were identified in all three samples. These changes were associated with the following phases: (i) coexistence between the monoclinic and incommensurate phases, (ii) incommensurate phase, and (iii) orthorhombic phase. The temperature at which these changes began was 700 °C, 500 °C, and 200 °C for LTO, LCTO1/32, and LCTO1/16, respectively. The incorporation of Ce^{3+} ions into a stable phase of high purity was successfully achieved. Its effect on phase transitions was observed, and due to its dimensions, the materials can be classified as 2D nanomaterials.

Keywords

Lanthanum titanate, Raman in situ, hidrotermal, layered, substitution.

Reference

Ojeda-Galván, H. J., Rodríguez-Aranda, M. del C., Rodríguez, Á. G., Alanis, J., Íñiguez, J., Mendoza, M. E., & Navarro-Contreras, H. R. (2021). Structural and Raman study of the thermoelectric solid solution Sr1.9La0.1Nb2O7. Journal of Raman Spectroscopy, 52(3), 737–749. https://doi.org/10.1002/jrs.6032.

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[NSN-34] OBTENTION OF HEXAGONAL BORON NITRIDE NANOSHEETS BY LIQUID PHASE EXFOLIATION AND THEIR USE FOR THE REMOVAL OF DYES FROM WATER

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Hexagonal boron nitride (hBN) is a layered lattice structure material that by its form of white powder also is known as “white Graphene”. It consists of boron and nitrogen atoms join to form a hexagonal structure, these atoms in a layer of hBN too alternately linked to each other by strong covalent bonds and the layers of h-BN are linked due to weak Van der Waals forces. Hexagonal boron nitride nanosheets (hBNNSs) exhibit excellent properties including high hardness, high mechanical strength, and exceptional thermal stability and have an excellent potential in fields such as catalysis, electronics, coatings, sensing, and water cleaning. In this study the obtention and characterization of hBNNSs and their application to remove different dyes (brilliant green, methylene blue, crystal violet, among others) from water are reported. The hBNNSs were obtained by liquid phase exfoliation method during 4 hours of ultrasonic treatment and using isopropyl alcohol and distillated water as dissolvents. The hBNNSs were characterized by X-ray diffraction (XRD), Raman spectroscopy, and transmission electron microscopy (TEM) and the removal of dyes was studied by ultraviolet visible spectroscopy (UV-Vis). TEM and Raman results confirmed the obtention of hBNNSs with a thickness of few layers. Whereas XRD patterns revealed the hexagonal phase of the hBN. UV-Vis spectra showed that the percentage removal of dye from aqueous phase increases with the increase of contact time between the dyes and hBNNSs. Results demonstrate the potential of hBNNSs for the efficient removal dyes from water.

Keywords
Nanosheets, boron nitride, removal, dyes.
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[NSN-9] ONE-DIMENSIONAL ZnO NANOSTRUCTURES FOR PHOTOCATALYTIC AND SENSING APPLICATIONS

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One dimensional zinc oxide nanomaterials (1DZnO) are widely studied due their tunable optical, morphological and structural properties witch make them suitable candidates for their implementation in multiple optoelectronic applications. Therefore, their synthesis through versatile and cost-effective process is a currently desired in the field of materials research science. In the present work, we synthetized 1DZnO using the Vapor-Liquid-Solid (VLS) technique on gold-coated silicon wafers. Manipulation of the growth parameters allowed the obtaining 1DZnO nanostructured coatings with different aspect ratio and surface area. Afterwards, the effect of the morphological and optical properties over the sensing performance and the photocatalytic activity of the nanostructured platforms were evaluated. The synthesized ZnO nanostructures were characterized by XRD, SEM, TEM, UV-Vis, FTIR, AFM, PL, XPS and EDS. After synthesizing and understanding these materials, different 1DZnO morphologies were evaluated as photocatalysts for hydrogen production through a photocatalytic proton reduction reaction. It was discovered that 1DZnO structures with random orientation and high aspect ratio exhibited the most stable and effective photocatalytic activity. Additionally, the CO2 gas sensing properties of the synthesized 1DZnO materials were investigated at various concentrations. The results demonstrated a strong sensing response for longer 1DZnO and a faster response time for shorter ones. Notably, these materials exhibited good selectivity towards oxidizing gases. Both applications align with the green transition agenda. Finally, by evaluating the impact of morphological and structural factors on 1DZnO biofunctionalization methodologies, an effective procedure for attaching antibodies was developed to construct an E. coli optical biosensing layer. The results showcased a successful approach to creating efficient biorecognition layers on top of 1DZnO materials without impeding optical response. Therefore, the results present study could open a gateway for the development of adaptable ZnO nanostructured materials for energy harvesting, gas sensing and biosensing applications.

Keywords
nano-ZnO, Photoluminescence, Biofuncionalization, Gas-sensing, Photocatalysis.

Reference

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[2] Int J Hydrogen Energy 2020;45:1–10. https://doi.org/10.1016/j.ijhydene.2020.08.247.
[3] Sensors Actuators B Chem 2021;337:129765. https://doi.org/10.1016/j.snb.2021.129765.

This work was supported by

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[NSN-116] FROM WASTE TO NANOMATERIALS: USE OF AGRO-INDUSTRIAL WASTES TO OBTAIN GRAPHENE OXIDE FOR CATALYTIC APPLICATIONS

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Graphene oxide (GO) is a useful and promising 2D carbon nanomaterial that contains oxygen functional groups in its basal and edge planes. These oxygen functionalities, confer GO a high hydrophilicity, this property makes GO a good candidate for many applications, such as drug delivery, treatment of harmful cells, and water purification. GO is usually obtained using Hummer's method, which consists of the chemical oxidation of graphite. However, during this synthesis method, an exorbitant volume of strong acid liquid waste is generated besides the long time needed to obtain the final product. For this reason, the use of green chemistry for the synthesis of GO aims to tackle the disadvantages of Hummer´s method and also decrease and eliminate the presence of toxic and polluting compounds during GO synthesis. In this direction, the use of agro-industrial waste as raw materials to produce high-quality nanomaterials is an eco-friendly alternative to obtain a value-added final product that can be used afterward in different applications.

In the present work, GO is produced through pyrolysis of different agro-industrial wastes, which are: peanut shells, post-use commercial, and artisanal coffee. The properties of GO obtained from agro-industrial waste are compared with the properties of GO produced by Hummer's method using different characterization techniques. Subsequently, GOs obtained from different raw materials are functionalized with magnetite by chemical coprecipitation for its application as a catalyst. The functional groups present in the obtained GO nanomaterial are used as nucleation centers for the formation of metal oxides. Therefore, a higher number of functional groups present on the GO surface will lead to the formation of metal oxide nuclei, obtaining metal oxide nanoparticles with good dispersion on GO films.

Keywords

Graphene oxide, agro-industrial wastes, nanoparticle, magnetite, nanocomposites.

Reference

Somanathan, T., Prasad, K., Ostrikov, K. K., Saravanan, A., & Krishna, V. M. (2015). Graphene oxide synthesis from agro waste. Nanomaterials, 5(2), 826–834. https://doi.org/10.3390/nano5020826

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[NSN-54] FABRICATION OF A MEMBRANE OF GO/FLG HETEROSTRUCTURES FOR THE REMOVAL AND INACTIVATION OF S. AUREUS FROM WATER

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Mexico is the second country that uses the most untreated water for irrigation. This type of water carries large amounts of pathogenic organisms, heavy metals, and residues that cause health problems. A membrane is a thin film of porous material that connects two reservoirs and allows or does not the passage of molecules, salts, metals, or particles from one reservoir to another. Thanks to their chemical and physical properties, membranes based on nanomaterials have emerged as important candidates to remove salts, metals, microorganisms, and other residues from water. For this reason, this project proposes the fabrication of membranes based on heterostructures of graphene and graphene oxide for the treatment of water contaminated with microorganisms. Graphene and graphene oxide were synthesized and characterized by different microscopy techniques. Membranes with different concentrations of graphene and graphene oxide were manufactured by vacuum filtration and evaluated in assays to remove strains of Staphylococcus aureus from water. In this work, it was observed that the formation of heterostructures of graphene and graphene oxide leads to significant retention and inactivation of microorganisms in the membranes and that in this way these pathogens can be removed from the water.

Keywords
Heterostructures, Membranes, 2D materials, Water.

Reference

R. Kanchanapally, B. P. V. Nellore, S. S. Sinha, F. Pedraza, S. J. Jones, and others, Antimicrobial peptide-conjugated graphene oxide membrane for efficient removal and effective killing of multiple drug resistant bacteria, RSC Adv. 5 (2015) 18881–18887. https://doi.org/10.1039/C5RA01321F.

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[NSN-135] OBTAINING TiO2 NANOPARTICLES USING STEVIA REBAUDIANA AND ITS ANTIFUNGAL EFFECT

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The objective is to synthesize NPs of titanium dioxide (TiO2) from the extract of Stevia rabaudiana. The methodology used for the biosynthesis of nanoparticles (NP`s) through plant extracts, is facilitated by functional groups such as total phenols, flavonoids, anthocyanins, proteins; They are powerful reducing agents and are mainly responsible for the formation of metal ions to metal NPs in a one-step green pathway, they are part of the specific secondary metabolism of the plant under study (Stevia rebaudiana). For which bromatological analysis was carried out, it was carried out according to the protocols proposed by the AOAC, while the determination of the antioxidant capacity was carried out according to the consulted literature. Once the extract of stevia rebaudiana was identified, the synthesis was carried out: Stevia extract and titanium isopropoxide were used at different concentrations, once mixed with vigorous stirring, the analysis of the colloid obtained using UV-Vis spectroscopy was carried out. Subsequently, the structural and morphological analysis and X-ray diffraction were carried out, obtaining the identified TiO2 band. Once the nanoparticles were obtained, their antifungal effect was carried out for the inhibition of the Botrytis cinerea fungus.

Keywords
Nanoparticles, TiO2, antifungal.

Reference

1.- M. Atif Irshad, R. Nawaz, M. Zia ur Rehman, M. Adrees, M. Rizwan, S.,Ali, S. Ahmad, S. Tasleem, (2021). Synthesis, characterization and advanced sustainable applications of titanium dioxide nanoparticles: A review. Ecotoxicol. Environ. Saf. 212 (2021) 1-14. https://doi.org/10.1016/j.ecoenv.2021.111978.

This work was supported by
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[NSN-239] STRUCTURAL AND OPTICAL CHARACTERIZATION STUDY OF MULTISTACKED InAs/GaAs QUANTUM DOT HETEROSTRUCTURES

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The development of multistacked InAs/GaAs quantum dots (QDs) heterostructures has been a topic of great relevance in the understanding for optimal optoelectronic devices such as: third generation solar cells, light emitters devices, infrared sensors, among others [1]. This work exposes the molecular beam epitaxy (MBE) growth of five and ten periods of InAs/GaAs QDs samples. The heterostructures were analyzed using high-resolution X-ray diffraction (HRXRD), ellipsometry spectroscopy, and photoreflectance spectroscopy to investigate their structural and optical properties. The HRXRD analysis revealed well-defined peaks corresponding to the symmetric crystallographic plane (004) and compressive strain due to the InAs lattice mistmatch. The peaks positions, widths, and intensities of the diffraction peaks were extracted, providing information about the increasing microstrain effects of the heterostructures as the InAs/GaAs periods increase. The ellipsometry spectroscopy (ES) data showed the pseudo-dielectric function of the heterostructures, which allowed to determine the optical bandgaps, and excitonic transitions were better identified as the InAs QDs increase from five to ten periods. The ES provided insights into the quantum confinement effects within the presence of multistacked InAs QDs. Photoreflectance spectroscopy was employed to further probe the optical properties of the heterostructures. The photoreflectance (PR) spectra exhibited characteristic oscillatory features corresponding to the interband transitions, enabling to determine the main transition energies around 1.0 eV as the period of QDs increase. The analysis of PR spectra provided information of quantum confinement effects, the electronic structure, and optical transitions in the QDs heterostructures. This characterization study revealed interesting information about the main features and changes in the the structural and optical properties of the multistacked InAs/GaAs quantum dot heterostructures. These findings contribute to the understanding and optimization of such heterostructures for potential applications in nanotechnology and optoelectronic devices.

Keywords
InAs, quantum dots, strain, multistacking, QDs, ellipsometry spectra, photorreflectance spectra.

Reference

C.A. Mercado-Ornelas et al. Nucleation and diffusion processes during the stacking of bilayer quantum dot InAs/GaAs heterostructures. J Cryst Growth, 555 (2021) 125959. https://doi.org/10.31349/RevMexFis.68.031002.

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[NSN-159] THERMOELECTRICITY IN NANOSTRUCTURED PHOSPHORENE

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Thermoelectricity allows the conversion of heat into electrical energy, the emergence of two-dimensional materials such as phosphorene has brought new impetus to this area because thermoelectric properties are improved by reducing the dimension of the material. In this work, the effect of nanostructuring by gated junctions on the thermoelectric properties of phosphorene is analyzed. Using the hybrid matrix methodology and the Landauer-Büttiker formalism, the electronic transport and thermoelectric properties of the system are obtained. Finding that the gated phosphorene junctions produce a high anisotropy of the thermoelectric properties between the amchair and zigzag directions of the phosphorene, where the electronic conductance, the power factor and the electronic thermal conductance are better in the armchair direction, and in the opposite way the Seebeck coefficient, figure of merit and efficiency have higher values in the zigzag direction. The increase in temperature causes an improvement in the thermoelectric response.

Keywords
Thermoelectricity, phosphorene, junctions.
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I. Rodríguez-Vargas, acknowledges CONACYT-Mexico for the financial support through Grant No. A1-S-11655.

[NSN-138] SYNTHESIS AND CHARACTERIZATION OF BINARY Fe2O3@TiO2 NANOCOMPOSITE FOR PHOTOCATALYTIC DEGRADATION OF DYES IN WATER

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Dye pollution in water is a serious environmental problem due to its high production quantity in several types of industries in the world and an inefficient wastewater treatment. Several materials have been synthesized to solve this environmental issue (Fawzi Suleiman Khasawneh & Palaniandy, 2021). TiO_2 is one of the most used photocatalyst in scientific research because it is not toxic, has a low cost and excellent photoconversion; nevertheless, it uses UV light rather than visible light. In order to improve its photocatalytic characteristics TiO_2 has been combined with other semiconductors, between all of them Fe_2O_3 has presented the best synergistic characteristics. The aim of this research is to synthesize Fe_2O_3@TiO_2 core-shell nanoparticles and use them as a photocatalyst for the degradation of methylene blue. The Fe_2O_3 nanoparticle core was synthesized by the coprecipitation method from Fe3+ iron salt. The TiO_2 shell was synthesized by solvothermal method, using titanium Isopropoxide as titanium source and absolute ethanol as solvent. The Fe_2O_3@TiO_2 core-shells were characterized using SEM-EDS, XRD and FTIR spectroscopy. Photocatalytic activity of methylene blue degradation was performed under Xenon lamp irradiation at different exposure times. The efficiency of photodegradation was measured by UV-Vis spectrophotometer. The XRD result showed that Fe_2O_3 nanoparticle has a single phase. The existence of Fe_2O_3 and anatase TiO_2 phases in the XRD pattern shows that the Fe_2O_3@TiO_2 nanoparticles are successfully synthesized. Based on SEM characterization, the Fe_2O_3@TiO_2 core-shells are agglomerated.

Keywords
Iron Oxide, Titanium Oxide, Core-Shell, Photocatalyst.

Reference

Fawzi Suleiman Khasawneh, O., & Palaniandy, P. (2021). Removal of organic pollutants from water by Fe2O3/TiO2 based photocatalytic degradation: A review. Environmental Technology and Innovation, 21(xxxx), 101230. https://doi.org/10.1016/j.eti.2020.101230.

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[NSN-119] SYNTHESIS OF FE2O3 NANOPARTICLES BY LASER ABLATION IN DIFFERENT LIQUID MEDIA

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Iron-based nanostructures are currently receiving significant attention in the field of nanotechnology due to their remarkable physical and chemical properties. Iron oxides are extensively studied for their diverse range of applications, including information storage, recording, photocatalysis, and solar energy conversion. These materials exhibit excellent biocompatibility, making them highly promising for various biomedical applications, such as targeted drug delivery and contrast agents in magnetic resonance imaging. Typically, these nanoparticles are synthesized using chemical methods, including hydrothermal and solvothermal routes. Although effective in controlling particle size, these methods involve multiple complex steps for implementation, Maneeratanasarn et al. (2013). In this study, our objective was to obtain Fe2O3 nanoparticles using a physical method and compare the samples obtained in different liquid media and with varying fluencies. The Fe2O3 nanoparticles were synthesized by ablating a Fe2O3 target using a Nd-YAG laser with a wavelength of 1064 nm and 6 ns pulse duration. The target was ablated within four different liquid media (ethanol, isopropanol, acetone, and DI-water) for a duration of four minutes each, using two fluencies (1.66 and 1.41 J/cm2) for each medium. The resulting samples were characterized using transmission electron microscopy (TEM), UV-visible absorption spectroscopy, and X-ray photoelectron spectroscopy (XPS). TEM characterization revealed the successful synthesis of nanoparticles with an average size of approximately 50 nm using this method, and the presence of possible core-shell structures was also observed. UV-visible absorption spectroscopy and XPS analysis confirmed that Fe2O3 was the only iron oxide synthesized in the samples. In conclusion, laser ablation of a Fe2O3 target in different liquid media is a suitable technique for obtaining Fe2O3 nanoparticles and core-shell structures, without requiring high fluencies.

Keywords
Laser ablation, Fe2O3, fluencies, core-shell

Reference

P. Maneeratanasarn, T. Van Khai, S. Y. Kim, B. G. Choi, and K. B. Shim, Synthesis of phase-controlled iron oxide nanoparticles by pulsed laser ablation in different liquid media, Phys. Status Solidi Appl. Mater. Sci., 2013. https://doi.org/10.1002/pssa.201228427.

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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-37] INFLUENCE OF TEMPERATURE ON THE OPTICAL AND ELECTRICAL PROPERTIES OF ZnO:Al THIN FILMS

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In semiconductor materials, their properties can be manipulated or controlled through impurification with certain elements, this of course influences their electronic properties such as the width of their band gap and conductivity. A semiconductor material with insulating characteristics is ZnO, which under appropriate doping conditions can considerably increase its conductivity, maintaining its high optical transparency, which makes it very suitable for use in various applications, such as: solar cells, anti-reflective coatings and touch screens in electronic devices. 6 samples were synthesized, one of them, without Al by means of PLD technique, ablating two targets simultaneously under an oxygen atmosphere keeping the Zn plasma constant and varying the Al plasma with the support Langmuir probe. This paper presents a study on the optical and electrical properties of ZnO:Al thin films subjected to heat treatments at 170°C, 310°C and 450°C. The films were analyzed by UV-Vis spectroscopy and later the resistance of the films was measured by the four-point technique to calculate their resistivity after each treatment. The results showed that the band gap width presents a decrease from 3.48 to 3.25 eV and the resistivity reports values from 10-2 Ωm without the presence of Al to 10-6 Ωm with Al, increasing its electrical conductivity. With this we can say that the films improved their electrical properties while maintaining their optical transparency as the temperature increased.

Keywords
semiconductors, plasma parameters, bandgap, laser ablation, thin films.

Reference

J.A. Guerrero de Leon and J.G.Quinñones-Galvan,ZnO thin films grown at different plasma energies by the laser ablation of metallic Zn with a 532 wavelength, Materials Research Express 7(2020). http://doi.org/10.1088/2053-1591/ab6773.

This work was supported by

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[PLV-123] STUDY OF INSULATING MATERIALS USING THE SPARK-INDUCED BREAKDOWN SPECTROSCOPY (SIBS) TECHNIQUE

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There are well-known techniques for determining the elemental composition of materials. Among these techniques, Laser-Induced Breakdown Spectroscopy (LIBS) and Spark-Induced Breakdown Spectroscopy (SIBS) can be mentioned. Like LIBS, the main advantages of SIBS are speed of analysis, minimal sample preparation, and the potential for portability. Additionally, SIBS offers more pulse energy per unit size and is comparably cheaper than LIBS [1]. Furthermore, SIBS is commonly used on conductive materials. The proposal of this work is to expand the use of SIBS to insulating materials. This study presents the results of the characterization of insulating materials through the study of optical emission lines generated by SIBS at atmospheric pressure. The following insulators were studied: Cerium oxide (CeO2) 99.5%, Lanthanum oxide (La2O3) 99.99%, Manganese oxide (MnO2) 99.9%, Niobium oxide (Nb2O5) 99.9%, Silicon oxide (SiO2) 99.5%, Titanium oxide (TiO2) 99.9%, Tungsten oxide (WO2.9) 99.99%, and Zirconium oxide (ZrO2) 99.9%. The results of the light emission of the oxides are presented, as well as the mixtures between some of them. The study aims to discriminate the proportion of trace elements in insulating materials.

Keywords
SPARK, SIBS, LIBS, oxides, CeO2, La2O3, MnO2, Nb2O5, TiO2, ZrO2.

Reference

Iyll-Joon Doh, Carmen Gondhalekar, Valery Patsekin, Bartek Rajwa, Keegan Hernandez, Euiwon Bae, and J. Paul Robinson, " A Portable Spark-Induced Breakdown Spectroscopic (SIBS) Instrument and its Analytical Performance ", Applied Spectroscopy, 2019, Vol. 73(6) 698–708. DOI: 10.1177/0003702819844792.

This work was supported by

This work was supported by PAPIIT- IG101220, A. Garzon acknowledges her postdoctoral fellowship from DGAPA-UNAM and M Martinez would like to thank CONACYT (Mexico) for his postdoctoral fellowship.

[PLV-246] CsPbBr3 THIN-FILMS DEPOSITED BY SINGLE-SOURCE THERMAL EVAPORATION

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$CsPbBr_3$ inorganic halide perovskite thin films have been employed in different optoelectronic devices such as light-emitting diodes (LEDs) and solar cells due to their excellent electronic properties. In general, perovskite thin-films are usually made by solution processing methods, such as conventional spin coating processes, however, it is difficult to control the thickness and form a smooth surface. On the other hand, vacuum thermal evaporation methods offer high reproducibility of large area and compact films[1]. In this context, in this work, perovskite $CsPbBr_3$ thin-films were deposited by single-source thermal evaporation using $CsPbBr_3$ crystal powder as evaporation source material. Thin-films were grown by varying the vacuum pressure of 10^{-5} Torr, 10^{-6} Torr and 10^{-7} Torr and significant differences in the crystal structure of $CsPbBr_3$ thin-films fabricated at different pressures were observed. Subsequently, the thicknesses of the films were varied at 350 nm, 500 nm, 600 nm and 800 nm and they were annealed at 300 °C for 20 minutes. The effect of annealing on the structural, optical and morphological properties of $CsPbBr_3$ thin-films was studied by X-ray diffraction, absorption spectroscopy, photoluminescence and SEM respectively. Finally, our results suggest that single-source thermal evaporation is a promising method for depositing high-quality inorganic $CsPbBr_3$ perovskite thin-films for optoelectronic applications.

Keywords
CsPbBr3 perovskite, thin-films, single-source thermal evaporation, vaccum.

Reference

Ullah, S., Wang, J., Yang, P., Liu, L., Yang, S. E., Xia, T., ... & Chen, Y. (2021). All-inorganic CsPbBr3 perovskite: a promising choice for photovoltaics. Materials Advances, 2(2), 646-683.

This work was supported by

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Sesión Oral

[PLV-35] THE SURFACE TEMPERATURE OF A 2" WATER-COOLED TI TARGET DURING DC MAGNETRON SPUTTERING IN Ar AND Ar/N2 GAS MIXTURES

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The temperature of a 2" diameter water-cooled titanium target was measured from the centre to close to the target edge, using an electrically floating fine, 0.005" wire, type K chromel-alumel thermocouple. The temperature measurements were performed as a function of the DC plasma power (power densities of 1.0, 2.2 and 4.1 W/cm2) and Ar gas pressures of 10 to 60 sccm. Typically, the temperature difference between the centre of the target and inside the racetrack was more than 200 oC, the racetrack temperature increased almost linearly with the applied power to a maximum value of ~840 oC. The target temperature was also investigated as a function of the N2 gas concentration in the Ar gas mixture (1 to 10%), and these measurements are compared with the elemental composition of the deposits produced.

Keywords
DC Magnetron Sputtering, Target temperature, titanium, titanium nitride.
Reference
Volume 171, Issue 2, 15 April 1989, Pages 307-311.
This work was supported by
PAPIIT IG101123

[PLV-88] CHARACTERIZATION OF THE PLASMA RESULTING FROM THE COMBINATION OF THE LASER ABLATION OF A Mo TARGET IN A N2 MICROWAVE ECR DISCHARGE

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The use of plasmas to modify the properties of various materials is a topic of great interest to specialists. Exposing different materials to plasma their mechanical, electrical, and magnetic properties can be modified by creating new phases within them. In the present work a hybrid plasma created by combining a stationary microwave discharge of the ECR type using nitrogen as the working gas, and a plasma formed during pulsed laser ablation of a solid molybdenum (Mo) target plasma was investigated. This hybrid plasma was generated at a working pressure of 6 x 10-4 Torr. To characterize the plasma, parameters such as density, electron temperature, and average kinetic energy were determined using Langmuir probes. Additionally, the chemical species present in the plasma were analyzed through optical emission spectroscopy (OES). The results of the OES measurements showed a significant increase in excited species within the hybrid plasma compared to individual plasmas. Finally, the hybrid plasma was used to deposit thin films of molybdenum nitride (MoN), opening the possibility of obtaining materials with specific properties and applications in various fields.

Keywords
Pulsed laser ablation, microwave plasma, Pulsed laser ablation, OES, MoN.

Reference

Camps, E., Campos-González, E. & Rivera-Rodríguez, C. Characterization of the combination of microwave and laser ablation plasmas. Surf. Coatings Technol. 4 2 2, 127509 (2021). https://doi.org/10.1016/j.surfcoat.2021.127509.

This work was supported by
CONAHCYT

[PLV-266] TERNARY COMPOUND THIN FILMS PRODUCED BY A NOVEL CYLINDRICALHOT REFRACTORY ANODE VACUUM ARC SYSTEM (CHRAVA)

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

Keywords
vacuum arc, plasma characterization, thin films, mechanical properties, tribology.

Reference

[1] J. Phys. D: Appl. Phys. 28(2) (1996) 353.
[2] Surf. Coat. Technol. 133-134 (2000) 91.
[3] Sci. Rev. Instrum. 89(9) (2018) 095109.

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[PLV-96] GRAPHENE OXIDE COATINGS OBTAINED BY ATMOSPHERIC PRESSURE PLASMA JET FOR PROTECTION OF ALUMINUM

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Graphene oxide is a carbon-based material, but unlike other graphene materials, graphene oxide has oxygen-based functional groups such as hydroxyl, alkoxy, carbonyl, and carboxyl, among others. It has been widely studied in recent years due to its electrical, anticorrosive, mechanical, and chemical properties, thermal stability, hardness, and hydrophobicity, which allow it to be applied in a wide variety of areas.

In this work, a novel graphene oxide coating modified with a coupling agent obtained by an atmospheric pressure plasma jet has been studied in its microstructure, chemical composition, thermal behavior, and protection against corrosion. This coating is obtained from a suspension of graphene oxide and a coupling agent, which is supplied to the plasma jet using an ultrasonic mist. The plasma projects the species in the ultrasonic mist onto the aluminum surface, allowing the coating to form in short treatment times compared to other deposition methods.

The coatings obtained are continuous, adherent, and homogeneous. The microstructure analysis shows continuous layers forming, making it viable as a protective barrier against corrosion. The chemical analyses show by EDS that the atmospheric pressure plasma jet does not generate contamination or elements foreign to graphene oxide and the coupling agent.

The XPS analyses show that the treatment with atmospheric pressure plasma does not chemically modify graphene oxide since it maintains its functional groups. However, by thermogravimetry analysis, the results indicate an increase in oxygen pyrolysis. Corrosion measurements show higher electrochemical activity in the coatings. This higher current activity is due to the combined response of the coating and the aluminum substrate. The contribution of the graphene oxide film is caused by the functional groups, which contain oxygen. This coating was able to protect the aluminum substrate from corrosion.

Keywords

Graphene oxide, APPJ, plasma, coatings, aluminum, corrosion, inhibitors, thin films.

Reference

J. A. Cabello Mendez, A. Arguelles Rojas, J. J. Pérez Bueno, Y. Meas Vong, Study of the anticorrosive behavior of samarium as a corrosion inhibitor in multilayer systems for aluminum alloy, Sci. Rep. 13 (2023) 3149. https://doi.org/10.1038/s41598-023-30193-y.

This work was supported by

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[PLV-260] THIN FILMS DEPOSITED BY THE ABLATION OF METALLIC SN AT DIFFERENT OXYGEN PRESSURES

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It is well known that SnO2 thin films have been widely used as transparent conductive oxides for applications in solar cells, light emitting diodes, flat panel displays, and in general, in optoelectronic applications. However, SnOx has attracted attention due to it can work with the multivalent Sn cation (ref) which ends up with a tunable conductivity type and bandgap semiconductor.
In this work SnOx thin films have been grown at room temperature on quartz substrates by pulsed laser deposition. The oxygen content on the samples was changed by varying the pressure (10, 20, 30 and 40 mTorr) of an Ar/O2 gas mixture.
The laser produced plasmas were analyzed by means of Langmuir planar probe measurements in order to determine mean kinetic ion energy and Sn ion density. Fluence was kept constant for all deposits. The plasma parameters changes as a function of deposition pressure was studied.

Resulting films were optically characterized by UV-Vis spectroscopy, in which it was found that absorption and transmittance are highly influenced by deposition pressure. The structural properties of the films were studied by XRD and Raman spectroscopy. Chemical composition and oxidation states were analyzed by XPS spectroscopy.

Keywords
SnO-thin films, PLD, Control-Oxygen-Pressure, Semiconductor, Band-Gap Variation.
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Universidad de Guadalajara

[PLV-340] SYNTHESIS AND CHARACTERIZATION OF STANNANE AND ITS IMPACT IN EXTREME ULTRAVIOLET LITHOGRAPHY AND VACUUM TECHNOLOGY

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Stannane (SnH_4) is an unstable molecule produced by the interaction of hydrogen radicals and tin in cleaning collector mirrors used in the Extreme Ultraviolet (EUV) lithography process. The physicochemical characteristics of this gas, its interaction in a plasma system, and its interaction with various materials have not been completely explored and understood. Even though this gas is important in EUV lithography technology, few works have focused on it for a few decades. With the aim to identify this compound, the electron ionization mass spectrum of stannane (SnH_4) was presented. The density of the liquid, cracking pattern, chemical surface, semiquantitative properties, and surface morphology of Stannane were examined. All ten natural abundance isotopes were observed experimentally for each set fragmentation ion such as Sn^+, SnH^+, SnH_2^+, and SnH_3^+ by mass spectrometry. Density functional electronic structure theory was executed to calculate the optimized ground state geometries of these gas phase species, and their relative stabilities behavior in the data and less observed signals for SnH4+. The surface of the deposited tin film resulting from the oxidation of this gas was constituted by metallic Sn and SnO, which were revealed by X-ray photoelectron spectroscopy. Finally, the SnH_4 deposition on Al_2O_3-coated QCM was performed.

Keywords
Stannane, Mass Spectrometry, EUV Lithography, Characterization, Synthesis.

Reference

Dren Qerimi, Andrew C. Herschberg, Gianluca Panici, Parker Hays, Tyler Pohlman, David N. Ruzic. Tin removal by an annular surface wave plasma antenna in an extreme ultraviolet lithography source. Journal of Applied Physics 132 (2022) 113302. https://doi.org/10.1063/5.0094375.

This work was supported by

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RENEWABLE ENERGY: MATERIALS AND DEVICES

CHAIRMEN

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

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

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

[RWE-39] GOLD RECOVERY FROM E-WASTE PROCESSORS LEACHED IN SEAWATER AND ITS RECYCLING FOR THE SYNTHESIS OF GOLD NANOPARTICLES

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It is 13 times more expensive to extract minerals from the Earth than to recycle them since obtaining and processing virgin resources requires industrial quantities of water, chemicals, and fossil fuels; it is expected that by 2030, 74.7 Mt of electronic waste will be produced worldwide, so, to counterbalance the environmental impact of the generation of e-waste, this work presents the recovery of gold from computer processors using nitric acid diluted in seawater instead of aqua regia, and proposes the reuse of this metal for the synthesis of nanoparticles. The seawater leaching method presents a much lower risk to the environment, compared to the aqua regia leaching method currently used to obtain gold from electronic waste since NO and Cl2 are not wasted during extraction. Furthermore, hydrochloric acid is not necessary, as HNO can oxidize Cl ions present in seawater into Cl2, which can transform Au0 atoms into Au3+ ions, allowing us to prepare HAuCl4, the precursor to synthesize bimetallic AuCu nanostars and semispherical gold nanoparticles that can be used for different applications, including SERS.

Keywords
SERS, seawater, gold nanoparticles, e-waste.

Reference

Sheng, P. P. & Etsell, T. H. Recovery of gold from computer circuit board scrap using aqua regia. Waste Manag. Res. 25, 380–383 (2007).

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División de Materiales Avanzados, IPICYT.

[RWE-149] STUDY OF THE INFLUENCE THE SUBSTRATE POSITION INSIDE THE REACTOR CONTAINER ON THE OPTOELECTRONIC PROPERTIES OF CdS ULTRA THIN-FILMS DEPOSITED BY CHEMICAL BATH DEPOSITION TECHNIQUE

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Cadmium Sulfide (CdS) n-type semiconductor is one of the most used as a window layer in thin films solar cells, such as CdTe, CIS, CIGS and CZTS. Optoelectronic properties are the most important properties for window materials, in this way, in the chemical bath deposition technique (CBD) these properties are influenced by the position of the substrates inside the reactor container and the pressure exerted by the solution column over them. In this sense, the aim of this work is to analyze the optoelectronic properties of CdS ultra thin-films deposited by DBQ technique considering different position inside the reactor container, carryng out a detail study of the optical, morphological, electrical and structural properties. CdS thin films were deposited on soda lime/SnO2:F (FTO) using CBD technique. CdS samples with areas of 4 cm2 and thickness of 27-48 nm were obtained; X-ray diffraction patterns show CdS thin films with different polycrystalline structures, SEM images reveal different surface formations, resistivity values around 105 Ω.cm were measured. Uv-Vis spectra show transmittance values around 45-94% in the visible region and the estimated energy band gap values around 2.1-2.36 eV. The best physical properties are obtained when the substrates are placed near the bottom of the reactor container with FTO side down, giving rise to an optimal configuration that allows reducing the amount of precursor solutions to reduce the amount of toxic waste generated, these results are important in the processes of photovoltaic technology and the reduction in environmental impact.

Keywords
CdS, ultra-thin films, CBD technique, Substrate position, solar cells.

Reference

(1) Lee T.D. and Ebong A. U. A review of thin film solar cell technologies and challenges, Renewable Sustainable Energy Rev. 70 (2017) 1286–1297 http://dx.doi.org/10.1016/j.rser.2016.12.028.

This work was supported by

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[RWE-155] SYNTHESIS AND CHARACTERIZATION OF QUANTUM DOTS SENSITIZED SOLAR CELLS

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In this work, quantum dots sensitized solar cells (QDSSC) have been prepared using SILAR. Quantum dots (QDs) with different configurations were incorporated into thin films of TiO2. Prototype solar cell configurations include: TiO2/CdZnS/ZnS, TiO2/PbS/CdZnS/ZnS. The aim of this work is to find the QD configuration which would provide a maximum of light absorption and thus generate a higher photocurrent. Light absorption measurements have been used to evaluate and compare samples. Prototype solar cells have been tested under one sun of illumination using asolar simulator. The characteristic J-V curves have been obtained for samples with different QDs composition. Light absorption and photovoltaic behavior results will be presented.

Keywords
Quantum Dot Sensitized Solar Cells, Composition of QDs, SILAR.

Reference

Esparza, D., Zarazúa, I., López-Luke, T., Cerdán-Pasarán, A., Sánchez-Solís, A., Torres-Castro, A., ... & De la Rosa, E. Effect of Different Sensitization Technique on the Photoconversion Efficiency of CdS Quantum Dot and CdSe Quantum Rod Sensitized TiO2 Solar Cells.

This work was supported by

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[RWE-203] GaAs-BASED SCHOTTKY SOLAR CELLS WITH EMBEDDED GaNAs/GaAs QUANTUM WELLS SYSTEM FOR MULTI-PHOTON ABSORPTION

T. A. Pérez-Oviedo B.S.E.[1], M. I. Bustos Ibarra B.S.E.[1], I.G. Pérez Ortiz B.S.E.[1], P. A. Vera-Gallegos B.S.E.[1], A. Belio Manzano P.H.D.[2], J. P. Olvera Enríquez M.S.C.[2], E. Briones P.H.D.[3], V. H. Mendez García P.H.D[2], L. I. Espinosa Vega P.H.D[2], I. E. Cortes Mestizo P.H.D[4]

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At present, increasing the conversion efficiency of solar cells is sought. In this task, a wide variety of strategies has been developed with the aim of reduce the cost of production and rising the working wavelength range of photovoltaic devices. One alternative to standard p-i-n solar cell structures is photovoltaic technology with Schottky barriers. A Schottky barrier solar cell is constructed by using a n-type or p-type semiconductor material, a metal-semiconductor rectifying contact, and an ohmic junction [1]. This project shows the development of Schottky solar cells composed of n-type GaAs with embedded GaNAs/GaAs quantum wells system for multi-photon absorption. Two multi-quantum wells sequences are explored where the GaAs barrier is kept at 18 nm while the GaNAs well is 6 nm for A-samples and 12 nm for B-samples, both with 15 periods of the quantum well sequence. Firstly, technology computer aided design (TCAD) is employed to develop a numerical model to obtain the theoretical current-voltage curve of this III-N-V Schottky barrier solar cell concept. The proposed designs were grown using molecular beam epitaxy on n-type GaAs (100) substrates. An Oxford-CNMX32 nitrogen radio-frequency plasma at 325W in conjunction with nitrogen flux of 0.25 sccms was employed to obtain GaNAs layers with nitrogen concentration ~ 0.5%. Then, it was characterized employing HRXRD, Raman, and photoreflectance spectroscopies where suitable structural, optical, and electrical properties were found. Physical vapor position technique (PVD) was used to fabricate rectifiers electrodes. The effect of the Schottky barrier is explored with different metals work functions (Sb, Cu, and Au) while InGa eutectic alloy is used to elaborate the ohmic contact. The current-voltage curves were taken under AM1.5D solar spectrum at 450 W/m2. Sb(Cu) Schottky contact solar cells exhibits the better VOC(Jsc) with values of 0.147V(7.72μA/cm2) and 0.172V(11.61μA/cm2) for A- and B-samples, respectively.

Keywords
Quantum-well solar cell, photovoltaic devices, Schottky solar cell.

Reference

Murat Soylu, Fahrettin Yakuphanoglu, Photovoltaic and interface state density properties of the Au/n-GaAs Schottky barrier solar cell, Thin Solid Films, Volume 519, Issue 6, (2011) 1950-1954. https://doi.org/10.1016/j.tsf.2010.10.030.

This work was supported by
The Laboratorio Nacional de Análisis Físicos, Químicos y Biológicos/UASLP, CONAHCYT CF-2023-I-1300, COPOCyT Fideicomiso 23871, and Investigadoras e Investigadores por Mexico.

[RWE-205] STUDY OF RAPID THERMAL ANNEALING EFFECT ON THE OPTICAL AND ELECTRICAL PROPERTIES OF III-N-V MULTI-QUANTUM WELLS HETEROSTRUCTURES FOR PHOTOVOLTAIC APPLICATIONS

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The GaNxAs1-x alloy is considered a promising material for photovoltaic and optoelectronic applications [1]. In the dilute regime (x ≤ 0.03) the lattice mismatch between GaNAs and GaAs is lower than GaAs with other III-V materials. Thus, this material is suitable in the development of multi-quantum well solar cell based on GaAs. Nevertheless, rising the x value produces detrimental effects on the electrical and structural properties that reduces the conversion efficiency of devices. In this work, p-i-n GaAs photovoltaic heterostructure with GaNAs/GaAs multi-quantum wells systems are analyzed. Molecular beam epitaxy was used to growth samples with 10, 20, and 30 periods of (4nm)GaAs/(6nm)GaNAs/(4nm)GaAs quantum wells. The diffraction of [004] plane obtained indicated two peaks intensities which correspond to GaAs and GaNAs, denoting a nitrogen composition of ~ 0.01. The current-voltage behavior indicates that the conversion efficiency decreases as the number of quantum wells is augmented. Rapid thermal annealing (RTA) treatments were explored with the aim to reduces the detrimental effects of the nitrogen inclusion in the optoelectronic properties of the GaNAs alloy. The samples were annealed at 700, 800, and 900 °C for 60 seconds in a N2 atmosphere. To analyses the effect of the RTA on the photovoltaic structure Raman spectroscopy was employed. Composition, doping, and crystallinity were evaluated through GaAs and GaNAs vibrational modes, founding changes in the LO and L- as indicative of the success/failure of the thermal process. The band structure was studied by ellipsometry employing pseudo-dielectric function and by Photoreflectance spectroscopy, employing the third-derivative lineshapes of the spectrum related to E- and GaAs gaps. Additionally, the presence of Franz-Keldysh oscillations on photoreflectance spectrum allows to study the electric field distribution modification by RTA. The current-voltage behavior of the proposed solar cells indicated that are improved by the annealing process.

Keywords

GaAs-solar cell, quantum-well solar cell, Rapid thermal annealing.

Reference

J.F. Geisz, and D.J. Friedman, III–N–V semiconductors for solar photovoltaic applications, Semicond. Sci. Technol. 17 (2002) 769–777. https://doi.org/10.1088/0268-1242/17/8/305.

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[RWE-215] PHOTOTHERMAL APPLICATIONS OF NANOFLUIDS OBTAINED THROUGH GREEN SYNTHESIS OF COPPER OXIDE AND THEIR POTENTIAL USE IN SOLAR COLLECTORS

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Nanoparticle synthesis is a topic of great interest due to its diverse applications in various fields. However, conventional synthesis methods can present environmental problems. In this regard, green synthesis emerges as a sustainable alternative that allows minimizing negative impacts on the environment. Metallic oxide nanoparticles have aroused significant interest in the scientific community due to their incredible potential in different fields. Among them, copper oxide possesses unique properties such as high electrical and thermal conductivity. The synthesis of copper oxide nanoparticles using green methods has become a promising alternative to reduce the environmental impacts of nanomaterial production. In this project, copper oxide nanoparticles were synthesized using the controlled precipitation method with Hibiscus sabdariffa (Jamaica) extract. The nanoparticles were mixed with water, ethylene glycol, and a 50% water and 50% ethylene glycol mixture to form a nanofluid with concentrations of 0.1, 0.2, 0.3, and 0.5% by weight of copper oxide nanoparticles, respectively. The obtained results demonstrate a successful synthesis of copper oxide, which was characterized using techniques such as X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), ultraviolet-visible spectroscopy (UV-VIS), and scanning electron microscopy (SEM). These techniques revealed a laminar morphology grouped in secondary agglomerates, with an average size of 24.6 nm and a pure phase. When the nanoparticles were mixed with the base fluid, they were characterized using a thermal lens technique, which showed an increase in thermal diffusivity compared to the base liquid. In this work, the proposal is to harness solar energy to generate heat by utilizing the obtained nanofluids with their high thermal diffusivity. Their potential application in solar collectors aims to enhance heat transfer and improve system efficiency. This methodology emphasizes the need to develop sustainable production methods that minimize environmental impact and maximize energy efficiency.

Keywords
nanoparticles, nanofluids, energy, efficiency, conductivity.
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This project was supported by the multidisciplinary SIP Project 2275 and module 20231669.

[RWE-247] STUDY OF THE INTERFACES BETWEEN POROUS SILICON AND CONDUCTIVE POLYMERS AS AN EFFECTIVE MEDIUM FOR CHARGE ACCUMULATION

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Electrical characterization results (i-v and impedance) are presented, showing the characteristic of charge accumulation of porous silicon layers infiltrated with conductive polymers (PANI and PYRROLE), which form an effective medium, which allows the movement of electrons, through the polymer chain. The I-V curves show an increase in reverse bias current over time, this indicates that charge accumulates within the effective medium. The impedance characterization shows Nyquist diagrams with half circles that allow modeling the medium as a system of two solution resistances Rs and charge transfer resistance Rt, a double layer capacitance (DLC) and a Warburg impedance (Z_W), which relates the oxidation-reduction characteristics of an electrolyte, in this case an adjustment is made to model the effective medium. This effective medium could be considered a solid electrolyte for application in batteries.

Keywords
conductive polymers, charge accumulation, Battery.

Reference

Ibanez, J. G., Rincón, M. E., Gutierrez-Granados, S., Chahma, M. H., Jaramillo-Quintero, O. A., & Frontana-Uribe, B. A. (2018). Conducting polymers in the fields of energy, environmental remediation, and chemical–chiral sensors. Chemical reviews, 118(9), 4731-4816.

This work was supported by
Proyecto VIEP.

[RWE-253] CdTe SURFACE MODIFICATION DURING $CdCl_2$ AND $MgCl_2$ THERMAL TREATMENT AND THEIR PERFORMANCE ON CdTe SOLAR CELLS

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CdTe thin films as part of CdS/CdTe photovoltaics solar cells has been studied, improving the efficiency of this by different routes. Annealing process are the most common procedures to activate the window and absorber materials. In this work $CdCl_2$ and $MgCl_2$ as activation processes of CdTe thin films was studied. The morphological, structural, and electrical properties of the activated CdTe thin films are reported. Scanning Electron Microscope (SEM) measurements reveal a morphological improvement, as CdTe grains become larger, increasing their grain size. Also, a noticeable decrease on the grain twins is observed. X-Ray Diffraction (XRD) study confirms the improvement of the structural composition of the CdTe grains, were a (111) orientation is enhanced. Finally, electrical measurements were done using the four-probe technique. A decrease on the resistivity of at least one order of magnitude is observed, compared with the as-grown CdTe thin film. Annealing at 420 ^{o}C seems to yield the best reduction on resistivity while enhancing the structural and morphological characteristics of CdTe.

Keywords
MgCl2, CdCl2, Thermal Treatments, CdTe, CSVT system, Sublimation, Surface Modification.

Reference

J. D. Major, et al, A low cost non-toxic post-growth activation step for CdTe solar cells, Nature 511 (2014) 334

Angeles-Ordoñez, et al, CdTe/CdS solar cell junction activation: Study using MgCl2 as an environment friendly substitute to traditional CdCl2.

This work was supported by
Projects SIP 20231014, SIP 20231027, SIP 20231026.

[RWE-257] MODELING AND ANALYSIS OF THE STRUCTURE OF A SOLAR TREE BY VECTOR CALCULATION

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It is common to find conventional solar panels in the city supplying energy to homes, parks or schools; unfortunately, these systems disturb the image of the environment generating visual pollution and affecting people's mood. In recent works, structures have been developed that maintain a balance between energy efficiency and design, focused on using conventional solar cell technology resulting in tree designs that look far from the real ones. The objective of this work is to model a tree-shaped structure assuming possible technologies that allow having solar cells with shape and curvature similar to that of a real leaf in order to design a structure according to the essence of the environment in which it is installed. For this purpose, parametric equations are used to generate the trajectories in space that define the shape of the trunk and branches by varying a scalar parameter; likewise, paraboloids are used to create the geometric locations of the leaves and shape them by manipulating concavity, curvature and rotation parameters. In addition, an algorithm was created in Python that models a paraboloid with the shape of a leaf where the distribution of solar energy on the surface is studied as a function of its curvature and the angle of incidence of the light rays; in this way, a graphic approximation of the energy efficiency of the structure was obtained, as a function of the curvature of the leaves, to seek a balance between maximum energy conversion and a design in harmony with the environment.

Keywords
Photovoltaic structure, parametric equations, visual pollution.

Reference

S. Dey, and B. Pesala, Solar tree design framework for maximized power generation with minimized structural cost, Renewable Energy (2020) 1747-1762. https://doi.org /10.1016/ j.renene.2020.07.035.

This work was supported by

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[RWE-267] IN-SITU SOLUTION-BASED DOPING OF CdS APPLIED ON THIN FILMS CAPACITORS

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CdS is an n-type semiconductor typically used in CdS/CdTe solar cells and thin film transistors (TFTs) due to its high mobility (>1 cm^2/V-s), low temperature deposition process (< 70 ºC) and compatibility with large area/flexible substrates. Usually, CdS is deposited by Chemical Bath Deposition (CBD), which is a simple and inexpensive solution-based process. Moreover, the ability of changing the doping concentration of CdS in-situ during the CBD process could lead to a potential optimization in device performance and will allow the development of other novel structures. However, one of the main drawbacks in CBD is the amount of water and CdS precursors wasted during the deposition as a result of the position of the substrate inside the reactor (substrate/reactor volume ratio). In this work, we propose a novel methodology used in the CBD process to deposit and evaluate in-situ Cu-doped CdS thin films, while reducing the water and CdS waste associated to the process. Polycrystalline CdS and CdS:Cu thin films were evaluated as active semiconductor layer using metal-insulator-semiconductor (MIS) capacitors. Capacitors were fabricated using a Al/Si^{++}/HfO_2/(CdS or CdS:Cu)/metal stack. A change in doping concentration (n-type) ranging from -1.0x10^{-17} cm^{-3} to -1.7x10^{-18} cm^{-3} was found when adding Cu dopants in the CdS lattice. Also, CdS and CdS:Cu thin films thermally annealed at room atmosphere showed an increasing changes in accumulation region behavior of C-V curve in the case of CdS capacitors. The XPS analysis reveals that Cu replaces Cd inside the CdS structure, resulting in CuS. Also, CuO was found in the film, which could be the result of the oxidation of Cu.

Keywords
Capacitors, CdS:Cu, charge carriers, CBD, MIS.

Reference

M.L. Albor Aguilera, J.M. Flores Marquez, et al., Cu doping concentration effect on the physical properties of CdS thin films obtained by the CBD technique, Materials Research Express 4 (2017) 086410. http://dx.doi.org/10.1088/2053-1591/aa810c.

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[RWE-307] MONITORING CONGO RED DISCOLORATION USING THERMAL PROPERTIES IN PHOTOCATALYTIC PROCESSES: A NEW APPROACH

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The photocatalytic process is an alternative remediation technology to counter the negative effects of dyes in aqueous solutions [1]. In this work, the photocatalytic potential of β-PbO nanoparticles to degrade Congo red was investigated. For the first time, monitoring of photocatalysis reporting thermal diffusivity measured by thermal lens spectroscopy and thermal wave resonator cavity techniques is reported. The reaction was carried out under alkaline conditions with UVC light irradiation and in the presence of lead oxide nanoparticles. It was possible to record a decrease of the characteristic peak of Congo red around 497 nm in the UV-Vis spectra. Likewise, a decrease in thermal diffusivity from $15.53\pm0.026x10^{-4}$ $cm^2 \cdot s^{-1}$ to $13.96\pm0.045x10^{-4}$ $cm^2 \cdot s^{-1}$ was observed as the irradiation time increased. The azo-derived dye degradation reaction follows pseudo-first-order kinetics. The model used allowed the calculation of an apparent rate constant of 0.0188 min^{-1} and the half-life of the Congo red of 36.8 min^{-1} in the presence of tetragonal lead oxide. The experimental conditions allowed the degradation of the dye in a percentage up to 90%.

Keywords
Photocatalysis, lead oxide, Congo red, thermal diffusivity.

Reference

V. Vaiano, I. De Marco. Removal of Azo Dyes from Wastewater through Heterogeneous Photocatalysis and Supercritical Water Oxidation, Separations 10 (2023) 230. https://doi.org/10.3390/ separations10040230.

This work was supported by
CONAHCYT

[RWE-323] HETEROGENEOUS CATALYSIS IN THE COPRODUCTION OF BIODIESEL AND HYDROGEN

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Currently, one of the main causes of environmental pollution is the excessive use of non-renewable resources, which increases greenhouse gas emissions such as CO_2, NO_x, and SO_x, leading to poor air quality and becoming one of the greatest challenges, as the death of millons of people a year in reported because of this.
A highlighted proposal to solve this problema is the production of bioenergies, with biodiesel production standing out. This biofuel has a significant impact due to the reduction of greenhouse gas emissions, and being biodegradable, it does not present major risks for the environment. Biodiesel is obtained through transesterification reaction, using a catalyts to optimized the reaction time. The types of catalysis reported for this reaction are homogeneous and heterogeneous catalysis. Homogeneous catalysis has disadvantages such as the separation of the catalyst and also increases costs due to the use of other products for biodiesel neutralization. On the other hand, heterogeneous catalysis has advantages such as easy separation of the catalyst from the reaction system, reusability, and obtaining pure biodiesel without further treatments. Transesterification reaction generates a by-product, glycerol, which is used in many industries, but requires further treatment to be suitable for use.

In this project, a circular economy using glycerol as a platform molecule for hydrogen production is proposed, as it is a biofuel with great energy potential. Therefore, the solid-state synthesis of sodium silicate (Na_2SiO_3) is developed, which is a layered oxide used as a heterogeneous catalyst for the co-production of biodiesel and hydrogen. The optimal conditions for catalyst synthesis were 6 hours at 900°C. The optimal conditions for obtaining biodiesel were 1 hour, a molar ratio of 1:8, and 3% wt.

Keywords
Biocombustible, biodiesel, catálisis, hidrógeno.

Reference

Martínez, A., Mijangos, G. E., Romero-Ibarra, I. C., Hernández-Altamirano, R., & Mena-Carvantes, V. Y. (2019). In-situ transesterification of Jatropha curcas L. seeds using homogeneous and heterogeneous basic catalysts. ELSEVIER, 235, 277-287. https://doi.org/10.1016/j.fuel.2018.07.082.

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[RWE-331] HETEROGENEOUS DIRECT TRANSESTERIFICATION TO PRODUCE BIODIESEL FROM CASTOR SEED

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In Mexico, the transport sector is driven by fossil fuels and is responsible for the emission of 148 million tons of CO2, representing the second source of greenhouse gas (GHG) emissions. This situation has stimulated the interest of biofuels in the country, particularly biodiesel.
Currently, the most common way to produce biodiesel is through transesterification by homogeneous catalysis. However, this method shows several drawbacks in its operation such as corrosion, soap formation or reusable catalysts, so there has been the need to implement a novel alternative production: direct transesterification by heterogeneous catalysis. This process presents competitive advantages such as lower costs, high purity, the use of feedstock that do not compete with the food sector, obtaining biodiesel from seed, and reuse of the catalyst.
The present work consists in the production of biodiesel through the reaction of direct transesterification of castor seed in the presence of a basic heterogeneous catalyst not reported so far. The results have shown so far that biodiesel was obtained within two hours, achieving a similar infrared spectrum like that is reported in the literature. Therefore, this method can be said to be effective in obtaining a pure substance in a shorter time range than expected.

Keywords
Biofuels, biodiesel, direct transesterification, heterogeneous catalyst, castor seed.

Reference

Mijangos Zúñiga, G.E., Producción sustentable y valorización energética de biocombustibles a partir de biomasa utilizando catalizadores básicos heterogéneos, PhD thesis, in Unidad Profesional Interdisciplinaria en Ingeniería y Tecnologías Avanzadas. 2022, IPN: Ciudad de México.

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[RWE-333] ELECTROCHEMICAL CHARACTERIZATION OF ELECTRODE MATERIALS TYPE PEROVSKITE ABO3 BY REPLACEMENT OF RARE-EARTH IONS

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This research project focuses on the characterization and determination of the electrochemical performance of rare earth-based manganites (ABO_3-type) [$La_{0.7-x}Ce_xCa_{0.3}MnO_3$]/YSZ (x=0.35, 0.52, 0.63), in order to investigate whether modification of the A-site in the ABO3 perovskite will help to improve the ionic conductivity in electrode materials for solid-state fuel cells (SOFCs). The synthesis of the perovskites was carried out using the Pechini method (a variant of the Sol-Gel method). Characterization was performed using high-temperature electrochemical impedance spectroscopy (EIS) with a temperature range of 300 °C to 1000 °C in measurement intervals of 50 °C. The most significant contribution during the analysis was the comparison of the impedance values obtained in this study with other rare earths that have been used for A-site substitution in the research group (RE = Sm, Pr), in order to determine which combination of rare earths have the best electrochemical properties to reduce cathode polarization and/or operating temperature in SOFCs.

Keywords
Solid oxide fuel cells, perovskites, Impedance spectroscopy, cathode, electrochemistry.
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[RWE-122] STRUCTURAL AND ELECTRONIC PROPERTIES OF $(CdTe)_{1-x}(In2Te3)_x$ FILMS, WITH x = 0.3 AND 0.7, GROWN BY RF SPUTTERING AND ITS EVALUATION AS PHOTOVOLTAIC MATERIAL

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CdTe is a semiconductor widely employed in production of solar cells and gamma ray detectors. Alloying with elements like sulphur, manganese, zinc, mercury, indium allows tailoring many of its electronic properties because the existence of respective tellurates. In particular alloying CdTe with indium made possible to modify the band gap in the infrared range [1].
The compounds In2Te3 and CdIn2Te4 are compounds related to CdTe with a crystallogrpahic structure in which sites in the structure have been identified as ordered vacancies.
(CdTe)1-x(In2Te3)x thin films with a nominal composition in weight of x=0.3 and x=0.7 were deposited employing RF sputtering. The films were deposited on glass, silicon, CdTe and CdS films at 180 C using argon as working gas.
The produced (CdTe)1-x(In2Te3)x thin films were uniform and characterized to obtain chemical composition and structural and electronic properties. Their electric properties were characterized to evaluate the potential in the production of photovoltaic devices.

Keywords
Thin films, semiconductors, ordered vacancies, optical spectroscopies, photovoltaics.

Reference

Santana, M., Luyo, J., Melendez, M., Zapata, M., Zapata, A., Jimenez, S., ... & Pena, J. L. (2013). Electronic properties of (CdTe) 1-x (In2Te3) x growth by closed space vapor transport combined with free evaporation.

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[RWE-152] HYSTERESIS INDEX FOR 2D/3D PEROVSKITE SOLAR CELLS

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Currently, perovskite solar cells are considered as the solution for solar energy in the future. These devices combine high efficiency and low cost of fabrication. The 3D structure is better in efficiency but with lower stability. The 2D structure is more stable but with lower efficiency. The use of 2D/3D perovskites as light absorbing materials attempts to combine the improved stability of 2D with the higher efficiency of 3D. The development of perovskite solar cells is limited by different parameters: low stability, humidity, heat, and current density-voltage (J-V) hysteresis. J-V hysteresis phenomena are observed as distinct J-V curves varying the scan direction, range and rate, during the J-V characterization. In this study, characterization of 2D/3D perovskite solar cells was performed obtaining their hysteresis J-V curves. These results might be used as a guide to improve the stability as well as the efficiency of 2D/3D perovskite solar cells.

Keywords
Perovskite solar cells, perovskite 2D/3D, hysteresis.

Reference

Valle-Pulido, J., Solis, O. E., Esparza, D., Rodríguez-Rojas, R. A., Turren-Cruz, S. H., Rivas, J. M., & Zarazúa, I. (2023). Degradation analysis of perovskite solar cells doped with MABr3 via electrochemical impedance. Solar Energy, 258, 148-155.

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[RWE-154] PEROVSKITE SOLAR CELLS UNDER LOW INTENSITY INDOOR LIGHTS

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Low-intensity indoor lighting is often wasted when electricity can be produced from it. Unfortunately, there are currently no solar cells that can efficiently collect this illumination. The implementation of 2D/3D Perovskites as light absorbing materials in photovoltaic applications has been a fast and productive technology, maintaining good efficiency but low stability. On the other hand, 2D perovskites have shown good stability, and efficiencies are very low compared to 3D perovskites.In this work, present a preliminar results to use of 2D/3D perovskite solar cells to collection of low intensity light analyzing the results in terms of efficiency, stability and low manufacturing cost are sought, combining the good stability to humidity of the 2D perovskite and the efficiency performance of 3D perovskite.

Keywords
Perovskite solar cells, low intensity, 2d/3D structure.

Reference

Rodríguez-Romero, J., Sanchez-Diaz, J., Echeverría-Arrondo, C., Masi, S., Esparza, D., Barea, E. M., & Mora-Sero, I. (2020). Widening the 2D/3D Perovskite Family for Efficient and Thermal-Resistant Solar Cells by the Use of Secondary Ammonium Cations.

This work was supported by
Financial support for this project was provided by COZCyT, and UAIE-Universidad Autonóma Zacatecas.

[RWE-158] XPS AND SIMS CHARACTERIZATIONS OF A NON-FULLERENE ACCEPTOR ORGANIC SOLAR CELL

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Organic solar cells represent an alternative for the use of solar energy due to their attractive promising characteristics: flexibility, semi-transparency, low cost, and diversity of organic semiconductors. However, these devices have short lifetimes because they are more susceptible to chemical degradation due to the presence of oxygen and water, which has made it necessary to investigate new materials used in the structural configuration layers to improve the efficiency and stability of the device. In this work we present the analysis of the chemical characterizations made by SIMS and XPS of bulk heterojunction inverted organic solar cells (iOSC), fabricated using a small molecule as acceptor material. The materials used for the fabrication of the active layer of the cell were the donor PM6 (polymer) and the acceptor Y7 (small molecule, non-fullerene acceptor) [1], for the electron transport layer (ETL) the material used was PDINO (polymer). The chemical characterizations were carried out on the organic solar cells without encapsulation and exposed to air at different times.

Keywords
Organic solar cell, PM6:Y7 blend, SIMS, XPS, non-fullerene acceptor.

Reference

M. Ramírez-Como, E. Moustafa, A. A. A. Torimtubun, J. G. Sánchez, J. Pallarès and L. F. Marsal, "Preliminary Study of the Degradation of PM6:Y7-based Solar Cells," 2022 IEEE Latin American Electron Devices Conference (LAEDC), Cancun, Mexico, 2022, pp. 1-5.

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CONAHCYT doctoral program 002906 adjudge to CVU No. 932821 and the 2022 program “Proyectos de Desarrollo Tecnológico o Innovación para alumnos del IPN”.

[RWE-202] DESING, GROWN PROCESS, AND ASSEMBLY OF A PHOTOVOLTAIC MODULE COMPOSED OF GaAs-BASED SOLAR CELL WITH EMBEDDED GaNAs/GaAs NANOSTRUCTURES

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The photovoltaic technology stills looking for high-efficiency devices and materials. In this task, one of the most important and currently strategies are the implementation of nanostructures inside solar cell with the aim of improve the conversion efficiency through increasing absorption range toward lower phonon energy than band gap energy of the host material [1]. In this work, the development of a photovoltaic module composed of p-i-n GaAs-based solar cell with embedded GaNAs/GaAs nanostructures is exhibited. First, the photovoltaic heterostructure was numerically designed by technology computer-aided design process. The design improved was grown using molecular beam epitaxy on GaAs n-type (100) substrate. Then, it was characterized employing HRXRD, Raman, and Photoreflectance spectroscopies where suitable structural optical and electrical properties were found. Next, physical vapor position (PVD) was employed to made Ag/InGa electrodes. Finally, ten cells were ensembled in series on a printed circuit board. Current-voltage behavior was obtained under a AM1.5D spectrum at 450 W/m2. The prototype shown the following electrical behavior: short-circuit current 0.36 mA, open-circuit voltage of 4.5 V, and maximum power of 0.403 mW. Measurements of quantum efficiency proven that this solar cell design is capable of utilize photons with wavelength lower than 872 nm.

Keywords
MBE, quantum-well solar cell, photovoltaic devices, electrical performance.

Reference

Nazmul Ahsan, Naoya Miyashita, Muhammad Monirul Islam, Kin Man Yu, Wladek Walukiewicz, Yoshitaka Okada; Two-photon excitation in an intermediate band solar cell structure. Appl. Phys. Lett. 23 April 2012; 100 (17): 172111. https://doi.org/10.1063/1.4709405.

This work was supported by

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[RWE-222] REDUCED GRAPHENE OXIDE SYNTHESIS AND CHARACTERIZATION FOR POTENTIAL APPLICATION AS TRIBOELECTRIC MATERIAL

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Reduced graphene oxide (rGO) is a versatile nanomaterial derived from obtaining graphene oxide (GO). rGO has contributed to a technological development because it shows new properties. Some of these properties are: hardness, elasticity and a high thermal and electronic conductivity.
In this project rGO is synthesized using modified Hummer's method. The first step is the oxidation of graphite to obtain graphene oxide. This modification involves the implementation of green chemistry to use reagents efficiently. After the oxidation process, the next step is the reduction of graphene oxide to produce rGO. It is a key step because it has a large impact on the pureness of the rGO produced. Besides, the nanomaterial was characterized by the techniques of XRD, FTIR and Raman to verify that the process was carried out correctly. Subsequently, rGO successfully synthesized is mixed with a biopolymer. The latter is a polyaniline whose composition has double bonds which allows electron flux. Therefore, a mixture of polyaniline with rGO might bring triboelectric properties to the synthesized material making it capable of performing energy harvesting.

Keywords
Reduced graphene oxide (rGO), Nanomaterial, Synthesized, Mixure and Triboelectric.
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Authors knowledge the support of SIP-IPN 20231669 project.

[RWE-322] PRODUCTION OF ACTIVE CHLORINE FOR THE DEGRADATION OF SULFAMETHOXAZOLE USING AN ELECTROCHEMICAL REACTOR

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A filter-press FM01-LC reactor electro-generating active chlorine on a synthesized Ti/RuO_2-ZrO_2-Sb_2O_3 anode is evaluated to account for whether the optimization of the active chlorine concentration in the elimination of 20 mg L^{-1} sulfamethoxazole (SMX). The three most important factors affecting the reactor performance (chloride concentration, current density and volumetric flow) are used in wide ranges via a Box–Behnken design (BBD) of experiments in the absence of SMX (4 h): 0.01 to 0.2 mol L^{-1} NaCl, 10 to 250 A m^{-2} and 1 to 5 L min^{-1}. An initial pH of 5.8 is utilized due to the HOCl predominance, presenting the most oxidizing potential among chlorine species. Higher chlorine concentrations are produced at higher NaCl contents (0.2 mol L^{-1} NaCl). Volumetric flows around 3.87 L min^{-1} should be enough to furnish chloride ions to the anode surface by convection. The current density strongly depending on pH is the decisive parameter to either maximize the chlorine concentration. A higher active chlorine production at 250 A m^{-2} eliminates the pollutant before 5 min, and a lower amount of intermediates remain after 90 min of electrolysis; since this condition effectively acts against the reducing character of SMX.

Keywords
Active chlorine, Sulfamethoxazole, Box–Behnken, Electrochemical reactor, Anode.

Reference

[1] B. Bonola et al., "Implications to enhance sulfamethoxazole degradation using statistical optimization of either active chlorine concentration or ORP in an electrochemical reactor," J Environ Chem Eng, vol. 8, no. 5, Oct. 2020, doi: 10.1016/j.jece.2020.104179.

This work was supported by

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[RWE-324] FUNCTIONALIZATION OF 3-AMINOPROPYLTRIMETHOXYSILANE SELF-ASSEMBLED MONOLAYERS ON ZnO/Au NANOWIRES: ROLE OF THE SEED LAYER

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In recent years, research on zinc oxide nanostructures has increased, driven by the harnessing of the optical and electrical properties of ZnO at the nanoscale This study examines the change in the optical response of ZnO nanowires due to the adsorption of molecules on their Surface. We grew two different types of ZnO nanowires (NWs), both grown using the vapor–liquid-solid (VLS) technique but with two distinct types of seed layers (Spray pyrolysis and sputtering). Morphology and crystal structure were studied using scanning electron microscopy (SEM) and X-ray diffraction (XRD) techniques. The seed layer and subsequent heat treatment resulted in the fabrication of NWs with different orientations and morphologies. To carry out the surface functionalization, hydroxyl groups are generated on the surface of zinc oxide nanowires by incubating them in a potassium hydroxide solution. After 3-aminopropyltrimethoxysilane (APTMS) functionalization, Photoluminescence (PL) spectroscopy revealed a shift in the spectra, whereas Fourier Transform Infrared Spectroscopy (FTIR-ATR) technique shown a characteristic peak of the Si-O-Si bond that is related to the APTMS multilayer. We have proposed a mechanism for the different crystal planes present on the surface of ZnO nanowires and their interaction with molecular species. This work could provide a basis for optimizing the specific orientation in ZnO NWs for their potential use as gas sensors or detect biological compounds for environmental applications.

Keywords
Nanowires, Zinc oxide, Functionalization, Seed layer, 3-aminopropyltrimethoxysilane.
This work was supported
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[RWE-326] ENHANCEMENT OF CIPROFLOXACIN DEGRADATION USING $BiVO_4$ CHEMICALLY MODIFIED WITH RUBIDIUM

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Nowadays safe water access is decreasing due to many factors as demographic explosion and water pollution. Among the principal water pollutants, there is the pharmaceutical compounds, e.i. ciprofloxacin, which after human consume, it is integrates to water as contaminant agent. This research is a contribution toward materials development for chemical compounds remotion. In this work, $BiVO_4$ chemically modified with Rubidium at different concentrations (1-10%) were synthetized by hydrothermal synthesis method. The present work aims to increment $BiVO_4$ photocatalytic properties. Catalysts powders were obtained in one-pot hydrothermal method, and characterized via X-Ray diffraction, Fourier-Transform Infrared spectroscopy, N_2 adsorption-desorption test, UV-Vis-NIR spectroscopy and X-Ray photoelectron spectroscopy. As results, for concentrations of 1 and 3% Rb on $BiVO_4$, the band gap value was reduced form 2.4 eV to ~2.25 eV, and photo-degradation of ciprofloxacin evaluated via UV-Vis spectroscopy reach to be more than 60% in 4 hours with rubidium implementation samples, compared with 48% of CIP degradation in 4 hours with pure $BiVO_4$. The influence of synthesis parameters in the physical and chemical properties is discussed.

Keywords
BiVO4, rubidium, ciprofloxacin, photodegradation.

Reference

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This work was supported by
The authors acknowledge the support of FORDECYT-PRONACES/6005/20, SIP-IPN-2275(module 20231669) and SECTEI/289/2019, CM 059/2021. The authors also thank the Centro de Nanociencias y Micro y Nanotecnologias of the IPN for the sample characterization facilities.

[RWE-330] DEVICE FOR OBTAINING DRINKING WATER THROUGH THE CONDENSATION OF AIR HUMIDITY

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The availability of water supplies in urban areas has been decreasing throughout the years, as analysed by several civilian and government organizations in Mexico and internationally. One proposed solution is the design of a machine prototype that can concentrate water vapour from the environment into an isolated cabin and then take it to its dew point, through the adjustment of the cabin temperature by means of a refrigeration cycle. The obtained water is then subjected to a potabilization process that reduces the number of dissolved particles present, especially in environments with substantial air pollution. The obtained water can then be used for various miscellaneous uses or be further purified into drinking water by external means. The proposed machine is intended to be used in humid areas with limited access to clean water. Preliminary results show that after 45 minutes of continuous work and 15 minutes on standby, the prototype was able to capture 1.5 litres of water, with an observed energy consumption of 1.072 kWh, in an environment with an average of 43.9% RH and standard deviation of 18.7% RH (measured during a 20.5-hour period). Furthermore, the prototype is an IoT-enabled device, whose machine-human interface can be accessed with a smartphone or computer either locally or remotely for diagnostics and power cycling of the components.

Keywords
Water capture, atmospheric water generation, internet of things, mechatronics engineering.

[RWE-332] VANADIUM OXIDE THIN FILMS BY ULTRASONIC SPRAY PYROLYSIS FOR ENERGY APLICATIONS

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In recent years Vanadium (V) has attracted great interest because it is an abundant element on the planet, which has various oxidation states, +2, +3, +4 and +5. This allows to produce different vanadium oxides as: VO, VO_2, V_2O_3, V_6O_{13}, V_3O_7 or V_2O_5, each of which has different properties. One of the biggest challenges is the pure synthesis of any of these oxides, without mixing the different phases. In particular, vanadium pentoxide (V_2O_5) presents greater interest due to its chemical stability and its photocatalytic properties. V_2O_5 has an energy bandgap of ~2.3 eV, which favors photocatalytic reactions for the decomposition of contaminants in water under visible light, hydrogen production or its use as hole transport layer in solar cells. In the present work, V_2O_5 was synthesized by ultrasonic spray pyrolysis. Three different concentrations of precursors were used and five different synthesis temperatures in order to observe how these parameters can influence the optical, morphological and structural properties. Thin films were characterized by X-ray diffraction, UV-vis, Scanning Electron Microscopy (SEM), FTIR and four points.

Keywords
ultrasonic spray pyrolysis, vanadium oxides, hole transport layer.
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Sesión Oral

[RWE-242] EFFECT OF SILVER DEPOSITS ON PINEWOOD FILTER RETENTION OF ANTIBIOTIC-RESISTANT ESCHERICHIA COLI

Denisse Fabiola Gonzalez Ramírez Sc. D in Biotechnology[1], Claudia Marissa Aguilar Melo Sc. D in Bioprocess[2], Mario Fidel García Sánchez Sc. D Physics[1], Issis Claudette Romero Ibarra Sc. D Chemistry[1]

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Wastewater reclamation is limited among other pollutants by biological contaminants. The exposition to fecal bacteria, viruses, or parasites leads to mild to severe disease in humans. Toddlers, immunocompromised people, and elders; are the most vulnerable to infections. Current research on pathogenic agents in water is focused on the inactivation of antibiotic-resistant bacteria. Especially physical methods like filtration in membranes of 22 micrometers are efficient for bacteria retention. However, applying such a process to potabilization plants is not feasible in comparison with chlorination. Disinfection operations using chlorine derivatives are associated with cancer cases in plant workers or water consumers if the dosage is mishandled. Research indicates that wood tissular structure retains particles of micrometric sizes [1]. This work evaluated pine wood as a filter for retaining a strain of *Escherichia coli* antibiotic-resistant. The pine wood sections were treated with silver nitrate. The results indicate that wood alone retains above 90% of the initial concentration of bacteria, while the impregnated material had a long-term effect preventing bacteria proliferation in the material.

Keywords
Antibacterial, biological filter, Silver nanoparticles, wood functionalization, antibiotic-resistant bacteria.

Reference

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This work was supported by

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[RWE-228] ULTRASOUND SYNTHESIS OF A BaTiO3@Bi CATALYST AND ITS PHOTOCATALYTIC ACTIVITY ON THE DEGRADATION WATER POLLUTANTS

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Water pollution occurs when harmful substances such as medicines, personal care, household cleaning products, pharmaceuticals, microplastics etc., make their way into bodies of water (streams, rivers, lakes, oceans, etc.) degrading water quality. Many of these substances have not been in the environment for long but have been found to cause known or suspected adverse ecological and human health effects. We refer to these compounds as emerging contaminants (EC) and due to the difficulty of removal in water treatment plants, is important to migrate to new technologies. Advanced oxidation processes (AOPs) are chemical treatment procedures designed to remove organic and inorganic materials in water and wastewater by oxidation through reactions with hydroxyl radicals(OH). $BaTiO_3$ is a semiconductor known for its ferroelectric properties and applications as a dielectric material. For catalytic applications: $BaTiO_3$ has a relatively large band gap, which means it requires high-energy photons (ultraviolet or higher) to generate electron-hole pairs. This limits its usefulness in practical applications since a significant portion of the solar spectrum lies in the visible range. In order to improve the catalytic performance of $BaTiO_3$, surface modification can be achieved by introducing dopants with other catalytic active materials. This study explores the synthesis, characterization and catalytic evaluation of a $BaTiO_3$@Bi catalyst prepared via a green synthesis approach. The obtained powders were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The band gap and surface area of the catalyst was also determined using a Uv-Vis Nir-spectrophotometer and the N_2 adsorption desorption isotherms were obtained using a volumetric N_2 adsorption analysis. The catalytic activity of the synthesized $BaTiO_3$@Bi powders was evaluated on the degradation of ibuprofen (IB) under various conditions. The results reveal that a pure $BaTiO_3$@Bi photo catalyst was successfully obtained in 30min, and the catalytic activity showed a 50% IB degradation in 120min.

Keywords
Green synthesis, Emerging contaminants, Barium Titanate, Ibuprofen, Pharmaceuticals.

Reference

J. Halder and N. Islam, “Water Pollution and its Impact on the Human Health,” Journal of Environment and Human, vol. 2, no. 1, pp. 36–46, Jan. 2015, doi: 10.15764/EH.2015.01005.

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[RWE-214] SYNTHESIS OF BISMUTH OXY-HALIDES WITH PHOTOCATALYTIC ACTIVITY FOR IBUPROFEN DEGRADATION

Daniel Flores-Ramírez Master's degree[1], Anel Ivonne Robles-Cortes Master's degree[1], Issis Claudette Romero-Ibarra PhD[1], Carlos Eduardo Santolalla Vargas PhD[2]

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The constant technological advance of mankind has improved notably the life quality. This has given people faster and better ways to perform activities that were not easy some ages ago, unfortunately, it is inherently attached to a pollution phenomenon. Wastewater is full of recalcitrant pollutants, one group of them are drugs of common use like ibuprofen. Among the main techniques used to reduce contamination, photocatalysis is regarded as a clean method for degradation and decomposition that only employs light or sunlight and a photocatalyst. These materials promote redox reactions by photogenerated carriers. There is a wide range of photocatalyst, from the well-known oxides like TiO2, ZnO, RuO2, FeO2, Bi2O3, which have been used extensively for almost all applications, to the novel ones such as the Bismuth based family. One subdivision of this group is the Bismuth Oxy-Halides like BiOF, BiOCl, BiOBr and BiOI. They have demonstrated to have a better efficiency in the degradation of drugs from water greater than those other common oxides. The structural composition of these compounds allows easier carrier separation. Furthermore, the bandgaps have been reported to be 3.5, 3.1, 2.7 y 2.1 eV, respectively. Other properties are fast carrier mobilities, and low cost. In this work, we report the facile synthesis of BiOBr and BiOI by solvothermal and hydrothermal method varying temperature reaction. The phases of both materials were confirmed by X-Ray Diffraction (XRD) and the bandgap was measured by UV-Vis-NIR spectroscopy. These semiconductors were used in the ibuprofen photocatalysis, which was monitored by UV-Vis spectroscopy, showing degradation rates about 60 % within one hour under visible light.

Keywords
Bismuth-based, Oxy-Halides, photocatalysis, Ibuprofen degradation.
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[RWE-38] TECHNOLOGIC TRANSFER OF FLEXIBLE ORGANIC SOLLAR CELLS BASED ON P3HT:PCBM/NP-CdS/TIO2 ABSORBER

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[2]Instituto Politécnico Nacional, Guanajuato, Mexico.

In this work we designed flexible organic solar cells (FOSC) using ITO/PET as a flexible substract, PEDOT:PSS as electron donor, P3HT:PCBM system as light absorber layer, TiO_2 as hole donor, and Al as electrode. The P3HT:PCBM system was modified by introducing semiconducting TiO_2/CdS nanoparticles (np) to enhance electrical and optical properties. The TiO_2/CdS np were obtained by sol-gel method, then they were incorporated into a P3HT:PCBM solution and finally the absorber layer was deposited by spin coating at room temperature. The TiO_2 layer was deposited by the spin coating technique from TiO_2 nanoparticles obtained through a developed sol gel procedure. XRD showed that TiO_2 layers obtained by sol-gel has anatase phase, similar to TiO_2 np. On the other hand, CdS np have hexagonal close-packed phase. Uv-vis spectroscopy measurements on PET/ITO/TiO2:P3HT:PCBM structures showed better light absorption when the TiO_2/CdS np are incorporated. The effect of the np on the electrical properties of the FOSC devices was analyzed through J-V curves and the optical active region was studied by means of the spectral quantum efficiency.

Keywords
flexible, organic, sol-gel, polymer.

Reference

M. Oviedo-Mendoza et al., Improving P3HT:PCBM layers by blending TiO2/CdS nanocomposites for application in photovoltaic solar cells, J. Mater Sci: Mater Electron (2021) 32:102-112. https://doi.org/10.1007/s10854-020-04705-9.

This work was supported by

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[RWE-69] EFFECT OF BISMUTH INCORPORATION ON STRUCTURAL, OPTICAL, AND ELECTRICAL PROPERTIES OF CuSbS2 NANOSTRUCTURES

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Chalcostibite $CuSbS_2$ has gained significant research interest as an absorber material in polycrystalline thin-film solar cells and as thermoelectric material. In this contribution, we report a simple solvothermal process for the synthesis of Bi-doped $CuSb_{1-x}Bi_xS_2$ (CABS) nanostructures with x = 0, 1.25, 2.5, 5, and 7 mol%. Powder X-ray diffraction analysis confirms the presence of single-phase chalcostibite in the orthorhombic crystal structure. With the increment of Bi concentration, the diffraction peaks shift towards a lower angle due to the substitution of larger Bi^{3+} ions at the Sb^{3+} site. Estimated chemical compositions by Energy Dispersive Spectroscopy (EDS) of the samples show that the nanoparticles are slightly Cu-rich and that the Bi atomic percentage in the nanoparticles increases with the increase in the Bi/Sb+Bi molar concentration in the precursor solution. Scanning Electron Microscopy (SEM) analysis revealed the formation of elongated particles with an average length and a diameter of around 350 nm and 80 nm for pure $CuSbS_2$, respectively. A few cuboid and oval-shaped particles are also observed in the micrographs. With the increase in Bi concentration, the density of cuboid particles increases The X-ray Photoelectron Spectroscopy (XPS) survey spectra exhibited a signal corresponding to the 4d orbital of Bi in the doped samples, along with the presence of other constituent elements. A rigorous analysis confirms the correct oxidation states of Cu, Sb, Bi, and S with +1, +3, +3, and -2, respectively. The estimated energy band gap decreased from 1.52 eV to 1.42 eV by increasing the Bi concentration from 0 to 7%. The electrical properties of CABS nanostructures are found to be affected by Bi doping.

Keywords
$CuSbS_2$ nanostructures, Bi doping, optical properties, XPS analysis, electrical parameters.

Reference

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This work was supported by

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[RWE-282] BISMUTH-BASED LAYERED OXIDE CATALYSTS FOR HYDROGEN PRODUCTION

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The reduction of greenhouse gas emissions is one of the main priorities in industries worldwide. Hydrogen has positioned itself as an ideal fuel in the transport industry since it helps reduce the emission of greenhouse gases. The atmospheric oxidation of hydrogen (H_2) produces energy, which makes it a clean fuel. Because of this, many countries have invested and searched for routes to obtain H_2 [1]. Currently, the production, storage, transport, and distribution of H_2 represent a significant challenge, but it is expected that in the coming years, H_2 will be the most widely used fuel worldwide. In this work, the mitigation of greenhouse gases is sought through the co-production of biofuels (biodiesel) and H_2 through heterogeneous catalysis. The synthesis, characterization, and evaluation of the catalysts in the production of hydrogen is presented. The proposed catalysts are based on abundant raw materials in Mexico and friendly to the environment, with an $MBiO_x$ type structure, where M=alkali metals.

Keywords
Biofuels, Hydrogen, Layer Oxides, Catalyst.

Reference

B. P. Sandaka, J. Kumar, “Alternative vehicular fuels for environmental decarbonization: A critical review of challenges in using electricity, hydrogen, and biofuels as a sustainable vehicular fuel,” Chemical Engineering Journal Advances, vol. 14. Elsevier B.V., May 15, 2023. doi: 10.1016/j.ceja.2022.100442.

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SIP project 20231669 (IPN)
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[RWE-274] INFLUENCE OF THE SUBSTRATE ON THE ELECTROCHEMICAL PROPERTIES OF NANOSTRUCTURED CERIUM OXIDE THIN FILMS

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Ultrasonic pyrolytic spray deposition is a versatile synthesis technique for depositing dense or porous, homogeneous films consisting of one or multiple layers. It offers the possibility of manufacturing multilayers and the freedom to modify deposition variables such as deposition temperature, substrate, precursor composition and concentration, solvent composition, among others. Changing one or more parameters in this synthesis method modifies the characteristics of the resulting materials.

In this work, nanostructured thin films of cerium oxide were prepared on FTO substrates, stainless steel, and titanium using ultrasonic pyrolytic spray deposition. X-ray diffraction (XRD) analysis revealed that the films obtained exhibited the cubic phase of CeO_2. The bandgap of the obtained films was estimated using ultraviolet-visible spectroscopy, yielding a value between 3.0 and 3.3 eV. Electrochemical measurements, such as cyclic voltammetry, chronoamperometry, and Mott-Schottky analysis, were performed to study the oxidation and reduction processes, as well as the potentials at which capacitive and faradaic processes occur. Additionally, the positioning of the conduction and valence bands relative to the oxidation and reduction potential of water was determined.

Keywords
Cerium oxide, thin films, Ultrasonic pyrolytic spray, FTO.

Reference

Reyes G. (2021). “Películas de óxido de cerio nanoestructuradas para aplicaciones electroquímicas.” Tesis de Maestría. IPN

Zumeta I., García J. (2021). "Strong texture tuning along different crystalline directions in glass supported CeO2 thin films by ultrasonic spray pyrolysis". Scientific Reports

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[RWE-24] EX-SITU MODIFICATION OF HEMATITE PHOTOANODES FROM POROUS CUO-SB_2O_5-SnO_2 CERAMICS FOR PHOTOELECTROCHEMICAL WATER SPLITTING

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Abundance, low cost and high performance are some of the principal requirements that a material must cover for large scale photoelectrochemical water splitting implementation. In theory, hematite is one of the most promising materials for achieving this assignment. However, a strongly low carrier mobility and hole recombination stop for reaching viability. Morphology design and chemical modifications are accepted techniques that would accomplish efficiencies close to the behavior of an ideal photoanode. In this regard, Sn doped hematite photoanodes grown via chemical vapor deposition on robust, conductive and porous ceramics of CuO-Sb_2O_5-SnO_2 are presented. A time-lapse of deposition of 25 min of hematite precursor and a posterior heat treatment for ex situ doping by substrate diffusion were used. Temperatures between 600-1000 °C were investigated at 10 min on top temperature and rates of 5 °C/min as well as two-step rapid thermal treatments of the same time. The best current density of 0.57 mA/cm^2 was obtained for 750 °C at 1.23 V vs RHE (reverse hydrogen electrode) under AM1.5G simulator (86.6 W/cm^2). A higher performance compared to undoped hematite is reveal. This approach, consisting of a 5 µm section of nanograins of the highly porous substrate cover on a nanofilm of hematite, is presented as an alternative for low cost and easy made promising modified photoelectrodes.

Keywords
Hematite, 3D nanostructured materials, water splitting, photocatalysis.

Reference

A. N. Bondarchuk, I. Corrales-Mendoza, F. Marken, L. Á. Arellanes-Mendoza, J. A. Aguilar-Martínez, L.G. Silva-Vidaurri, G. Curiel-Olivares, F. Montejo-Alvaro, Hematite photoelectrodes grown on porous CuO-Sb2O5-SnO2 ceramics for photoelectrochemical water splitting, Solar Energy Materials & Solar Cells, 221, (2021).
DOI: https://doi.org/10.1016/j.solmat.2020.110886

This work was supported by

This work was supported by the National Council of Humanities, Science and Technology of Mexico (CONAHCYT), grant #A1-S-20353.

[RWE-218] HYDROGEN PRODUCTION USING Ni-BASED CATHODE PRODUCED FROM WASTE NiMH BATTERIES

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Due to technological and economic development, energy requirements are increasing (electricity, batteries, fuels, etc.), and most of the energy produced is obtained from fossil fuels, which leads to the concomitant generation of CO_2. An attractive option is the use of hydrogen, which has an energy yield of 140 MJ/kg, three times higher than the hydrocarbons usually employed. Nickel is one of the non-noble metals used as a catalyst for hydrogen generation and one of the main components of NiMH (Nickel-metal hydride) batteries, which become a pollutant at the end of their useful life. Since they are disposed of in municipal landfills, where their metal casing suffers corrosion and leachates are generated containing metals such as Ni, Co, Cd, Mn, Zn, Cr, rare earths, among others, which contaminate surface and groundwater, their recovery and subsequent use to generate a value-added product is essential. As a result of the above-mentioned problems, in the present research, Ni-based electrodes were generated to catalyze the hydrogen evolution reaction. For this purpose, Ni was recovered in NiMH battery leaching liquors and then deposits were generated by direct current (DC) on a carbon steel support, varying the current density applied for each test. These, Ni-based electrodes were characterized by scanning electron microscopy (SEM) and energy dispersive X-ray analysis (EDX) to know the morphology and determine the elemental composition. To observe the performance of the electrodes, an electrochemical evaluation was performed using techniques such as: open circuit potential (OCP), linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS), using different electrolytes such as: $HClO_4$ and KOH. The results indicate that the current density obtained decreased when KOH was used compared to $HClO_4$.

Keywords
Hydrogen production, NiMH, nickel-based cathode, alternative energy.
This work was supported by
We aknowledge the financial support of SIP project 2275 and the module 20231669. I want to extend my grattitude to CONAHCyT for the PhD scolarship. We thank Adolfo Lopez Angeles for the technical support provided with EIS.

[RWE-249] PREPARATION OF M-LSCF (M= Ag,Co) CATALYST AND ITS CATALYTIC PERFORMANCE FOR SOOT COMBUSTION

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Diesel engine exhaust emissions produce a large number of pollutants, mainly CO, HC, NO_x, PM, in which the main component of diesel engine PM (particulate matter) is soot. Soot particles emitted by diesel vehicles have significant adverse effects on air quality, human health and global climate change, which are worthy of careful study. Soot catalytic combustion is one of the most economical and effective methods to reduce carbon emissions, which requires the use of high-performance catalysts. Perovskite catalysts are widely used in the field of soot catalytic combustion. This material is a mixed ionic electronic conductor with comparatively high electronic conductivity (200 S/cm) and good ionic conductivity (0.2 S/cm). In order to control high emissions of soot diesel engines, this research utilizes highly efficient perovskite oxide catalysts to remove soot. The selected system was the $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-\delta}$, the powder was synthesized via the liquid citrate method, they were finally loaded with different active phases such as Ag and Co by an in-situ vapor-phase dissociative process, all with a percentage of 3% wt. The obtained catalysts were physicochemical, structural, and microstructurally characterized. Different samples were tested by thermogravimetric analysis (TGA) looking forward to elucidating both the effect of the composition, temperature and other features of the catalyst on the soot combustion. The results in the samples impregnated with Ag and Co, which showed T10 and T50 of 333°, 390 °C for the case of silver and 386° and 438 °C for cobalt.

Keywords
soot, catalyst, perovskite, oxidation.

Reference

Chemical synthesis and evaluation of Co3O4/Ce0.9Zr0.05Y0.05O2-δ mixed oxides for the catalytic-assisted combustion of soot

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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-41] SIMULATION OF GALLIUM NITRIDE AND ALUMINUM GALLIUM NITRIDE STRUCTURES FOR UV-C PHOTODETECTORS

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We have designed and simulated ultraviolet C (UV-C) photodetectors, three structures were proposed; the first one is based on a GaN homounion, the second is based on an AlGaN homounion, and the third structure is based on a nAlGaN/pGaN heterounion. A physical model approach was used to design each layer's detector dimensions and doping concentrations. So, after resolve the ambipolar and poisson equations the photocurrent, reverse saturation current due difussion and recombination, and the depletion capacitance were estimated to supply a SPICE model. The calculated properties were used to perform a simulation program with emphasis on integrated circuits (SPICE) equivalent circuit models to integrate the photodetection capabilities of the different structures in an electronic CAD simulator. The model allows to calculate the transport properties in the dark and under ultraviolet (UV) illumination conditions. In addition, the effect of the depletion capacitance was considered by considering the circuit's amplification stage.

Keywords
UV-C, AlGaN, GaN, Modeling, Photodetectors.

Reference

Lizette A. Zebadua-Chavarria, Jorge L. Camas-Anzueto, Vicente León-Orozco, and Carlos A. Hernandez-Gutierrez "Theoretical modeling and design aspects of cubic-phase GaN homojunction-based UVC light sensor," Optical Engineering 61(10), 107102 (6 October 2022). https://doi.org/10.1117/1.OE.61.10.107102.

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[SEM-57] STUDY OF POWER INFLUENCE IN THE PERFORMANCE OF BROADBAND PHOTODETECTORS BASED ON SPUTTERED NiO_X/n-Si HETEROJUNCTION DIODES OBTAINED AT ROOM TEMPERATURE

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Nickel oxide (NiO_x) belongs to the group of metal oxide semiconductors, which are attractive for optoelectronic applications and thin film devices due to their electrical and optical properties [1]. In this work, NiO_x thin films were deposited on corning glass (CG) substrates and Si wafers by rf sputtering using 40, 60 and 80 W of power. High-performance broadband photodetectors based on NiO_x/n-Si heterojunction were fabricated using n-type (100) Si wafers with resistivity of 4–10 Ω·cm. Semitransparent Au layer was used as a top contact, while Al was used as a back contact. Current-Voltage (I-V) measurements indicated photoresponse of the heterojunction diodes under illumination with red, green, blue and UV light in self-powered mode and under reverse bias. The photocurrent at bias voltage V_b = 0 V, depends on the radiofrequency (RF) power used to deposit the NiO_x layer, while the open circuit voltage is almost independent of the power. The responsivity (R) at V_b = 0 V of the 60 W diodes was 0.39, 0.61, 0.67 and 0.95 A/W under illumination with red, green, blue and UV lights (optical powers of 3.71, 1.03, 1.31 and 0.335 mW/cm^2). The obtained R values are higher than previously published results for self-powered broadband photodetectors based on NiO. The On/Off ratio of these diodes at Vb = 0 V is 1.5×10^4, 6.7×10^3, 9.4×10^3, 9.4×10^3 for illumination with the four lights. Capacitance-Voltage measurements indicated high quality of the NiO_x/Si interface with low interface defect density and low density of bulk traps in NiO_x for diodes obtained at the three powers. The quality of the RF sputtered NiO_x layers and the low deposition temperature make them attractive for application in flexible optoelectronic devices.

Keywords
Broadband, photodetector, high responsivity, rf sputtering, nickel oxide.

Reference

[1] Yu, X., Marks, T. J., & Facchetti, A. (2016). Metal oxides for optoelectronic applications. Nature materials, 15(4), 383-396.

This work was supported by
E. Osorio (CVU: 1057649), gratefully acknowledges CONACYT for Ph.D. scholarship.

[SEM-59] SÍNTESIS DE NANOCOMPOSITES TiO2-Au MEDIANTE ABLACIÓN LÁSER DE SÓLIDOS EN LÍQUIDOS Y PRECIPITACIÓN

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Titanium dioxide with the formula TiO2 is an inorganic solid, chemically stable, inert and insoluble. Regarding its crystalline structure, titanium dioxide occurs in three types: anatase, rutile and brookite. For the synthesis of TiO2 there are various methods such as the sol-gel, the hydrothermal, and the precipitation; we will focus on the synthesis by precipitation that is generation and growth of particles in a liquid medium. Gold nanoparticles (Au NPs) have unique properties, such as the presence of a strong absorption band in the visible region. In the present work, the synthesis and characterization of titanium dioxide (TiO2) is carried out before and after being decorated with gold (Au) nanoparticles, using the solid-in-liquid laser ablation method to obtain the nanoparticles. In a solution of 15 ml of bidistilled water we add a gold coin to later irradiated with ns pulses of Nd:YAG laser using a wavelength of 1064 nm; To obtain TiO2, the precipitation method was used using titanium isopropoxide (Ti (OC3H7)4) as a precursor, we added 1 ml to 10 ml of bidistilled water and stirred for 15 min with a magnetic mixer. Heat at 60°C until the liquid is completely evaporated to recover as much of the powder as possible. All the samples were analyzed by means of X-ray diffraction and Raman spectroscopy to know their structure and composition where we were able to conclude that the chosen synthesis produces TiO2 with crystalline structures with a mixture of anatase and brookite phases.

Keywords
TiO2, gold nanoparticles, laser ablation of solids in liquids, precipitation.

Reference

Murillo Romero, Herman Alfredo. “Obtención de un compósito de dióxido de titanio y carbón activado aplicado a la oxidación foto catalítica del ion cianuro”. Tesis de Licenciatura, Escuela Politécnica Nacional. Quito, 2015. Disponible en: http://bibdigital.epn.edu.ec/handle/15000/9253.

This work was supported by
Dr. José Guadalupe Quiñones Galván.

[SEM-61] INFLUENCE OF DOPAJE WITH TRANSITION METALS ON PROPERTIES OF CdS0.5Se0.5 THIN FILMS

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The objective of this project is to determine the structural and optical properties of CdS0.5Se0.5 thin films doped with Ni, Co, Cu, and La, grown using Chemical Bath Deposition (CBD), with the dopant element concentration as a variable of study. Thus, concentrations of 1%, 3%, 5%, and 10% were used within the chemical bath, relative to the amount of Cd present in the solution. The thin films were studied using Uv-Vis spectroscopy and X-ray Diffraction (XRD), to determine structural and optical properties. The pure CdS0.5Se0.5 film exhibits a crystal size of 10 nm, while the films with Ni, Cu, Co, and La have crystal sizes of 6, 7, 8, and 12 nm, respectively. By increasing the concentration of dopant elements, more translucent films are deposited (compared to the pure film), and this is confirmed by the percentage of transmittance at higher energy wavelengths. Additionally, a variation in the edge of the transmittance spectra is observed, indicating a change in the value of the bandgap (Eg). Similarly, regarding the value of Eg, a value of 2.05 eV was obtained for the CdS0.5Se0.5 film, with the Ni and Co doped films oscillating around this value but without showing any clear trend. On the other hand, as the concentration of Cu and La in the films increases, the value of Eg increases to 2.16 eV and 2.18 eV, correspondingly.

Keywords
CdS0.5Se0.5, thin films, CBD, band gap, doping.

Reference

Z. Ye, L. Yang, M. Qin, X. Lu y X. Xiao, «Doping and orientation regulation of p-type Cu:CdS1−xSex/Pt thin film photocathodes for enhanced photoelectrochemical water splitting,» Applied Surface Science, vol. 566, nº 150723, 2021.

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[SEM-141] PHOTOCURRENT IN NANOSTRUCTURED ZINC OXIDE FILMS WITH GOLD NANOPARTICLES

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In this work analyzes the photocurrent of zinc oxide films with gold nanoparticles. Zinc oxide films were obtained by thermal evaporation of zinc on different substrates and subsequent thermal oxidation in laboratory atmosphere. The gold nanoparticles were deposited on zinc oxide films by thermal evaporation. However, the presence of nanoparticles was not detected through the surface plasmon. A strong influence of gold nanoparticles on the absorption edge of the semiconductor and on the electrical characteristics of the zinc-gold oxide compound is observed. The current-voltage ratio was measured in the dark, with natural light, as well as with lamps of 408, 370 and 532 nm. In all cases, it is observed that the current decreases when the composite material is exposed to natural light, while with nanoparticles it decreases up to 2 orders of magnitude with respect to the current observed in the dark with only zinc oxide. In the experiments it was observed that the photocurrent is independent of the plasmonic effect.

Keywords
Photocurrent, Zinc oxide films, Gold nanoparticles, Thermal evaporation, Plasmonic effect.

Reference

Weiwei Zhang, Wenzhong Wang, Honglong Shi, Yujie Liang, Junli Fu, Min Zhu (2018) Surface plasmon-driven photoelectrochemical water splitting of aligned ZnO nanorod arrays decorated with loading-controllable Au nanoparticles, Solar Energy Materials and Solar Cells, Vol. 180, Pages 25-33.

This work was supported by

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[SEM-169] THIN FILMS OF SnO2/TiO2 PHOTOCATALYSTS FOR BLUE METHYL DEGRADATION

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To carry out wastewater treatment, it is necessary to use oxidative processes for its degradation, such as heterogeneous photocatalysis. Currently, binary photocatalysts of SnO_2 with TiO_2 are used for the degradation of complex molecules. SnO_2 thin films were obtained by heat treatment at 400°C for 1 hour. Through X-ray diffraction analysis, the SnO_2 and TiO_2 phases were verified. The Eg values of both materials were also calculated, being 3.8 eV and 3.2 eV, respectively. Once the SnO_2/TiO_2 film junctions were deposited, they were immersed in solutions with different concentrations of the indicator methylene blue, with direct exposure to the sun. Preliminary absorbance results indicate catalytic photodegradation of this indicator. Comparing the photodegradation results with those obtained by W. Vallejo et al [1].

Keywords
degradation, SnO2/TiO2, blue methyl.

Reference

[1] W. Vallejo, C. Díaz-Uribe, A. Cantillo, J. Photochem. Photobiol. A Chem. 299, 80 (2015).

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[SEM-223] INFLUENCE OF GRAPHENE ON THE GROWTH OF GaSb FILMS

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Semiconductor compounds from the antimonide family provide a good alternative to be applied in the fields of microelectronics and optoelectronics due to their electrical, structural and optical properties, including high electron mobility and a direct band gap. Recently, there has been an increased interest in improving the crystal quality of III-V semiconductors, leading to the study of coupling gallium arsenide (GaAs) alloys with 2D materials such as graphene (G) [1]. In this work, gallium antimonide (GaSb) heterostructures were coupled onto Graphene by the close space vapor transport (CSVT) technique. The GaSb films were deposited by CSVT for 5 min, at a temperature of 610 °C, under a constant flow of H_2. The substrates used were G/GaAs (100) and GaAs (100). The samples were characterized by scanning electron microscopy (SEM), Raman and high-resolution X-Ray diffraction (HR-XRD). Raman measurements confirmed the growth of GaSb on the mentioned substrates, evidencing the LO and TO phononic modes. The FWHM of the LO phononic mode was determined, being narrower for the GaSb grown on G/GaAs. Additionally, a uniform surface was found by SEM.

Keywords
III-V semiconductors, GaSb, graphene, CSVT.

Reference

[1] Y. Alaskar et al., "Towards van der Waals Epitaxial Growth of GaAs on Si using a Graphene Buffer Layer," Adv. Funct. Mater., vol. 24, no. 42, (2014), pp. 6629–6638, doi: 10.1002/adfm.201400960.

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CONAHCYT, CINVESTAV, project number CF-2023-I-1117

[SEM-245] SYNTHESIS AND CHARACTERIZATION OF CDS THIN FILMS WITH THE ADITION OF CARBON QUANTUM DOTS FROM GARLIC BY THE CHEMICAL BATH METHOD (DBQ)

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Cadmium sulfide is an inorganic compound soluble in acids. It has a yellow to orange color and a wurzite crystal structure. This structure gives the compound its optical and electrical properties. Due to its energy bandgap, CdS can absorb and emit light at various wavelengths, making it important in semiconductors. Its wide bandgap is useful in electronics, often used in thin films on glass.
Carbon quantum dots are common nanomaterials with unique electronic and optical properties. The majority of carbon quantum dots have a size ranging from 2 to 10 nanometers in diameter. They absorb light, causing electrons to jump to higher energy levels, and emit light when those electrons return to lower levels, releasing energy as photons.
For this study, cadmium sulfide was synthesized and used as a thin film layer with garlic carbon quantum dots. The garlic carbon quantum dots were obtained by heating garlic peel at 200°C, then mixing 5 mg of the dots with 20 ml of deionized water. The mixture underwent agitation and ultrasound processes. Glass substrates were used for the thin films. To create the cadmium sulfide layer, a chemical bath deposition method was employed using cadmium chloride, ammonium hydroxide, and ammonium chloride in a solution volume of 17 ml of carbon quantum dots, which was agitated.
After agitation, the glass substrates were divided into two groups. One group was heated in a microwave oven for 5 seconds, while the other was exposed to ultraviolet light for 30 minutes. Both groups were then kept in a dark place for 5 days. The resulting films were analyzed using photoluminescence.

Keywords
Carbon quantum dots, semiconductors, photoluminescence, thin films, chemical bath deposition.

Reference

Zhao, S., Lan, M., Zhu, X., Xue, H., Ng, T., Meng, X., Lee, C., Wang, P. (2015). Green synthesis of bifunctional fluorescent carbon dots from garlic for cellular imaging and free radical scavenging. Applied Materials & Interfaces, 7(31), 17054-17060. https://doi.org/10.1021/acsami.5b03228.

[SEM-263] SPECTROSCOPY CHARACTERIZATION OF AlGaAs/GaAs MULTI-QUANTUM WELLS

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Low dimensional semiconductor quantum systems (LDS) have undoubtedly been the best promotors of the recent advances in science and technology, and have shaped the vision of the world that can be perceived as it is now in our daily life. In order to get LDS at least two materials of mismatched energy band gaps are required, and the large band offset allows for strong carrier confinement in a potential well at high temperature, enabling the fabrication of temperature-insensitive optical and/or electronic devices [1]. However, usually a material with a large (small) bandgap has a small (large) lattice constant. Therefore, there is a large lattice mismatch inherent in a heterostructure with a large band offset, which introduces defects in multiple stacked nanostructures. In this context, diluted GaNAs is a unique alloy, it can be easily grown on AlGaAs without the formation of strain-related defects. In this work, ex-situ non-destructive optical characterization of GaNAs/AlGaAs QWs by molecular beam epitaxy is presented. The Raman spectra (RS) were fitted by Lorentzian curves to assess for frequency shifts, and changes in of FWHM and intensity. RS showed high crystallinity quality with no-modification of the vibrational modes in comparison with the substrate, and with minimum strain effects. The band structure was analyzed by ellipsometry spectroscopy (ES). ES displayed several overlapped transitions of GaNAs and AlGaAs such as E, E_0, E. + Δ_0, E_0 + Δ_0 and E_+ + Δ_0, E_1, E_1 + Δ_1, $E´_1$. The confined electron states determined by photoreflectance spectroscopy showed that E- is the main confined band with scarce contribution of E+.

Keywords
Low Dimensional Systems, Molecular Beam Epitaxy, Multi-Quantum Wells, Optical Spectroscopy.

Reference

Takaaki Mano, Masafumi Jo, Fabrication of GaNAs/AlGaAs Heterostructures with Large Band Offset Using Periodic Growth Interruption, (2011) Appl. Phys. Express 4 125001, http://dx.doi.org/10.1143/APEX.4.125001.

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[SEM-287] ESTIMATION OF CARRIER CONCENTRATION OF P-TYPE InGaAsSb QUATERNARY ALLOYS FOR APPLICATIONS IN INFRARED DEVICES

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The antimonide family has become one of the most potential semiconductor materials to develop a new generation of applications in the infrared, such as laser diodes, thermophotovoltaic cells, and detectors. These devices are promising for a large variety of biomedical, environmental, and industrial applications. The antimonide family is compounded by binary, ternary, and quaternary alloys. One of the most promising is InGaAsSb because its band gap energy can be tuned in a wide range from near-infrared (1.7 μm) to mid-infrared (3.5 μm). This alloy is doped to achieve p-n junctions; normally, Zinc (Zn) or Silicon (Si) is used for p-type doping, and Tellurium (Te) is used for n-type doping. Using photoluminescence spectroscopy (PL), and Raman spectroscopy, we analyzed the optical and structural properties of novel p-type doped $In_{0.145}Ga_{0.855}As_ySb_{1-y}$ films. These alloys were grown on GaSb (100) substrates by liquid phase epitaxy (LPE) modifying the type of doping between Zn and Si content. The PL spectra presented excitonic emission at ~1.9 μm with a small Full Width and a Half Maximum (FWHM). The Raman spectra presented the LO (GaSb-InAs) and TO (GaSb-InAs) modes vibrational for the $In_{0.145}Ga_{0.855}As_ySb_{1-y}$ alloys. The hole concentration was determined by analyzing the surface depletion region and its relationship with the phonon-plasmon coupling. In order to verify the carrier concentration found in p- type $In_{0.145}Ga_{0.855}As_ySb_{1-y}$ layers by Raman, PL was employed to estimate these concentrations; both techniques determined similar results.

Keywords
InGaAsSb quaternary alloy, infrared, liquid phase epitaxy.

Reference

G. Villa-Martínez, D. M. Hurtado-Castañeda, Y.L. Casallas-Moreno, M. Ramírez-López. M. A. González-Morales, M. L. Gómez-Herrera, P. Rodríguez-Fragoso, J. L. Herrera-Pérez, J. G. Mendoza-Álvarez, Si-doped In0.145Ga0.855As0.123Sb0.877: A novel p-type quaternary alloy with high crystalline quality, Solid State Sciences 123, 106797 (2022).

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[SEM-339] OPTICAL-THERMAL CHARACTERIZATION OF CUBIC InGaN THIN FILMS GROWTH BY MBE

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The study of InGaN thin films allow the exponential development of optoelectronic devices such as photoelectric cells and light-emitting diodes due to their high heat capacity and low sensitivity to ionizing radiation as other group III nitrides. In this work we present and optical-thermal characterization of InGaN thin film samples on GaAs substrates grown by the molecular epitaxy method (MBE). the samples in cubic phase were studied using by photoluminescence, photoreflectance and photoacoustic for optical and thermal characterization. X-Ray diffraction was used for structural characterization and for determination of the Indium concentration on the samples. These thin film samples were found to have concentrations from 21 to 27%. By means of the open cell photoacoustic technique we can determine the thermal diffusivity coefficient. This study will allow us to relate thermal, optical and structural parameters of InGaN thin films.

Keywords
InGaN, Photoacustic, Photoluminisence, Photorreflectance, Thermal difussivity.

Reference

Macias, M., Casallas-Moreno, Y.L., Camacho-Reynoso, M., Zambrano-Serrano, M.A., Pérez-Hernández, B.G., Yee-Rendón, C.M., Gurevich, Y.G., López-López, M. and Cruz-Orea, A., 2020. Thermal properties of cubic GaN/GaAs heterostructures grown by molecular beam epitaxy. Journal of Applied Physics, 128(13).

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[SEM-341] OPTICAL-THERMAL CHARACTERIZATION OF ALUMINIUM NITRIDE THIN FILMS GROWTH BY MBE

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Aluminum Nitride (AlN) is a semiconductor material of great interest in various applications due to its unique properties. Its high thermal conductivity and good electrical conductivity make it suitable for power electronics devices such as high-frequency transistors and high-power diodes. Therefore, the characterization of these properties in this material under different growth conditions is of significant interest. This study presents estimations of the thermal diffusivity of AlN films grown by molecular beam epitaxy on silicon(111) substrates, where the growth temperature has been varied. Additionally, a topographical analysis was performed using an atomic force microscope. Optical characterization was carried out using photoreflectance, reflectance, and photoacoustic techniques, enabling a detailed analysis of the thermal and optical properties of AlN.

Keywords
AlN, MBE, Thermal diffusivity, Photorreflectance, Photoacoustic.

Reference

Solís-Cisneros, H.I., Hernández-Gutiérrez, C.A., Anwar, A., Sevilla-Camacho, P.Y., Camas-Anzueto, J.L., Grajales-Coutiño, R., Trejo-Hernández, R., Casallas-Moreno, Y.L. and López-López, M.,2022. Physical and technological analysis of the AlGaN-based UVC-LED: An extended discussion focused on cubic phase as an alternative for surface disinfection.

This work was supported by

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[SEM-353] STUDY OF THE EFFECTS OF EXPOSURE TIME TO UV/OZONE ON GaAs SURFACES

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Gallium Arsenide (GaAs) is one of the most important semiconductors with extensive applications in device fabrication due to its excellent electrical and optical properties. Surface preparation is crucial to ensure optimal device performance that is why lots of efforts have been focused on this issue. In this work, we studied the changes to the surface of GaAs wafers before desorption and growth by molecular beam epitaxy (MBE) technique, due to the UV/Ozone treatment.

UV/Ozone treatment has been widely studied to modify the surface of semiconductors such as GaAs and Si, but there are some parameters that need to be clarified and specified such as the exposition time. Therefore, we built a UV/Ozone exposure system, which employs UV light of 185 nm to produce ozone and 253.7 nm wavelength to dissociate it. As a result of this, atomic oxygen is formed.

Sample are mounted over an aluminum sample holder ensuring that the distance between the sample and the UV bulb was constant and time exposition was varied from 15 to 3600s. Our anlysis focuses on the characterization of two types of GaAs wafers doped with silicon, one with (100) orientation and n-type carrier concentration in the order of (1-10)x10^{17} cm^{-3}. The other with 10° of disorientation off toward (111) A and n-type concentration of (1-2.7)x10^{18} cm^{-3}.

Different techniques were used to study the GaAs surface. Such as atomic force microscopy (AFM), photoreflectance, photoluminiscence and X-Ray photoelectron spectroscopy (XPS). Results revealed significant surface changes in rugosity, built-in internal electric field, bandgap energy and oxide compostion due to UV/Ozone treatment as a function of exposure time which could have important implications for the surface preparation of GaAs as well as for the development of future studies on GaAs surfacer characterization.

Keywords
GaAs, Uv/Ozone, Surface Preparation, Surface Characterization, GaAs surface.

Reference

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This work was supported by
The autor Luis Vargas Hernández would like to thank Alejandra García Sotelo, Dr. Sergio Jímenez Sandoval and Dr. Rogelio Fragoso Soriano, for the support in the characterization process. As well as CONACYT now CONAHCYT.

[SEM-84] CuCo2O4 FILMS AS A PROPOSAL OF SENSITIVE MATERIAL FOR CO DETECTION INSIDE A COMMERCIAL AIRCRAFT

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CuCo2O4 films were synthesized by means of sputtering assisted by sonochemistry, with alcoholic solution of acetyl acetonate of Cu at 7, 5 and 3 mmol of Cu+2, as a proposal of sensitive material in CO detection. Actually, only the gas sensing properties of this material have been reported for ammonia and ozone, and briefly for H2S, NO2 and CO; the latter with poor response. The films were heat treated in air at 600 ° C and were characterized by SEM, DRX, TEM and FTIR, determining the evolution of the surface morphology and crystal structure throughout the process. The evaluation of CO exposure was performed in a static environment at 100, 150, 200 and 300 ° C and concentrations of 0 ppm to 500 ppm of CO in samples M0, M1, M2, M3 and M4. The M2 sample with 7 mmol of Cu+2 is proposed as the best option of sensitive material because it was the only one that responded to 100 ° C with good sensitivity, although M0 and M1 presented better sensitivity at 300 ° C; the results indicate mainly the exchange of ions Co+2 by ions Cu+2 in the structure of Co3O 4, through the sonochemical process and an improvement in the detection of CO because it offers more active sites by the different valences of the 2 metals (Cu+1, Cu+2, Co+2 and Co+3), which favors the oxidation of CO.

Keywords
CuCo2O4; films; sputtering; sonochemical synthesis; CO detection.

Reference

S. Jain, A. Patrike, S.S. Badadhe, M. Bhardwaj, and S. Ogale, ACS Omega 3 (2018) 1977-1982. https://doi.org/10.1021/acsomega.7b01958.

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[SEM-86] AUTOMATION OF A ROBOTIC DEVICE FOR THE CHEMICAL DEPOSITION BYSPRAY PYROLYSIS TECHNIQUE

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Automation is described as the process of controlling and classifying components [1]. Applied in the elaboration of devices for the synthesis of semiconductor materials either, by physical or chemical methods. CBD, CVD, SILAR and spray pyrolysis (SPD) are examples of chemical techniques used, emphasizing the SPD method in this project. Consists of placing a glass in a thermal panel at a temperature of 400 C° [1], followed by the generation of a spray by means of a drag gas connected to the spray nozzle, which with a movement sprays the aqueous precursor solution intermittently onto the glass. The process gives off gases that are expelled with a hood as waste [2]. An example of a commercial device of this type would have a cost of $15,357.00 dollars [3], therefore the motivation of this work in addition to incorporating a mobile nozzle is the possibility for many laboratories to acquire such equipment, the device developed in this project, reduces manufacturing cost, by using available components and programming on IDE Arduino in order to obtain an affordable equipment for the research on the deposition of semiconductor thin films. As results, in the design of the prototype it incorporates the measurement of velocity in translation of the rail, where the sprayer is located and the control of flow in the carrier gas that goes through and electrovalve. The assembly of the prototype and its characterization by means of a functionality test synthesizing a film thin layer of SnO2, where its thickness and opto-electric, crystallographic and morphological characteristics will be measured using gravimetric differences method, X-ray diffraction techniques, scanning electron microscopy and Raman spectroscopy.

Keywords
Automation, spray pyrolysis, semiconductors.

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[SEM-120] CO-SPUTTERING OF CdTe AND ALUMINUM TO PRODUCE SEMICONDUCTOR ALLOYS

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Co-sputtering of CdTe and Aluminum targets were co-sputtered in an Ar atmosphere to evaluate the production of the ordered vacancies semiconductor CdAl2Te4. The power of the CdTe gun was employed to modify the proportion of Al in the films deposited on glass and silicon substrates.
Chemical, structural and electronic characterization results were obtained for the films employing AFM, SEM, EDX, UV-Vis, Raman and PL spectroscopies. Semiconductor properties were evaluated to determining conditions to produce semiconductor films.

Keywords
Thin films, semiconductors, ordered vacancies, optical spectroscopies, sputtering.

Reference

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[SEM-148] ACQUISITION DATA DEVICE FOR MEASURING RESISTIVITY IN SEMICONDUCTOR MATERIALS

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In semiconductor research electrical properties are fundamental, which define the use of the material. The difficulty is in measuring such properties in nanostructures, define as flat and reduced dimensions structures. The electrical properties of the thin films, generally in the order of the ohm's centimeter and microamps for the sheet resistance and current value respectively involves precision of the measuring devices coupled with interference signals, complicate the measurements of these properties [1]. The 4-point method, also known as the "Kelvin Method", consists of measuring electrical impedance using two linked circuits powered by a direct current source, in the first current flows from the adjustable source to the exterior points and measured by a ammeter, the second is connected in parallel to the internal points in which voltage circulates measured by a voltmeter [2]. A laboratory prototype was apply using a circuit arrangement as follows: the inner leads implement voltage and the outer leads implement current, using two multimeters, it was implemented on a 2.5 X 7.6 mm commercial ITO board, collecting different sheet resistance data that they were plotted, obtaining the IV curve and by means of a linear adjustment the values approximate to the reported by the manufacturer ≈ 10. Subsequently, the optimization was planned using a data acquisition card, FZ0430 module for voltage measurement, ACS712 module for current and a regulable power supply of 24 V. The development of an affordable device to measure sheet resistance values in a range of 106-10-6 [3], as well as eliminate the contribution of interference signals in the connections and the contact between the points with acceptable precision is the main objective of the project.

Keywords
resistivity, semiconductors, kelvin method.

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JO Sígala Valdez, H. Martell Puente , L. Pérez-Arrieta , A. Del Río De Santiago.

[SEM-206] ELECTRICAL EVALUATION OF GaNAs/GaAs SEMICONDUCTOR NANOSTRUCTURES FOR SCHOTTKY DIODES

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In the obtention of intermediate band concept for photovoltaic devices, the GaNAs material has been studied and applied to take advantage of the behavior that its electronic structure of bands acquires with the percentage of nitrogen used in the alloy, %N. Nevertheless, a lack of information related to optical and electrical properties of GaNAs is currently a bottle neck, avoiding the appropriated design process of GaNAs-based devises and increased by the fact that a small variation in the %N is translated into a wide modification of their electrooptical parameters. In this work, efforts on the obtention of electrical parameters such as semiconductor work-function and the formation of Schottky and Ohmic junctions are shown. GaNAs/GaAs epilayers were grown by molecular beam epitaxy (MBE), obtaining samples with %N between 0.5 to 2%. To evaluate the GaNAs work-function Schottky and Ohmic metal-semiconductor junctions were realized thought physical vapor deposition technique, PVD. Metals like Ag, Cu, In, Mn, Sb, Sn, and Zn were employed to create a 500nm-thick electrodes on the GaNAs surface. On this way, MBE and PVD are used to create a two-terminal device in which two rectifying contacts are present. The Schottky behavior is dependent on both parameters the %N and the metal work-function. The current-voltage behavior of the devices was obtained and contrasted with a numerical analysis obtained by TCAD. Additionally, the experimental I-V curves are used in conjunction with a current–voltage model for double Schottky barrier devices [1] to extracting both Schottky Barrier heights simultaneously. The preliminary results indicated that cupper makes ohmic junctions in the GaNAs alloy in the %N range explored here. On the other hand, silver electrodes represent a strategy in the obtention of rectifier junctions.

Keywords
GaNAs alloy, Schottky diode, Ohmic junction, Molecular Beam Epitaxy.

Reference

Grillo A., Di Bartolomeo A. (2020). A current–voltage model for double Schottky barrier devices. Advanced Electronic Materials, 7(2), 2000979. https://doi.org/10.1002/aelm.202000979.

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[SEM-208] MODULATION OF THE OPTICAL PROPERTIES OF Sn-DOPED GaNAs THIN FILMS GROWN BY MOLECULAR BEAM EPITAXY THROUGH ANNEALING TREATMENT

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Adding of nitrogen atoms to GaAs to form the GaNxAs1-x compound is one of the most outstanding strategies to use the so-called highly mismatched alloys in the development of photovoltaic devices. One of the most interesting properties of GaNxAs1-x is the division of conduction band in two sub-bands know as E- and E+, so that the alloy can be employ in the development of intermediate band [1]. Nevertheless, optical, structural, and electronic properties of the GaNAs are reduced with the rise of the of the nitrogen mole concentration (x), compromising the efficiency of GaNAs-based devices' performance. Thus, the study of mechanism to improve the optoelectronic properties of the GaNAs alloy are mandatory. Here, GaNAs layers doped with Sn were grown by molecular beam epitaxy (MBE) to overcome the degradation of the electrical properties of the III-N-V material. GaNAs:Sn/GaAs epilayers are achieved where the Sn incorporation is controlled by the tin effusion cell temperature. The HRXRD technique indicates the presence of a x value ~ 0.001 in the ternary layer. RS and PR were employed to assess the tin incorporation on the GaNAs lattice. Additionally, Rapid Thermal Annealing (RTA) was applied for 60 seconds at 700, 800, and 900 °C to modify the structural properties of the sample as ex-situ scheme and evaluate the tin-atoms segregation. The LO mode presents a redshift related with a strain state on the lattice, increasing with the RTA. The L- vibrational mode intensity is also modified by the RTA, implying changes in the carriers' distribution. The effect of annealing in the band structure of the alloy was also analyzed by photoreflectance spectroscopy where a redshift of the transition related to E- was measured. Furthermore, the spectral region of Franz-Keldysh oscillations was modified toward higher frequencies, as an indicative of modification on the carrier distribution.

Keywords

GaNAs, photoreflectance, Rapid thermal annealing.

Reference

H.F. Liu, N. Xiang, S.J. Chua, S. Tripathy, Effect of rapid thermal annealing on the properties of GaNAs thin films grown by molecular beam epitaxy, Journal of Crystal Growth, Volume 288, Issue 1 (2006) 44-48, https://doi.org/10.1016/j.jcrysgro.2005.12.045.

This work was supported by

The Laboratorio Nacional de Análisis Físicos, Químicos y Biológicos/UASLP, CONAHCYT CF-2023-I-1300, COPOCyT Fideicomiso 23871, and Investigadoras e Investigadores por Mexico.

[SEM-220] DEVELOPMENT OF GaAs/G HETEROSTRUCTURES BY THE CSVT TECHNIQUE

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The integration of gallium arsenide (GaAs) with graphene has emerged as a promising avenue for advancing electronics and photonics technologies. The direct epitaxial growth of GaAs on graphene (G) has demonstrated remarkable performance in devices due to the matching lattice constants and low density of defects at the interface. Furthermore, the GaAs/graphene structure enables the realization of efficient and compact optoelectronic devices such as photodetectors, modulators, solar cells, and light-emitting diodes. Additionally, the compatibility of graphene as flexible substrates opens up opportunities for flexible electronics. Therefore, in this work, GaAs films were grown on G/GaAs(100). Graphene was deposited on Cu by Chemical Vapor Deposition (CVD) and subsequently transferred to GaAs(100) substrates. Raman spectroscopy was performed, obtaining the characteristic peaks of graphene, G and G' at 1569 and 2709 cm^{-1}, respectively. The growth of GaAs films was achieved by the Close-Spaced Vapor Transport (CSVT) technique and characterized using Raman, XRD, and SEM. In the Raman spectrum, both TO and LO vibrational modes were presented. However, comparing the spectrum with a sample without graphene, the LO mode is more intense indicating fewer defects in the material.

Keywords
Heterostructures, CVD, CSVT, Graphene, GaAs.

Reference

J.J. Cruz Bueno, G. García Salgado G, R. Balderas Valadez, et al. Effect of the Gaseous Atmosphere in GaAs Films Grown by Close-Spaced Vapor Transport Technique. Crystals. 2019;9(2):68. doi:10.3390/cryst9020068.

This work was supported by

This work has been supported by Conahcyt and for the project: CF-2023-I-1117.

[SEM-226] THERMAL, STRUCTURAL, AND OPTICAL CHARACTERIZATION OF GaAs SURFACE PASSIVATION

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The arsenide family, which includes GaAs and InAs along with other binary and ternary compounds, plays a crucial role in the advancement of optoelectronic devices like photovoltaic cells and light-emitting diodes (LEDs). However, this family is highly reactive with the environment, producing oxidation reactions on the alloys surface that extend to several atomic layers. These reactions directly impact the efficiency of radiation emission and absorption in the devices. Different surface passivation methods involving chemical compounds and plasmas have emerged as proposals to reduce the surface states. In this study, two chemical methods were used for passivation: sodium sulfide and ammonium sulfide, after the surface cleaning process. The plasma method involved degreasing, followed by deoxidation using UV lamp. Subsequently, an alkaline chemical compound was used for the passivation process. The effect of the three passivation methods on the optical, thermal, and morphological properties was evaluated by photoluminescence (PL), photoacoustic (PA) and atomic force microscopy (AFM) techniques, respectively. the study, it was found that the GaAs passivated samples present a higher efficiency in radiative recombination, as evidence by an increased intensity in the band-band transition obtained from the PL spectra. Likewise, the PA spectra indicated a decrease in the surface recombination velocity (VRS). The passivation treatments also influenced the surface roughness, in the passivated samples.

Keywords
GaAs, chemical passivation, UV lamp, photoluminescence, photoacoustic, AFM.

Reference

Tyagi, P. (2021). Review of Sulphur Interaction based GaAs Surface Passivation and Its Potential Application in Magnetic Tunnel Junction based Molecular Spintronics Devices (MTJMSD). NSF-CREST Center for Nanoscale Science and Technology, 1-21.

This work was supported by

CONAHCYT, CINVESTAV, project number: CF-2023-I-1117.

[SEM-262] DIMENSIONALITY EFFECTS ON THE CONFINED ENERGY STATES OF MULTI QUANTUM WELL HETEROSTRUCTURES GROWN BY MBE

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The mastery over growth of III–V semiconductor compounds and the possibility of tailoring their properties have conducted a large variety of electronic and optoelectronic devices that are already immerse in our daily life. For example, AlGaAs/GaAs heterostructures are widely used in the manufacture of visible light-emitting diodes, laser diodes, solar cells, HEMTS, etc. All the former appliances though are based in thin films grown with a high purity and precision in thickness by molecular beam epitaxy (MBE). However, the next generation devices are envisioned to comprise nanotechnology to improve their properties by further reducing the dimensionality of the heterostructures. On this regard self-assembly on high-index (HI) substrates is a promising technique that has been used in the last few decades to achieve QWRs with high density and high optical quality [1]. Quasi-one-dimensional behavior can be produced in structures where a thin layer of GaAs is sandwiched between layers of a compound with a larger gap (e.g., AlGaAs), where both electrons and holes generally are confined in the low bandgap layer. In this work, we present the optical properties of AlGaAs-GaAs multi-quantum well heterostructures grown by MBE simultaneously on singular (100) and high-index (631) substrates. The energy transitions of photoluminescence spectra were fitted to Viña and Pässler models. The deviations of the fittings for the (631) samples could be related to the change in dimensionality of the confinement. Another interesting behavior also ascribed to the changes of dimensionality is that for thin QWs (<45 Å) the PL energy lines redshifs as compared with the (100) reference sample which is supposed to present solely 2D confinement, and blue-shifts for thicker QWs (>45 Å). Finally, the distribution probability and eigenfunctions were estimated by employing numerical simulations of quantum wire arrays.

Keywords

MBE, Photoluminescence Spectroscopy, Band Structure, Quantum Well, Quantum Wire, Heterostructures.

Reference

F. E. Perea Parrales et al. Characterization of eigenstates interface-modulated in GaAs (631) multi-quantum well heterostructures. Journal of Applied Physics, Vol. 128, Issue 24, (2020). https://doi.org/10.1063/5.0029103.

This work was supported by

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[SEM-352] ANALYSIS OF TWINNING IN ZINCBLENDE GaN THIN GILMS GROWN ON GaAs BY PLASMA-ASSISTED MBE

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Zincblende nitride semiconductors, with gallium nitride (GaN) as their most prominent representative, are a promising alternative to solve problems in optoelectronic devices due to the built-in polarization of the more common wurtzite phase. Nevertheless, the zincblende phase usually exhibits a lower crystal quality compared to its wurtzite counterpart due to its metastable nature and is much less studied. Due to this, the growth of zincblende GaN suffers from a large number of wurtzite inclusions and other defects such as twinning. Since these two phenomena negatively affect device performance, it is imperative to identify and quantify them, in order to identify optimal growth conditions for obtaining high-quality materials.

To achieve this objective, X-ray diffraction studies were carried out on samples of zincblende GaN grown on GaAs (001) substrates by plasma-assisted molecular beam epitaxy, using different Ga/N ratios controlled by plasma power. Pole figure measurements of the zincblende 113 and wurtzite 10-13 reflections allowed for the determination of wurtzite inclusions as well as the amount of twins and their crystallographic relationship with the substrate.

For this, the experimental pole figures were compared with simulations carried out using a Python script that calculates the angles between planes of a material given its crystal system and lattice parameters. The results were also related to calculations of crystal quality by omega scans and to the roughness obtained by atomic force microscopy.

We found that the nucleation temperature is deeply linked with the number of twins and wurtzite inclusions generated, obtaining from about 60 % and up to >99 % of phase purity.

Keywords
XRD characterization, GaN Growth, Pole Figures.

Reference

Frentrup, M., Lee L.Y., Sahonta, S.-L., Kappers, M.J., Massabuau, F., Gupta, P., Oliver, R.A., Humphreys, C.J., Wallis, D.J. (2017), J. Phys. D: Appl. Phys. 50, 433002.

This work was supported by

CONAHCYT

Sesión Oral

[SEM-53] REVISITING THE CHARGE TRANSPORT PROPERTIES OF HIGH PERFORMANCE TANDEM SOLAR CELLS THROUGH THE SHOCKLEY MODEL FOR A PN JUNCTION

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The charge transport properties of solar cells of outstanding performance are rarely reported, strongly limiting the information on the device physic properties and technological issues. Often, just a current-voltage curve under illumination and its open circuit voltage (V_{OC}), short circuit current (J_{SC}), fill factor (FF) and efficiency are provided. However, pn junction(s) charge transport parameters as saturation current (J_0), ideality factor (n), parasitic series resistance (R_S), which are important to understand and assess the quality and behavior of the device and its technology, are neglected. Notwithstanding the high quality of some solar cells whose performance even constitute the state of the art, obtaining and providing some of the parameters qualifying their important physical properties allows a better assessment of the device quality and its technology. In this presentation it will be demonstrated that with those solar cells reported parameters: J_{SC}, V_{OC}, FF and the efficiency, properly used in the Shockley's model for a pn junction, some valuable physic information that is not given can be obtained. Such physic information might constitute interesting feedback to reshape the cell design and its technology in the search of a higher efficiency. The method developed here has been applied to data of some of the most efficient solar cells reported, clearly reveling their main issues. Besides a non-fitting method to extract the saturation current, ideality factor and the parasitic series resistance will be presented.

Keywords
Solar Cells, High Performance, Charge Transport, Shockley Model, Tandem.

Reference

J. Benick, A. Richter, R. Mūller, H. Hauser, F. Feldmann, P. Krenckel, S. Riepe, F. Schindler, M. C. Schubert, M. Hermle, A.W. Bett, and S.W. Glunz, High-Efficiency n-Type HP mc Silicon Solar Cells, IEEE J. Photovolt. 7 (2017) 1171-1175. https://doi.org/10.1109/JPHOTOV.2017.2714139.

[SEM-60] CORRELATION BETWEEN PHYSICAL AND STRUCTURAL PROPERTIES OF PURE CdS AND DOPED WITH DIVALENT AND TRIVALENT CATIONS

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Chalcogenides semiconductors are an important material, in last decades the study was increases because they can be used in multiple applications trough the modulated properties, this control can be done by varying the experimental parameters, using ternary materials and because of doping. The influence of doping on CdS thin films was studied using the chemical bath deposition technique, it was employed Cu, La, Co Ni and La as dopants; the experimental conditions were at 75°C, stirring at 240 rpm, 120 min of the time deposition, pH was controlled at 10, and the doping ratio was varied from 1 to 10%. The CdS thin films doped with the different elements obtained from the various experiments, the optical properties, surface morphology and structural were studied. In the transmittance spectra the absorption edge showing different trends, particularly in the La film, the slope increases this due to the increase in disorder in the semiconductor lattice. The value of Eg decreases with the increase of doping for the case of Cu, Ni and La, while for Cobalt it increases. The films are made up of hemispherical particles, the size of the particles change with the percentage of doping and with the cation. The films are formed by a mixture of cubic and hexagonal phases, there is a small displacement of the highest intensity peak, towards a greater angle in divalent cations, and towards smaller angles for La. The Cu doped films showed the highest current in response to UV light, in contrast Co and La doped CdS-ITO thin films interfere with the photoelectric property of the composite, and there is no considerable change in the incidence of UV light. The Ni and Cu doped films showed photoelectrochemical stability at constant potential.

Keywords
CdS, doping materials, optical properties, electrochemical properties, CBD.

Reference

A. Aboud, A. Mukherjee, A. A. Mohamed y N. Revaprasadu, «The effect of Cudoping on CdS thin films deposited by the spray pyrolysis technique, » Journal of Materials and Technology, vol. 8, nº 2, 2019.

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SIP Project contract 20230370,20230123.

[SEM-235] SYNTHESIS AND CHARACTERIZATION OFDOPED ZNO THIN FILMS VIA SOL-GEL METHOD FOR SOLAR CELL APPLICATIONS

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Research focuses on the synthesis and characterization of thin films of ZnO incorporating carbon quantum dots (CQDs) derived from black garlic. The objective is to develop thin films that can be used in solar cells, taking advantage of the UV light absorbed by the CQDs and their ability to emit light in a broad spectrum.

The synthesis process involved two solutions of 10 ml of methanol, each containing 0.05 g and 0.015 g of black garlic powder, respectively, and 0.5 g of zinc acetate. The thin films were deposited on glass substrates using the sol-gel method. The substrates were immersed in the CQD solution in methanol for a few seconds and then subjected to a temperature of 120°C for 2 minutes. This process was repeated five times for each film. Two films were prepared for each CQD concentration and were heat-treated at 200 and 400°C for three hours, resulting in a total of four films.

The carbon quantum dots possess unique properties, such as their ability to absorb UV light and emit white light. These properties make them suitable for various applications, including solar cells. Zinc oxide (ZnO) is a semiconductor material that also exhibits desirable properties for solar cell applications.

The resulting films were characterized using UV-visible spectroscopy and photoluminescence techniques. These characterization methods provided valuable information about the optical properties and performance of the ZnO thin films incorporating carbon quantum dots.

In conclusion, this study successfully synthesized and characterized thin films of ZnO incorporating carbon quantum dots derived from black garlic. The characterization techniques provided insights into the optical properties and performance of the films, contributing to the understanding of their potential applications. The sol-gel method was used for the deposition of the films, offering a versatile approach for fabricating thin films with tailored properties.

Keywords
Thin films, CQDs, garlic peel, ZnO.

Reference

Jeevika A, Alagarsamy G, Celestina JJ. Biogenic synthesis of carbon quantum dots from garlic peel bio-waste for use as a fluorescent probe for sensing of quercetin. Luminescence. 2022 Nov;37(11):1991-2001. doi: 10.1002/bio.4381. Epub 2022 Sep 19. PMID: 36063384.

[SEM-146] DESIGN AND AUTOMATED DEVICE FOR THE DEPOSITION OF THIN FILM EMPLOYING SUCCESSIVE IONIC LAYER ADSORPTION AND REACTION (SILAR) METHOD

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Posgrado en Ingeniería Grupo de Opto-Mecatrónica, Tecnológico Nacional de México/Instituto Tecnológico de Tuxtla Gutiérrez, Chiapas, Mexico.

Non vacuum techniques are being applied to deposit thin film for the last decades. They are convenient, simple, and inexpensive to obtain thin film by solar cells. In recent years techniques like Electrodeposition, chemical bath deposition, spin coating, pulsed laser deposition, spray pyrolysis, Successive Ionic Layer Adsorption and Reaction (SILAR), are being automatized through a low-cost microcontroller open source (ARDUINO) which are adapting in an electromechanical system, where the challenge is performance the growth parameter of process. Here we present the design and development of a mechanical device using a SILAR process. The system has been controlled by an open-source Rasp berry Pi Pico with a Micropython language into the Thonny IDE (Integrate Development Environment). The thickness, optical and structural thin film has been controlled by number of cycles, dip time, rinse time, the horizontal axis speed. The machine performance was assessment by depositing Cu2ZnSnS4 (CZTS) compound. UV-Vis spectroscopy demonstrated a band gap of 1.34 eV for 40 cycles, X-ray diffraction, show the formation of CZTS in (220) phase orientation, RAMAN spectroscopy, revealed CZTS material in the range from 323 to 333 cm-1. The secondary phases disappear with 350ºC for 20 min in Nitrogen atmosphere.

Keywords
SILAR, CZTS, Solar Cell, design, automation.

Reference

Tsin, F., Venerosy, A., Vidal, et al. (2022). Design, implementation, and characterization of an automated SILAR system: validation with ZnO thin film deposition. The International Journal of Advanced Manufacturing Technology, 123(3-4), 1189-1201.

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[SEM-349] RESISTIVE HUMIDITY SENSOR BASED ON MCM-41 AND POLYMER

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Presently, sensors are used and demanded to develop diverse monitor systems making the humidity sensor one of the most used, because its measurement and control are essential not only for human comfort but also for technologies and industry applications. In this work, we developed a resistive device by depositing polymer and MCM-41 layers over cloth using a spin-coating technique. Electrical characterizations show that we have an electrical sensibility to humidity because the polymer conductivity changes when a moisture stimulus is applied.

Keywords
MCM-41, Polymer, humidity sensors.

Reference

Y. P. Bernal, «Síntese e Caracterização do Material Mesoporoso MCM-41 para o Desenvolvimiento de Capacitores MOS,» Pernambuco, 2015.

This work was supported by
CONAHCYT.
Proyectos VIEP BUAP.

[SEM-347] MOLECULAR BEAM EPITAXY OF InAs SEMICONDUCTOR QUANTUM DOTS CAPTURED WITHIN ASYMMETRIC (Al)GaAs CONFINEMENT BARRIERS

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The first solid state transistor successfully demonstrated in 1947 at Bell Laboratories is a good example of a bulk semiconductor device. At that decade, in spite that how primitive the devices and their production process can now be considered, undoubtedly revolutionized the electronics industry and provided of countless reliable applications like radio, tv, computers, and some others. ¾ of a Century later, a new era in semiconductor industry is envisioned to offer sort of the same innovations in electronic appliances, the Quantum devices. Recently emerged frontier knowledge areas entitled as quantum computing, quantum communication, quantum photonics, quantum encryption, and so on. The fundamental lego brick part to build up the former technologies is the Quantum Dot (QD), and to get them applied is becoming necessary to explore mechanisms to successfully stack several QDs layers. Nevertheless, during encapsulation effects such as intermixing, diffusion, segregation, and the strain itself change the nanoislands geometry and composition affecting the structural, optical and optoelectronic properties. In this work an in-situ study of self-assembling and encapsulation of InAs quantum dots (QDs) within asymmetric barriers of (Al)GaAs is presented. It is found that the reduced mobility of In adatoms conduced to larger QDs density, relieving interface strain and delaying the 2D to 3D growth mode transition for QDs grown on AlGaAs. The in-situ analysis shows that the mobility of In atoms decreases the mass transport of 2D and 3D precursors that leads to the self-assembling of QDs, modifying the rate of formation. During QDs capping it is observed that intermixing plays a predominant role. The nanoislands are less affected if covered by AlGaAs in comparison to the GaAs capping, preserving the QDs morphology and avoiding materials alloying. Lastly, numerical simulations were performed to evaluate the strain fields using the experimental information as input data.

Keywords
Quantum Dots, InAs, Strain, multistacking, asymmetric barriers.

Reference

C. A. Mercado-Ornelas, et al. In-situ study of InAs quantum dots encapsulated in asymmetric (Al)GaAs confinement barriers, Rev. Mex. Fís., 68, 3, (2022) 031002. https://doi.org/10.31349/RevMexFis.68.031002.

This work was supported by
The Laboratorio Nacional de Análisis Físicos, Químicos yBiológicos/UASLP, CONAHCYT CF-2023-I-1300, COPOCyT Fideicomiso 23871, and Investigadoras e Investigadores por México.

[SEM-264] ANALYSIS OF THE MOSS-BURSTEIN EFFECT IN TIN N-TYPE DOPED GaAs(631) AND GaAs(100) LAYERS GROWN BY MBE

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Self-assembly of nanostructures is a process where atoms or molecules spontaneously organize into ordered nanoscale structures or patterns without any human intervention. The spontaneous assembly is a consequence of interactions between the species reaching a thermodynamic equilibrium and reducing the system's free energy. At macroscale the researcher task consists to buildup the scenario that may propitiate the nanoscale interactions, throughout carefully varying macroscopic variables like, temperature, pressure, species density, etc. Therefore, for the synthesis of low dimensional semiconductor nanostructures, high precision over any variation of the macro variables is required, a demand that is fully satisfied by growth techniques like molecular beam epitaxy (MBE). The synthesis of self-assembled quantum wires (QWRs) attaining quasi-one-dimensional or fractional dimension eigenstates is a notorious example of the capabilities of MBE [1]. On the other hand, further applications in electrical and optoelectronic devices demand of the realization doped layers preserving the 1D order. The aim of this work is the investigation of the optical properties of Sn doping GaAs layers grown by MBE. n-type doping was observed despite of the crystallographic orientation. By analyzing the PL lineshape spectra of the tin-doped samples in the range of 1x1017 cm-3 to 1x1019 cm-3 a significant blueshift of the emission peak was observed as large as 150 meV. The shift, Moss-Burstein effect, is a phenomenon in which the apparent band gap of a semiconductor is increased as the absorption edge is pushed to higher energy. Nevertheless, the PL spectra analysis indicated that the emission energy present deviations of the well-known dependence of n1/3. Here we show that the PL emission is in fact composed by additional lines associated to the band-to-band transition (1.42eV) and tin-clustering (1.38eV). Finally, we propose a novel mechanism to acquire the actual fermi energy for high doped samples presenting the Moss-Burstein effect.

Keywords
MBE, Moss Burstein Effect, Photoluminescence, Tin-dopped, Quantum Wire.

Reference

F. E. Perea Parrales et al. Characterization of eigenstates interface-modulated in GaAs (631) multi-quantum well heterostructures. Journal of Applied Physics, Vol. 128, Issue 24, (2020). https://doi.org/10.1063/5.0029103.

This work was supported by

The Laboratorio Nacional de Análisis Físicos, Químicos y Biológicos/UASLP, CONAHCYT CF-2023-I-1300, COPOCyT Fideicomiso 23871, and Investigadoras e Investigadores por Mexico.

[SEM-91] GROWTH OF GaAsSb TERNARY EPITAXIAL LAYERS ON THE GAAS SIDE OF THE L-S PHASE DIAGRAM AT LOW TEMPERATURE

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Sb-containing III-V semiconductor materials are of interest for optoelectronic devices for the mid and far infrared range of electromagnetic waves. The devices structures require a precise control of the thickness of the growing epitaxial layers. In the liquid-phase epitaxy, the best thickness control occurs at lower temperatures. In this work we used supersaturated Ga-rich liquid phases, having the liquidus temperature of 580 C, to grow GaAsSb epitaxial layers on GaAs (100)-oriented substrates. The maximum allowed concentration of Sb in the solid phase was 7.5 % according to X-ray diffraction measurements.

With this composition, 3 epitaxial layers were grown for different times tgr of 30, 90, and 120 sec. AFM images showed that the surface relief of the samples is grain-structured or undulating in two perpendicular directions with the formation of islands elongated in the <110>. The undulation period and the base of the granules vary from 0.2 to 2 μm, and their heights are in the range of 5-30 nm.

In addition, the surfaces of the epitaxial layers contain nano-islands with the bases from 20 to 50 nm and the heights from 1 to 15 nm, which reach their maximum density of 109 cm-2 in the epitaxial layer grown for 120 seconds.

Positions of the photoluminescence spectra peaks taken at 14 K correspond to the transition energies between the conduction and valence bands for the samples grown at longer times of 90 and 120 sec. The photoluminescence line is significantly shifted toward higher energy for the epitaxial layer grown at the shortest time of 30 sec, that we attribute to the quantization of the state levels for electrons and holes.

Keywords
III-V semiconductors, LPE growth, Sb-contained materials, photoluminescence, low-dimension structures.

Reference

V.Donchev, M.Milanova, K.Kirilov, S.Georgiev, K.L.Kostov, G.M.Piana, G.Avdeev, Low-temperature LPE growth and characterization of GAAsSb layers for photovoltaic, Journal of Crystal Growth

This work was supported by
CONAHCYT, EL FONDO FAI DE UASLP

[SEM-325] QUASI-VAN DER WAALS EPITAXY OF ALUMINUM ARSENIDE (AlAs) ON GRAPHENE/GaAs SUBSTRATES: TEMPERATURE-DEPENDENT MORPHOLOGY

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Two-dimensional (2D) materials, such as Graphene (G), have garnered significant attention in the field of nanoscience and device engineering. Graphene, a single layer of carbon atoms arranged in a honeycomb lattice, exhibits extraordinary mechanical strength, high electrical conductivity, and exceptional electron mobility. The discovery of graphene has had a profound impact on various branches of science, including epitaxial techniques that utilize 2D materials for enabling van der Waals epitaxy of many types of III-V semiconductors, including nitride and arsenide families. Aluminum arsenide (AlAs) has emerged as a highly promising semiconductor material with unique properties and wide-ranging applications in advanced electronic devices. Its compatibility with other III-V semiconductors enables its integration into heterostructures to create optoelectronic devices [1]. In this work, we present the quasi-van der Waals epitaxy of AlAs using molecular beam epitaxy (MBE) for the first time. We utilized G/GaAs and GaAs substrates. The growth temperature of AlAs was varied within the range of 135 to 471°C, while maintaining a constant beam equivalent pressure (BEP) of Al and As in all growths, using migration-enhanced epitaxy (MEE) technique. Diffraction patterns of AlAs on both types of substrates were observed by Reflected High Energy Electron Diffraction (RHEED). Raman spectroscopy confirms the presence of a single graphene layer, with signals at 1591 and 2703 cm-1, corresponding to G and 2D bands, respectively. Scanning electron microscopy (SEM) images show the temperature-dependent behavior of AlAs morphology; we found that lower temperatures, as low as 135°C, promote a smoother surface, while higher temperatures, such as 471°C, show island nucleation.

Keywords
Graphene, Quasi-Vander Walls epitaxy, MBE, AlAs.

Reference

[1] Butkutė, R., Skapas, M., Selskis, A., Bukauskas, V., Stanionytė, S., & Niaura, G. AlAs as a Bi blocking barrier in GaAsBi multi-quantum wells: structural analysis. Lithuanian Journal of Physics, 57(1), 2017

This work was supported by
This work was supported by CONAHCYT project number CF-2023-I-1117.

[SEM-306] SYNTHESIS AND CHARACTERIZATION OF 3:1 BiOBr/BiOCl COMPOSITES IN THE PHOTOCATALYTIC DECOMPOSITION ON METHYL ORANGE

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Photocatalysts based on bismuth oxyhalides (BiOX, X=Cl, Br, I) have recently attracted the attention of the scientific community due to the possibility of efficiently exploiting visible light, in addition to their high chemical stability and being environmentally friendly, which makes them excellent candidates for the degradation of pollutants present in water. In particular, heterojunctions formed by the combination of BiOX compounds, such as BiOCl/BiOBr have proven to be an effective strategy to enhance photocatalytic activity. In this work, four samples of BiOBr/BiOCl with a 3:1 molar ratio were prepared using precipitation synthesized BiOBr and BiOCl, and their photocatalytic activity was compared with a $BiOBr_{0.75}Cl_{0.25}$ precipitation sample, and commercial TiO_2 P25. Samples were analyzed by XRD, TEM, Raman, and UV-Vis absorption, and their activity in photocatalytic decomposition of methyl orange was evaluated.

Keywords
BiOX composites, BiOCl, BiOBr, Heterojunctions, Precipitation.
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Universidad de Guadalajara

TRIBOLOGY, SURFACES AND INTERFACES

CHAIRMEN

Dr. Edgar Enrique Camps Carvajal (ININ), enrique.camps@inin.gob.mx
Dr. Enersto David García Bustos (CONAHCYT-UPVM), edgarciab@conahcyt.mx

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

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

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

[SIT-77] SYNTHESIS AND CHARACTERIZATION OF Al_xO_y THIN FILMS BY PULSED DC MAGNETRON SPUTTERING AT CONSTANT CURRENT AND CONSTANT POWER

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Reactive magnetron sputtering is a commonly used technique in the synthesis of coatings and thin films for industrial and technological applications. Typically, the optimal deposition conditions are determined through trial and error. Therefore, to ensure the reproducibility and efficiency of the process, it is important to understand the correlation between sputtering variables and their effects on the synthesized coatings. Optical emission spectroscopy (OES) has been utilized as a diagnostic and control technique in sputtering to monitor changes in plasma composition when experimental parameters are modified. In this study, Al_xO_y films were deposited using a pulsed DC power source under various duty cycles and with different reactive gas contents in the chamber. We investigated changes in the optical emission of the plasma during the synthesis of films at constant power and current, and examined their correlation with the optical and morphological properties of the films.

Keywords
Pulsed DC Reactive Magnetron Sputtering, OES, plasma, Al_xO_y thin films

Reference

P. J. Kelly, P. S. Henderson, R. D. Arnell, G. A. Roche, D. Carter, Reactive pulsed magnetron sputtering process for alumina films, J. Vac. Sci. Technol. A Vacuum, Surfaces, Film. 2000;18(6):2890-2896. https://doi.org/10.1116/1.1319679

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[SIT-195] STUDY OF THE WEAR OF CHITOSAN FILMS PRODUCED BY ELECTROCHEMICAL DEPOSITION ON A COPPER SUBSTRATE

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The electric isolation used on copper cables and wires in low voltage applications is a thermosetting polymer, which, when the cable or wire loses its usefulness, the polymer is not recycled, generating an abundant source of waste. This work presents the initial results of using a biodegradable polymer material (chitosan) like electric isolation. For this, chitosan coatings were prepared on copper substrates using an electrolytic process. The electrolyte consisted of a chitosan solution mixed with acetic acid, deionized water, and ethyl alcohol. The electrochemical cell consisted of the chitosan solution as the electrolyte, using copper as the cathode and a graphite cylinder as the anode. Deposits were made at different process times at 20 V, with and without an electrochemical surface preparation process before the deposition. The samples were characterized by XRD and optical microscopy. Also, their properties were studied by sliding wear, using a variant of microabrasion test without abrasive material. The marks were characterized by optical microscopy, which determined the wear mechanism as its wear resistance. The XRD pattern obtained from the prepared surfaces presented the Cu and CuO phases, while the coated surfaces presented the chitosan peaks. The wear rate was bigger on the coated surfaces because the chitosan coating offered a lower wear resistance than the copper substrate. The main wear mechanisms observed on the surfaces were abrasion, plastic deformation, and material transfer.

Keywords
Chitosan, Wear, Copper, Electrochimical cell, Copper oxide, Electrochimical process

Reference

Navarro, C. H., Moreno, Morquecho, A. A., Valdez, A. C., & Miranda, S. G. (2012, 16 noviembre). Preparation and tribological properties of chitosan/hydroxyapatite composite coatings applied on ultra high molecular weight polyethylene substrate. Journal of Plastic Film & Sheeting. https://journals.sagepub.com/doi/10.1177/8756087911434183.

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[SIT-219] ANALYSIS OF ADHESION ON COATING USING NORM ISO STANDARD

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The adherence of borided AISI 01 steel was analyzed to substantially optimize its occupation in the manufacturing industry. The boriding treatment was realized by dehydrated boron paste on AISI O1 steel; The treatment temperatures used at 850°C, 900°C, 950°C and 1000 °C for 1, 2, 3 and 4 h. The evaluation of the adhesion on the iron boride coating was using Rockwell indentation in accordance by the norm ISO 26442: 2008-06. Type class using optical microscopy evaluated craters and/or indentations produced with Rockwell indentation. The coatings generated at 850 °C with the permanence times show class 1 and 2, due to the presence of small radial cracks and low presence of delamination. The coatings formed at 900 °C with the exposure times indicated a class 1 and 0 adhesion, due to absence of delamination and low radial cracks or fissures. For the coatings obtained at 950 with the permanence times, evidence class 1 and 2, due to delamination around the indentation mark. The coatings obtained at 1000°C are classified as class 1 and 2, due to the type of delamination and crack propagation. The study contributes the adhesion classification, based on the ISO 26443: 2008-06 standard for adhesion classification on hard coatings

Keywords
Adhesion, Boriding, Rockwell indentation

Reference

Zhiquan Huang, Jianming Wang, Ann Zammit, Joseph Buhagiar, Glenn Cassar, Xiyu Zhang, Jian Chen, Investigation on the failure mechanism of graphite-like carbon coatings under cavitation erosion in distilled water, Surface and Coatings Technology, 467 (2023), pp 129686. doi.org/10.1016/j.surfcoat.2023.129686.

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Universidad de Sonora and Universidad Politecnica del Valle de Mexico, Grupo ciencia e ingenieria de materiales.

[SIT-20] OPTIMIZATION OF POLYMERIC MIXTURE WITH REUSED AND NEW MATERIALS FOR THE MANUFACTURING INDUSTRY.

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The present assignment has of purpose the analysis of the micro hardness of the polystyrene with black masterbatch, so that we can find the differences between using different percentages of material new-recycled. The 5 samples that were obtained were injection inlet channels, that go from 100% of recycled material till 100% of new material (virgen) with intervals of 25% between each simple. After performing 50 indentations under the method of micro hardness Vickers, the results show that there does exist differences in using more than 50% of recycled material against using 100% therefore we can conclude that if we use a mixture with the 75% of recycled material or more, we obtain less resistance to penetration on the colored polystyrene and from using a mixture with 50% recycled and 50% virgin, a greater resistance to penetration is obtained. At the beginning of this assignment, the proposol was that the ideal mixture would be 75% recycled and 25% virgin, but based on the data obtained this is not possible.

Keywords
Polystyrene, micro hardness, material new-reused, hardness Vickers, resistance to penetration

Reference

Chanya Chuenarrom, P. B. (2009). Effect of Indentation Load and Time on Knoop and Vickers Microhardness Tests for Enamel and Dentin. Materials Research,476.
Hao Wu, F. D. (2022). On the Application of Vickers Micro Hardness Testing to Isotactic Polypropylene. polymers,16.

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Universidad Politécnica del Valle de México (UPVM)

[SIT-182] FINITE ELEMENT STUDY OF CUTTER ROLLS WITH DIFFERENT SURFACE TREATMENTS USED IN THE MANUFACTURING INDUSTRY

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Universidad Politecnica del Valle de México, Estado de México, Mexico.

One of the main objectives and challenges that the industry currently faces is to achieve high levels of performance and efficiency of the processes, however the complexity and number of sub-process, that are involved in this complicated task, so the behavior of a D2 types steel cutting roller will be analysed in detail with various surface treatments to evaluate the useful life of the blade without losing mechanical properties that make this steel one of the most used in the industry.

Therefore, in this article the analysis, behaviors and functionality will be shown in a computational way by FEM to AISI D2 steel with two types of surface coatings.

Keywords
FEM, Steel D2, cutter rolls, surface treatments, borurado

Reference

Medina, A.L. (2013). Endurecimiento superficial por nitruacion en baño de sales de un acero grado herramienta AISI H13. Escuela superior de ingeneria Mecanica y Electrica

This work was supported by
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[SIT-216] STUDY OF THE CORROSION ATTACK ON BORIDE AND NON-BORIDE SURFACES OF AISI 8620 IN NaCl SOLUTION

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The maritime industry is a high-demand work environment, especially for the high corrosion attack produced during the operations. Several parts of the mechanical system that work under this environment are made of AISI 8620 steel, showing a low lifetime due to the corrosion wear of the surfaces. For that, several projects have been dedicated to reducing these effects on the surfaces by modifying the surface characteristics with the deposition or generation of a layer that reduces the corrosion effects of the parts. This work studies the corrosion effects of the boride and non-boride surfaces in an electrochemical cell using a NaCl solution. The boride surfaces were produced with a thermochemical using recycled dehydrated paste at 1123, 1173, 1223, and 1273 K for 2 and 4 hrs. The structure and morphology of the surfaces were characterized using XRD diffraction and optical microscopy. At the same time, corrosion tests were carried out with an electrochemical cell using NaCl solution in deionized water at 3.5% (volume) with a graphite electrode at 3 and 9 VDC for 10 min. The wear marks were studied with optical microscopy on the surfaces and transversal section. These tests showed that the sample at 1223 K at 4 hr presented the best corrosion resistance because this layer had the higher thickness.

Keywords
Boride, corrosion, steel AISI 8620, abrasion, galvanic cell

Reference

M.Y. García-Santibañez, J.G. Quiñones-Galván, N. López-Perrusquia, M.A. Doñu-Ruiz, E. García, Study of wear processes generated by cavitation phenomena produced by laser induced dielectric breakdown on borided and non-borided 316L stainless steel surfaces in bi-distilled water, Materials Letters, 343, 2023, 134397

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Sesión Oral

[SIT-82] MICROSTRUCTURAL BEHAVIOR OF THE Ti-Al-Mo-N SYSTEM CONTROLLED BY Mo CONTENT: IMPACT ON THE MECHANICAL AND ANTICORROSIVE PERFORMANCE

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Transition metal nitrides (TMNs) are one of the most exploited coatings to improve the lifetime of a wide variety of industrial machining tools. To follow the growing demands of hi-Tec industrial machining, TMNs have been upgraded from the representative binary compound Ti-N to pseudo-binary (e.g., Ti-Al-N) and even pseudo-ternary (e.g., Ti-Al-Mo-N) systems. However, the final performance of the TMN coatings depends upon the elemental composition, together with their microstructure and morphology. Here, we show that Mo content variation from 14 to 33 at.% controls the mechanical and anticorrosive behavior of Ti-Al-Mo-N sputtering coatings. We found that, for the lower Mo contents explored, a B1 NaCl-type phase is predominant, leading to columnar morphology in those coatings. For the highest Mo content, a phase mixture containing B1 and tetragonal β-Mo_2N-type leads to dramatic changes in key morphological parameters due to the crystal growth evolution. The best mechanical performance (20.96 GPa hardness, 366.49 GPa Young's modulus, and highest scratching resistance) was achieved with the coatings with B1 structure, while the lowest corrosion rate (6.2 μA/cm^2) was shown by the coating with β phase. These results could contribute to tailoring tool protective coatings based on selection and optimization of alloying elements with specific purposes, showing a path to control their performance through the variation of the Mo content. Our findings could have a significant impact on the design and optimization of more complex systems, suggesting other applications such as anticorrosive coatings based on multi-element nitrides.

Keywords

Ti-Al-Mo-N coatings, B1 to β-Mo2N phase transition, Microstructural evolution

Reference

T. Gao, L. Yu, G. Lu, et al., Influence of Mo content on properties of Ti–Al–Mo–N films, Surf Eng. 0 (2020) 1–8. https://doi.org/10.1080/02670844.2020.1807814

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[SIT-112] DESIGN OF IMMISCIBLE AND ISOMORPHIC METALLIC ELEMENT INTERFACES

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Elements with compact hexagonal lattice structures have attracted the attention of the scientific community by reporting that: on the surface, at the grain boundary, and at the different interfaces, they inhibit considerable damage generated by continuous exposure to ionizing radiation, such as the so-called radiation induced embrittlement. Elements with this behavior and structure are among others: titanium and magnesium, which in addition to being light and having high resistance, make them highly desirable elements, both in science and in industrial and technological applications. In particular, this work focuses on generating nanostructured films (≤100 nm) of these high-purity elements, completely separated from each other, with the purpose of generate well-defined interfaces between them, to later build a greater number of these interfaces between them and achieve maximum efficiency for the desired purpose, which is: to inhibit damage by ionizing radiation.

Through a Pulsed Laser Ablation System, which has the necessary equipment to support totally independent targets, it has been possible to generate high purity magnesium nanostructured films with a preferential crystallographic structure, as reported by XRD analyses. However, in the case of nanostructured titanium films, this has not been the case, since they tend to oxidize at low ion kinetic energy during the Pulsed Laser Ablation process, a necessary condition to generate multilayers and therefore interfaces, a situation that has led to detailed studies of the nanostructured layers generated from each element separately.

Keywords
Nanostructured films, Titanium Magnesium, Pulsed Laser Ablation
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[SIT-100] DEPOSITION OF GaN THIN FILMS USING A HYBRID PLASMA SYSTEM

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The hybrid plasma used in this work was created by combining a stationary microwave ECR (with magnetic field) discharge using nitrogen as the working gas, and the plasma formed during the pulsed laser ablation of a GaAs solid target. The pulsed plasma propagates perpendicularly through the microwave plasma flux. The hybrid plasma was created at a working pressure of 6 x 10-4 Torr. Plasma parameters such as density, electron temperature and mean kinetic ion energy were determined using Langmuir probes. The optical emission spectroscopy measurements showed a significant improvement of the excited species present in the hybrid plasma in comparison with the individual plasmas. The characteristics of the GaN thin films deposited at different experimental conditions, such as the proportion of nitrogen in the working gas, the mean kinetic energy of ions produced during the ablation process were studied by means of XPS, Raman spectroscopy and XRD.

Keywords
GaN thin films, microwave plasma, pulsed laser ablation
This work was supported by
National Institute for Nuclear Research

[SIT-181] STUDY OF CAVITATION PRODUCED BY LASER-INDUCED DIELECTRIC BREAKDOWN ON BORIDED AND NON-BORIDED AISI 316L STAINLESS STEEL SURFACES

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The cavitation wear process is one of the main phenomena in hydromechanical systems due to the reduction of its efficiency in generating noise, vibration, and cavitation erosion. Nevertheless, this process has several useful applications, such as ultrasonic cleaning, mixture, and homogenization of different solutions. For that, this work presents the study of the wear produced on boride and not-boride surfaces of AISI 316L stainless steel (SS) surface, produced by the cavitation phenomena generated by a dielectric breakdown in bi-distilled water. Several samples of AISI 316L SS were boride at 800°C with a time of 1, 3, 5, and 7 hr, using dehydratase boron past. The boride and non-boride samples' structure, morphology, and topography were characterized using XRD and SEM. At the same time, the cavitation wear tests were carried out using a Nd:YAG laser emitting at 1064 nm, with the output energy of 750 mj in a parallel configuration of the sample with the focused beam. The wear resistance was determined using the lost weight of the samples. The boride surfaces presented the FeB and Fe2B phases combined with layer thickness from 4.8 to 28 μm for the films at 1 and 7 hr. The cavitation produced on the non-boride samples caused the erosion of surfaces with the combination of thermal and mechanical marks. In contrast, on the boride surfaces, the erosion of material revealed the microstructure of the films, being the sample with 7 hrs of treatment presented the best wear resistance.

Keywords
Cavitation, Boride, Wear, Dielectric breakdown.

Reference

Study of wear processes generated by cavitation phenomena produced by laser induced dielectric breakdown on borided and non-borided 316L stainless steel surfaces in bi-distilled water, Materials Letters, 2023, ISSN 0167-577X, https://doi.org/10.1016/j.matlet.2023.134397.

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THEORY AND SIMULATIONS OF MATERIALS

CHAIRMEN

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

The topics include (but are not limited to)

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

[TSM-95] OPTIMIZATION OF LINEAR AND NON-LINEAR CLUSTER-CHAINS OF Au AND Ag NPs FOR SERS APPLICATION

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Clusters of plasmonic nanoparticles (NPs) have been used as SERS substrates for the detection of different molecules. In particular, clusters of a few particles form chains or necklaces where the main feature is a small gap between adjacent NPs [1]. Moreover, the length of all gaps is not the same in a cluster-chain. In the gaps is located the spatial section where the electric field is intense (hot spots) related to the SERS enhancement factor under the fourth power approximation. In this work, we show the results of the near-electric field of chains up to 10 NPs of Au and Ag. In order to optimize the SERS enhancement factor, we have considered as parameters the size and separation distance between the NPs. We varied the NPs position parallel and perpendicular to the chain axis. The chains were modeled by using the discrete dipole approximation and an excitation wavelength of 632 nm. For all the cases, the chains presented a higher near-electric field strength in the gaps between the metallic NPs. We present color maps showing E vs dg vs N, where E is the field intensity, dg is the gap length and N is the NPs number. The separation distance, the size, and the number of NPs in a chain is relevant because it affects the near-electric field, and subsequently the SERS enhancement factor.

Keywords
hot spots, DDA, chains, Au, Ag

Reference

[1] D. Majumdar, A. Singha, P. K. Mondal, and S. Kundu. DNA-Mediated Wirelike Clusters of Silver Nanoparticles: An Ultrasensitive SERS Substrate, ACS Appl. Mater. Interfaces 5 (2013) 7798-7807. https://pubs.acs.org/doi/10.1021/am402448j.

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[TSM-183] AB INITIO STUDY OF THE ELECTRONIC AND OPTICAL PROPERTIES OF $BiFeO_3$ BY GGA+U

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Density functional theory (DFT) using the on-site Hubbard U correction (DFT+U) was implemented within the generalized gradient approximation (GGA) to investigate the structural, electronic and optical properties of the strongly correlated $BiFeO_3$ (BFO) insulator system. Because in each FeO_6 octahedra of the BFO structure the Fe-O bonds generate a strong correlation between the 3d states of Fe and the 2p states of the oxygen atom, the Hubbard correction has been used for both the O-2p and Fe-3d states. The effective values of the U parameter were obtained in a self-consistent procedure, using linear response theory as it is implemented in Quantum ESPRESSO (QE) package. We have found that the effective U-values, of 4.06 eV for both the Fe-3d and for the O-2p states in the trigonal structure of $BiFeO_3$, results in a direct band gap of 2.50 eV. Our obtained values, within this DFT+U framework, are discussed and compared with available experimental and theoretical data.

Keywords
Hubbard correction, Linear response theory, $BiFeO_3$, GGA, Band Gap

Reference

S. Ghosal et al., "Importance of the Hubbard U parameter to explore accurate electronic and optical behaviour of $BiFeO_3$", J. Phys. D: Appl. Phys. (2022) 55 375303 DOI 10.1088/1361-6463/ac761a

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[TSM-213] AB INITIO STUDY OF SO_2 ADSORPTION ON Ag-DOPED $BaTiO_3$(001)2X2 SURFACE

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SO_2 emissions due to industrial processes and natural sources have caused significant environmental and human health effects. Numerous experimental and theoretical studies have been performed to acquire insight into the adsorption and transformation mechanism of SO_2. In this work, an ab initio study of the SO_2 adsorption on the $BaTiO_3$(001)2x2 surface has been performed. Total energy calculations have been done in the PWscf code of Quantum Espresso within the density functional theory. The exchange-correlation energies are treated within the generalized gradient approximation (GGA). Pseudopotentials were employed for representing the interaction between ionic cores and valence electrons. Different configurations were considered for SO2 adsorption. To study the dissociation process of SO_2 on the Ag-doped BaTiO3(001)-2x2 surface, the Nudge Elastic Band (NEB) calculations were performed.

Keywords
$BaTiO_3$, SO_2, NEB, adsorption, DFT

Reference

G. Rakotovelo, P.S. Moussounda, M.F. Haroun, P. Légaré, A. Rakotomahevitra, M. Rakotomalala, J.C. Parlebas, Adsorption of CO, CO_2 and NO molecules on a $BaTiO_3$ (001) surface, Surface Science, Volume 603, Issue 9, (2009). https://doi.org/10.1016/j.susc.2009.03.006.

This work was supported by

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[TSM-12] A CANDIDATE EXCHANGE-BIASED VDW HETEROSTRUCTURE BASED ON Cr_2NO_2 AND Cr_2CF_2 MXenes

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Centro de Nanociencias y Nanotecnologia CNyN-UNAM, Baja California, Mexico.

By spin-polarized first-principles calculations, we investigated the Van de Waals heterostructure Cr2NO2/Cr2CF2. The aim is to create 2D FM/AFM heterostructures where the exchange bias effect can occur. Cr2NO2 MXene is a half-metal ferromagnetic material, while Cr2CF2 MXene is an antiferromagnetic semiconductor. The lattice mismatch of both MXenes is ~4%, good enough to construct the heterostructure. Three different stackings were considered in the heterostructure: H3, T4, and Top. Also, three different cell parameters are considered: larger lattice constant a(Cr2CF2), shorter lattice constant a(Cr2NO2), and both relaxed. In all cases, T4 staking is the most favorable interaction configuration. Non-covalent interactions show that Van der Waals forces dominate in the heterostructure. Also, the average electrostatic potential along the z-axis explains the stability in the T4 stacking. Antiferromagnetic coupling is the most stable when fixing a(Cr2CF2) as the heterostructure lattice parameter, while for the short lattice constant, a(Cr2NO2), the magnetic coupling becomes Ferromagnetic. Band diagrams evidence that both MXenes preserve their electronic properties after the interaction, so the antiferromagnetic alignment is intrinsic in the heterostructure for the larger lattice constant. Our theoretical findings open the door to consider the versatile MXenes as promising candidates for the new generation of information storage nanodevices.

Keywords
MXenes, Exchange Bias, Magnetism, Heterostructure
This work was supported by
We thank DGAPA-UNAM projects IA100822 and IN101523 for partial financial support. Calculations were performed in the DGTIC-UNAM Supercomputing Center projects LANCAD-UNAM-DGTIC-150, LANCAD-UNAM-DGTIC-368, and LANCAD-UNAM-DGTIC-422.

[TSM-174] ADSORPTION OF THE SCl_2 MOLECULE ON THE DOPED-BORON PHOSPHIDE MONOLAYER

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The growing population as well as the rapid development of the industry have substantially affected the environmental quality. Nowadays, special importance has been placed on the management of chemical sub-products that cause environmental contamination and affect human health. For example, sulphur dichloride (SCl_2) is widely used in the industry as insecticide and in organic synthesis. This pollutant is highly toxic for human health as well and it could induce burning, sore or even fatal consequences. In recent decades, atomic two-dimensional (2D) materials are gaining great attention due to their superior electronic, optical, and mechanical properties [1]. Motivated by the current problems of environmental contamination and the excellent physical properties of 2D materials, we have studied the structural and electronic properties of the doped-boron phosphide monolayer interacting with the SCl_2 molecule, using the density functional theory (DFT). The results showed that the SCl_2 molecule has a high adsorption energy and the electronic structures after doping show wide variety of properties that differ from the pristine BP. Therefore, our results suggest that the BP monolayer can be considered as a promising candidate to solve different current environmental pollution problems.

Keywords
Monolayer, DFT, electronic properties, SCl2, Adsorption, sensors

Reference

[1] W, Shao-feng; W, Xiao-jun, First-Principles Study on Electronic and Optical Properties of Graphene-Like Boron Phosphide Sheets. Chinese J. Chem. Physics, 28(5), (2015) 588–594.

This work was supported by

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[TSM-186] AB INITIO BOND ELASTIC CONSTANTS IN β12-BOROPHENE

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In recent years, the exploration of two-dimensional (2D) materials has unveiled a fascinating realm of unique properties and promising applications. Among these emerging materials, borophene has attracted significant attention due to its remarkable electronic, thermal, and mechanical characteristics. Specifically, β12-borophene, which is composed of a single layer of boron atoms arranged in a hexagonal lattice, has exhibited exceptional mechanical properties that make it an intriguing candidate for various nanoscale applications. Understanding the mechanical behavior of β12-borophene is essential for its successful integration into future nanodevices and nanomechanical systems. With its unique atomic structure and exceptional properties, β12-borophene has the potential to outperform other 2D materials, such as graphene and molybdenum disulfide, in certain applications that demand high strength, flexibility, and stability.

Elastic bond constants are useful in finite element-based predictive models for nanostructures. In this work we calculate the mechanical properties, in particular the bond constants Kr and Kɵ that are obtained from isotropic and axial strains, respectively. We perform calculations using density functional theory (DFT), in VASP code, using the GGA correlation exchange potential without spin polarization, 400 eV cutoff energy, and a 10x10x10 k-point grid for all calculations.

Keywords
Borophene, bonding elastic constants, nanomaterials.

Reference

Mortazavi, B. et al. (2016) 'Mechanical responses of Borophene Sheets: A first-principles study', Physical Chemistry Chemical Physics, 18(39), pp. 27405–27413. doi:10.1039/c6cp03828j.

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Universidad Autónoma de Yucatán, Facultad de Ingeniería.

[TSM-188] FIRST PRINCIPLES INVESTIGATION OF MOLECULAR HYDROGEN ADSORPTION ON β12-BOROPHENE

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In recent years, two-dimensional (2D) structures have garnered significant attention due to their unique electronic, mechanical, and chemical properties. borophene, a single-layer boron sheet, has emerged as a promising 2D material due to its exceptional strength, high thermal conductivity, and intriguing electronic characteristics. One particular form of borophene, known as β12-borophene, exhibits a honeycomb lattice structure with alternating hexagonal and triangular boron rings.

The efficient storage and controlled release of hydrogen are vital for a wide range of applications, including hydrogen fuel cells and energy storage devices. Therefore, investigating the adsorption properties of hydrogen on 2D materials like borophene has become an active area of research. Understanding the interaction between hydrogen molecules and β12-borophene at the atomic level is crucial for designing efficient hydrogen storage materials and enhancing their performance. In this investigation we present the results of our first principles calculations, utilizing density functional theory (DFT) methods, to investigate the adsorption behavior of molecular hydrogen on β12-borophene, using VASP code with GGA for exchange correlation energy and Van del Waals D3 correction.

Keywords
Borophene, hydrogen, adsorption, storage, nanomaterials.

Reference

Ledwaba, K., Karimzadeh, S. and Jen, T.-C. (2023) 'Emerging borophene two-dimensional nanomaterials for hydrogen storage', Materials Today Sustainability, 22, p. 100412. doi:10.1016/j.mtsust.2023.100412.

This work was supported by
Universidad Autónoma de Yucatán, Facultad de Ingeniería.

[TSM-200] STRUCTURAL AND ELECTRONIC PROPERTIES OF CARBON AND BORON NANOTUBES (BC_2NNTS) WITH CISPLATIN: A DFT STUDY

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Currently, different drugs are used in the treatment of diseases such as cancer. It is known that platinum coordination complexes are antineoplastics. Their anticancer activities are related to the alteration of the DNA configuration since they prevent damage to cells. However, the complexes make no distinction between healthy and damaged cells, therefore their encapsulation in nanotubes would represent a solution to the interactions with the healthy cells. In this work, the structural and electronic properties of boron carbon nitride nanotubes (BC_2NNTs) and their interaction with the anticancer drug (cisplatin) have been investigated. Studies have been done by calculating the total energy using first principles theories within the density functional theory (DFT) as developed in the PWscf code of the Quantum ESPRESSO package. The exchange–correlation energies are treated within the generalized gradient approximation (GGA). The electron-ion interactions are treated by using pseudopotential methods.

Keywords
Nanotubes, cisplatin, DFT

Reference

R. Klingeler, R.B. Sim, Carbon nanotubes for biomedical applications (2011) Springer Berlin, Heidelberg.https://doi.org/10.1007/978-3-642-14802-6.

This work was supported by

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[TSM-278] SURFACE MORPHOLOGY EFFECTS ON THE MECHANICAL AND ELECTRONIC PROPERTIES OF HALOGENATED POROUS 3C-SIC: A DFT STUDY

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Silicon carbide nanostructures have been widely studied due to its potential technological applications. However, the theoretical characterization, especially the effect of surface on the mechanical properties of this material is still underexplored. In this work, we report the electronic and mechanical properties of 3C-SiC nanopores with different pore surfaces and different passivation schemes using a density functional theory approach and the supercell technique. The nanopores were modelled by removing columns of atoms in the [0 0 1] direction, thus creating four types of pores, two with an Only C or Si pore and two with a C or Si-Rich pore surface. All surfaces were passivated with hydrogen, then some atoms of H were replaced with fluorine and chlorine. Results show that pores with a higher concentration of C on the surface have a larger bandgap compared with the Si cases. Moreover, only few changes can be observed due to passivation. For the mechanical properties the Bulk and Young's modulus were calculated and show that the Only C structures were the most brittle and, for almost all the pores, the H + Cl passivation improve the Bulk modulus.

Keywords
Porous-Silicon-Carbide, Mechanical-Properties, DFT.

Reference

R. Bermeo-Campos *et al,* Applied Surface Science, 631 (2023), 157481,0169-4332, DOI: https://doi.org/10.1016/j.apsusc.2023.157481.

This work was supported by

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[TSM-296] GEOMETRIC QUANTIFICATION OF CHIRALITY IN CARBON NANOTUBES

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Chirality is very important property in nanomaterials due to the possible implications in asymmetric catalysis processes and chiroptical phenomena. Carbon nanotubes can be classified according to their chiral vector, with several important properties depending on it. In this work we use the Hausdorff chirality measure (HCM) to geometrically quantify the chirality of several carbon nanotubes with different chiral vectors, in order to get insights into the optical response of carbon nanotubes.

Keywords
HCM, chirality, quantification, carbon nanotubes.

Reference

J. Jesús Pelayo, Robert L. Whetten, and Ignacio L. Garzón. Geometric Quantification of Chirality in Ligand-Protected Metal Clusters**,** The Journal of Physical Chemistry C 2015 119 (51), 28666-28678**.** DOI: 10.1021/acs.jpcc.5b10235

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[TSM-318] THEORETICAL STUDY OF THE RELATIONSHIP BETWEEN THE STRUCTURE AND THE ELECTRONIC PROPERTIES OF SrZrO3 NANOWIRES USING DFT

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The theoretical study was carried out using the Quantum Espresso code supported by the density functional theory (DFT) determining the relationship of the electronic properties in one-dimensional systems (nanowires, 1D) of SrZrO3 with respect to its structure [1] with directions of growth [100] and [110] and various sizes of formation units (FU) of 2x2 and 3x3. In the first part of the study, the test wavefunction and the k-point network were optimized for a pseudopotential of the generalized gradient approximation (GGA) of type PBE, with the aim of performing the geometric optimization of the systems in the axis of growth (Z), obtaining the lattice parameters that minimize energy, with values of 4.035 and 4.109 Ang for the direction of growth [100] 2x2 and 3x3 respectively, while in the direction of growth [110] values of 5.810 and 5.810 were obtained. 5,869 Ang for 2x2 and 3x3. For the second part of the study, the calculation of the electronic properties of the system was carried out, obtaining the band structure and the density of electronic states [2], to know the behavior of the forbidden energy band of the systems, before structural changes when increasing the number of FU, resulting in an indirect forbidden energy gap in the grown in the direction [100] with values of 2.268 and 2.095 eV for 2x2 and 3x3, while for the grown in the direction [110] a direct transition was obtained with energies of 1.624 and 1.059 eV in 2x2 and 3x3 respectively, thus determining the strong link of electronic properties with the shape, structure and number of atoms of a multielectronic system.

Keywords
Nanowires, DFT, electronic gap, Fermi

Reference

[1] Nazir, G.;et al, S. Putting DFT to the trial: First principles pressure dependent analysis on optical properties of cubic perovskite $SrZrO_3$. Comput. Condens. Matter 2015.

This work was supported by
Laboratorio Nacional de Supercómputo del Sureste de México.

[TSM-334] THERMAL FINITE DIFFUSION TIME SOLUTION OF THE ONE-DIMENSIONAL WAVE EQUATION FOR THE LASER INDUCED ULTRASOUND

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In this work a thermally corrected solution of the one-dimensional acoustic wave equation for the laser induced ultrasound (LIU) is presented. The conversion of electromagnetic radiation from the Laser into heat on a semi-infinite plane sample is modeled via de Maxwell-Cattaneo-Vernotte (MCV) differential equation, which introduces a heat diffusion time, into consider a finite propagation speed for heat, known in the literature as second sound; opposite to the instantaneous heat diffusion process characteristic of the widely used Fourier heat diffusion equation. The coupled differential equations for temperature and pressure are exactly solved in the frequency domain. This model is then compared with Fourier thermal propagation with and without thermal confinement approximation.

Keywords
Photoacoustics, Utrasound, Mathematical modelling

Reference

Misael Ruiz-Veloz, Geminiano Martínez-Ponce, Rafael I. Fernández-Ayala, Rigoberto Castro-Beltrán, Luis Polo-Parada, Bartolome Reyes-Ramírez, Gerardo Gutiérrez-Juárez; Thermally corrected solutions of the one-dimensional wave equation for the laser-induced ultrasound. Journal of Applied Physics 14 July 2021; 130 (2): 025104. https://doi.org/10.1063/5.0050895

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[TSM-338] GEOMETRICAL METHODS TO BUILD THEORETICALLY VAN DER WAALS HETEROSTRUCTURES: A REAL AND RECIPROCAL SPACE APPROACH.

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The vertical stacking mechanism of atomic layers, with different electronic properties to build a novel two-dimensional (2D) heterostructure with applications in nanoelectronics and optoelectronic industry, is of current interest since the success of mechanical exfoliation of graphene monolayer in 2004 [1]. Theoretically, this means to build and then study a commensurate 2D layered heterostructure where the Fourier transformations and the Bloch theorem can be applied as in Solid State Physics. This is due to a common periodicity in every layer in a heterogenous multilayer system. Hence, the goal of this work is to show a general Python computational code which generates commensurable 2D van der Waals heterostructures with more than 2 layers, different Bravais lattices, initial stacking, and chirality. The methodology is based on basics of crystallography, geometrical and algebra concepts developed with Python code. This implementation can be considered better than other previous developments such as CellMatch, Twister y Supercell-Core packages due to simplicity and flexibility for the users. The computational code delivers basic information such as lattice vectors, atomic positions in fractional coordinates in real space, and representation of every monolayer primitive cell in terms of the supercell lattice vectors in reciprocal space. This is essential to quantify the number of Bragg diffractions in reciprocal space resulting in the formation of minigaps shown in the electronic band dispersion. A hot topic currently in Solid State Physics and Electronic Structure of Materials. Finally, some results of graphene multilayer systems will be discussed to show the potentiality of this computational approach.

Keywords
Two-Dimensional, Heterostructures, Periodic Supercell, Multilayer, Python code

Reference

Geim, A. K., & Novoselov, K. S. (2007). The rise of graphene. Nature materials, 6(3), 183-191.

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Sesión Oral

[TSM-285] PREDICTION OF POTENTIAL MAGNETIC TUNNELING JUNCTIONS WITH SPIN POLARIZATION IN VAN DER WAALS MONOLAYER HETEROSTRUCTURES MA_2X_4: A FIRST-PRINCIPLES STUDY

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Currently, the widespread adoption of technology and its rapid advancement contribute to the disposal of millions of tons of electronic devices every year. These devices contain rare earths and heavy metals, which, when improperly discarded, can contaminate soil and groundwater. Moreover, the processing of these materials during manufacturing exacerbates the environmental impact. Within this context, spintronics, a technology that is still undergoing refinement, also faces similar challenges. In order to explore an alternative, this study investigated van der Waals heterostructures composed of MA_2X_4 monolayers for their potential use as magnetic tunnel junctions in spintronic devices. The first step involved utilizing a 1x3 supercell for the stacking of monolayers, and the Grimme method was employed to correct for van der Waals dispersion considerations. Furthermore, spin polarization and spin-orbit coupling tests were conducted at various angles, both transverse to the heterostructure in a general sense and atomically for magnetic elements such as Mn and Fe. Subsequently, electronic properties and density of states were calculated to identify atoms and their orbitals with a greater contribution to the magnetic effects.

Keywords
MXene, heterostructure, nitrides, magnetic moment, MTJ's

Reference

Wu, Q., & Ang, L. K. (2022). Giant tunneling magnetoresistance in atomically thin VSi2N4/MoSi2N4/VSi2N4magnetic tunnel junction. Applied Physics Letters, 120(2). https://doi.org/10.1063/5.0075046

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[TSM-17] STUDY OF THE THERMOELECTRIC PROPERTIES OF $AGBI_3S_4Se$ AND $AgBi_3SSe_4$ BY FIRSTPRINCIPLES METHODS.

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The electronic and thermoelectric properties were calculated for the thermoelectric materials $AgBi_3S_4Se$ and $AgBi_3SSe_4$, using Density Functional Theory (DFT) and the recent BoltzTraP2 program for the calculation of transport coefficients in a Semiclassical way. These materials are intermediate systems of the $AgBi_3S_5$ and $AgBi_3Se_5$ materials which are promising for materials science, because they present very good thermoelectric properties. The aim is to determine the thermoelectric properties of $AgBi_3S_4Se$ and $AgBi_3SSe_4$. For the calculation of the density of states, the method of first principles LAPW+lo was used. The 2009 Becke-Johnson modified Tran-Blaha potential (TB-mBJ) was used for the exchange-correlation potential. The study of the electronic properties shows that the total DOS of $AgBi_3S_4Se$ and $AgBi_3SSe_4$ are similar in the region close to the Fermi energy. The Seebeck coefficient, electrical conductivity, thermal conductivity and ZT of $AgBi_3S_4Se$ and $AgBi_3SSe_4$ corresponded with the experimental results. $AgBi_3SSe_4$ presents better ZT values in the temperature range from 1500 to 800 K, because in this temperature range this material presents a better Seebeck coefficient. The highest value for ZT was 0.528 for $AgBi_3SSe_4$ at the temperature of 800 K.

Keywords
Density of states; Thermoelectric properties; thermoelectric materials.

Reference

[1] W. Yutian, S. Xianli, Y. Dongwang, Z. Qingjie and T. Xinfeng, ACS Appl. Mater. Interfaces, **13**, 4185–4191, 2021.
[2] G. K. Madsen, J. Carrete, and M. J. Verstraete, Computer Physics Communications, **231**, 140–145,2018.

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[TSM-298] AB-INITIO STUDIES OF THE INITIAL STAGES OF THE EPITAXIAL GROWTH OF GaN/GaAs SUPERLATTICES IN (*hhl*) Si SUBSTRATES ORIENTATIONS.

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The III-Nitride (GaN, AlN, etc) exhibits unique properties that excel other III-V materials. These properties include the high dielectric breakdown voltage, wide bandgap, and high thermal conductivity. However, the monolithic integration of these compounds in Si substrates has been hindered by the mismatch in its fundamental physical properties such as their lattice constant, coefficient of thermal expansion and polarity. Many efforts have been made to overcome these challenges, as the growth of superlattices which, in addition to being able to enhance the crystal quality, can generate attractive new properties as phonon confinement effects related to lattice strains [1]. Therefore, we can infer that the interaction between to promising materials as GaN (cell parameter 5.186 Å) and GaAs (cell parameter 5.653 Å) superlattices growth in Si substrates could present very interesting properties.

In this work, we present an ab initio study of theinitial growth steps of different superlattices of GaAs/GaN on Si(111), Si(110) and Si(001) substrates. The structural changes, energy density differences and interfacial energy were calculated by using density functional theory.

Keywords
DFT, MBE, EPITAXY

Reference

[1] Y.Zhao et al., “Strain evolution and confinement effect in InAs/AlAsshort-period superlattices studied by Raman spectroscopy,” Sci. Reports2023 131, vol. 13, no. 1, pp. 1–9, Jan. 2023, doi:10.1038/s41598-022-26368-8.

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This work was supported by: CONAHCyT México – Estancias postdoctorales por México 2022 of J. Alanis Perez CVU 557499.

[TSM-284] *AB INITIO* PREDICTION OF MAGNETIC PROPERTIES OF DOPED TiS_2N_4: POTENTIAL APPLICATION IN SPINTRONIC DEVICES

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Most known magnetic devices are nanoscale-designed materials based on oxides, nitrides, or arsenides of rare earths. The strong interaction of mobile charge carriers with the localized magnetic moments of the d- and f-shells leads to a number of features of the electrical and optical properties of this compounds. However, the extended use of rare earths has raised concerns about human health and ecology since mining them generates tons of toxic waste. In order to predict green alternatives to produce magnetic devices, we have studied magnetic properties of TiS_2N_4 using first principles calculations. The TiS_2N_4 was doped with Mn, Fe, and Co to understand the magnetism in this material with high electron mobility. For geometry optimization, the supercell method was used to introduce the magnetic dopants in different arrangements. Spin-orbit coupling was used to calculate structural, electronic and magnetic properties.

Keywords
MXene, monolayer, doping, TiS_2N_4, magnetic moment

Reference

Ren, K., Shu, H., Wang, K., & Qin, H. (2023). Two-dimensional MX_2Y_4 systems: ultrahigh carrier transport and excellent hydrogen evolution reaction performances. Physical Chemistry Chemical Physics, 25(6), 4519–4527. https://doi.org/10.1039/d2cp04224j

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[TSM-176] MANGANESE DEPOSIT ON THE BP (111)-(2X2) SURFACE: DENSITY FUNCTIONAL THEORY STUDIES

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The technology development to improve the human being life generates the need of new materials with improved properties to expand their applications. The incorporation of metallic elements into semiconductors may transform the material physical properties. In view of these, in this work the structural, electronic, and magnetic properties of the manganese (Mn) adsorption and incorporation into the boron phosphide (BP) (111)- (2 × 2) structure have been investigated. Studies have been done using spin-polarized first-principles total-energy calculations. The exchange-correlation energies are treated within the generalized gradient approximation. The magnetic properties have been investigated considering different coverages and different magnetic configurations. To explore the Mn adsorption and incorporation, it is considered coverage ranging from ¼ to 1 monolayer (ML), with results displaying: Ferromagnetic (FM), antiferromagnetic (AFM), and non-magnetic (NM) behavior at low, intermediate, and high coverages, respectively. The surface formation energy (SFE) formalism is used to determine the structure stability. It is found that the 1 ML of Mn deposit may yield a stable structure. The electronic properties are explored considering the total density of states (DOS) and the projected density of states (PDOS). It is noted that the contribution of the Mn-d orbital modifies the metallicity of the surface. Finally, the charge density of the Mn-saturated surface is analyzed to show that the surface displays a metallic phase.

Keywords
Boron phosphide, manganese, first-principles, monolayer, adsorption, incorporation.

Reference

N. Hanani, “C.1. Semiconductor band structure and heterostructures,” An Autom. Irrig. Syst. Using Arduino Microcontroller, no. May, 2018, doi: 10.1088/978-1-6432-7028-9ch1.

E. Durgun, “Tuning Electronic Properties of Monolayer Hexagonal Boron Phosphide with Group III−IV−V Dopants ¨,” 2017, doi: 10.1021/acs.jpcc.6b10334.

This work was supported by

Computations were performed, the supercomputer Miztli of DGTICUNAM, Laboratorio Nacional de Supercómputo del Sureste de México, and the Instituto de Física BUAP computer center. CONAHCYT for the postdoctoral scholarships through program "Estancias posdoctorales por México - Modalidad 1".

[TSM-234] COMPUTATIONAL SIMULATIONS STUDIES OF BORON PHOSPHIDE NANOTUBES (BPNTs) WITH ANTI-CANCER DRUGS

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After the carbon nanotubes (CNTs) synthesis, these nanostructures have attracted the attention of scientists provided that they may be used in the molecules transportation. There are several theoretical and experimental reports that deal with CNTs and other similar inorganic nanotubes for drug transportation. Nanotubes analogous to CNTs, such as boron phosphide nanotubes (BPNTs), in the zigzag chirality are important because theoretical predictions indicate that they are soluble in polar solvents, therefore they may be appropriate for applications in biological systems. In this work, we have investigated the structural and electronic properties of the (14,0) BPNTs, in the pristine form and doped with different elements. In addition, we have analyzed the interaction and encapsulation of anticancer drugs (cisplatin and nedaplatin exploring different configurations). First-principles total-energy calculations have been employed to calculate the structural and electronic properties of the nanotubes. Studies are performed within the periodic density functional theory (DFT) as developed in the PWscf code of the Quantum ESPRESSO package. The exchange–correlation potential energies are treated according to the generalized gradient approximation (GGA) with the Perdew, Burke, Enzerholf (PBE) gradient corrected functional. The electron–ion interactions are modeled with the Vanderbilt ultra-soft pseudopotentials. Results show that the drug molecules may be encapsulated within the NTs suggesting that in this way they may be transported within a biological body.

Keywords
Boron phosphide Nanotubes, cisplatin, nedaplatin, density functional theory

Reference

D. García-Tora, V. M. Vázquez-Báez, R. Mendoza-Báez, E. Chigo-Anota, A.Flores-Riveros, G. Hernández Cocoletzi, J. F. Rivas-Silva, "Structural Stability and Electronic Properties of Boron Phosphide Nanotubes: A Density Functional Theory Perspective", Symmetry 14 (2022) 964. https://doi.org/10.3390/ sym14050964

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[TSM-251] LAYERED DEPENDENT SURFACE STATES IN BiSb

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The discovery of topological materials has been one of the most important events in the last years. Starting with the work of Liang Fu and his team [1] published in 2007, the interest in the study of topological materials growth exponentially. The emergence of the topological materials changes the understanding of the electronic and magnetic properties of materials. Topological materials have a high carrier mobility and almost null border effects dispersion, in comparison with other materials, which make them suitable for electronic applications, and recently, reports show the benefits of using topological materials in catalytic applications when compare to traditional materials. For this reason, the structural and electronic properties of few layers of BiSb were investigated. Studies were done using the density functional theory (DFT) considering the spin-orbit coupling. It is interested that only the monolayer is the one that show the direct band gap semiconductor character, from two monolayers onwards a semi-metallic character is found. This semi-metallic behavior is due of the existence of valance and conduction bands crossing the Fermi level near Gamma point. The existence of these band crossing is related to the topological surface states (TSS). It is expected that defects, like deformations, vacancies or doped atoms, do not affect the TSS, desirable property for magnetic-topological junctions with cell mismatch for applications in spintronics and solid-state storage. Also, the robust TSS make all the BiSb surface and active catalytic point, making it suitable for catalytic applications as well.

Keywords
Topological materials, layered dependent, spin-orbit coupling, DFT

Reference

[1] L. Fu, C. L. Kane, E. J. Mele Topological Insulators in Three Dimensions, Phys. Rev. Lett. (98) 2007, 106803. https://doi.org/10.1103/PhysRevLett.98.106803.

This work was supported by

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[TSM-232] HEAVY METALS ADSORPTION ON SRTIO3(111) A DFT STUDY

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Heavy metal pollution in water produces health problems in humans. Currently, pollution is an important global problem. Therefore, several experimental and theoretical groups have been investigating different methods for removing contaminants from water. Adsorption is a suitable process that can be used to remove dangerous contaminants such as heavy metals. This work reports Density Functional Theory (DFT) calculations to explore the heavy metals adsorption on strontium titanate (SrTiO3) surface (111). Calculations were performed using the PWscf code of the quantum ESPRESSO package. The work focuses on the Pb adsorption to investigate its remotion. Adsorption energy at different high symmetry sites is studied. Structural and electronic properties of selected systems are reported and compared. Understanding the mechanism in adsorption processes can help to propose improvements that lead to more efficient pollutant removal methods.

Keywords
heavy metals, strontium titanate, adsorption, DFT
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[TSM-265] AN EXPERIMENTAL-COMPUTATIONAL STUDY OF THE LP GAS DETECTION MECHANISMS ON TiO_2-GRAPHENE NANOHYBRID

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The growth by atomic layer deposition (ALD) in situ of the titanium dioxide-graphene nanohybrid (TiO2-GR) will be evaluated through infrared spectroscopy, employing an array conditioned to the growth parameters compatible with an infrared spectrometer by Fourier transform (FTIR). Additionally, the non-covalent interaction index (NCI) schemes will be obtained by computational simulation for the evaluation of the interactions involved in the growth of the material; this is to understand at the atomic level the growth of the TiO2-GR nanohybrid by the ALD technique.

Once the analysis and understanding of the growth of the TiO2-GR hybrid structures have been completed, the hybrid material will be synthesized for its subsequent assembly in an electrode array that allows us to monitor the response of the material when exposed to the components of the liquefied petroleum gas (LP gas). In parallel, a computational study of the interaction between the molecules that integrate the LP gas (butane, propane, and methanethiol) and the surface on the TiO2-GR hybrid material will be carried out; helping to understand the detection mechanisms, and, together with the experimental results, to evaluate the feasibility of the material to be used in a high-performance LP gas sensor device.

Keywords
TiO_2, DFT, GAS LP, SURFACE

Reference

Paez-Ornelas, J. I.; H. N.; Borbón-Nuñez, H. A.; Tiznado; Guerrero-Sánchez, J. A. First-principles study of the atomic layer deposition of ZnO on carboxyl functionalized carbon nanotubes: The role of water molecules, Physical Chemistry Chemical Physics, 2021, 23(5), 3467–3478.

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[TSM-259] ATOMIC SCALE ANALYSIS OF THE PERPENDICULAR MAGNETIC ANISOTROPY IN MnAl/CoAl HETEROSTRUCTURES

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As technology reaches the nanoscale, scientists constantly seek new materials to construct novel nanoscale devices. Information storage is vital since storing large amounts of information in smaller devices is necessary. This way, non-volatile information storage devices based on perpendicular magnetic anisotropy (PMA) materials allow easy scaling and large amounts of information in 3D arrays. Magnetic tunnel junctions (MTJs) based on PMA MnGa are a reality. On the other hand, tau-MnAl -a similar material with intrinsic ferromagnetic properties- still needs to be studied in detail. Recently, an experimental work appeared demonstrating PMA on a MTJ based on CoAl/MnAl/MgO/Ru [Takeuchi et al. Appl. Phys. Lett., 2022, 120(5)]. Although PMA was measured in the CoAl/MnAl interfaces, no atomic scale understanding of the PMA was demonstrated by computational simulations. In this work, we modeled the CoAl/MnAl interfaces through the use of Density Functional Theory (DFT). The results indicate the most stable interaction occurs between the last Al layer of CoAl and the first Mn layer of MnAl. In addition, we demonstrated a PMA effect in the CoAl/MnAl comes mainly from the MnAl structure, while CoAl does not show magnetic properties. CoAl only reduces the lattice mismatch between MnAl and the substrate (MgO), so the PMA is unaffected.

Keywords
Interfaces magnetic, magnetic properties, termodinamic stability, computational simulation

Reference

Takeuchi, Y., Okuda et al. 2022. Nanometer-thin L10-MnAl film with B2-CoAl underlayer for high-speed and high-density STT- MRAM: Structure and magnetic properties. Applied Physics Letters, 120(5), pp. 052404. doi: 0.1063/5.0077874

This work was supported by

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[TSM-15] UNDERSTANDING CARBOXYLIC ACID SURFACTANT ADSORPTION AND INHIBITION EFFECT IN AREA SELECTIVE ATOMIC LAYER DEPOSITION OF ZnO ON Cu AND Cu2O.

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Electronic device fabrication involves multiple steps, mainly thin film deposition, lithography, and etching. As the fabrication scale moves toward smaller sizes, achieving patterns <5 nm has become a significant challenge. In this context, it is necessary to study novel fabrication approaches that can either reduce the steps or processing in patterning methods[1].

The atomic layer deposition (ALD) process relays strongly on surface chemistry, providing an opportunity to limit growth to specific areas. One of the most studied approaches to accomplishing selective ALD is locally deactivating growth using self-assembled monolayers (SAMs)[2].

However, removal of the residual SAM is necessary for many applications, but it has not been well studied [3]. In this context, the search for novel molecules that can deactivate a specific surface stably and are easily removable is a major interest in improving selective deposition techniques. A promising candidate is a carboxylic acid SAM, which in contrast to other typically used SAMs, is quickly removed when immersed in water [4]

The aim of this work was to study the adsorption of the molecule acetic acid (AA) as a model of head group of carboxylic acid SAM on the Cu (111) and the Cu_2O (111) surface and assess the impact of diethylzinc (DEZ) ALD precursor in blocking effect based on the self-consistent periodic density functional theory (DFT) calculations. We included the most stable conformations for adsorption. Every selected configuration was assessed considering the electron-donating nature of the functional groups in the molecule and electron-withdrawing sites on the surface. The comparison between arrangements revealed interactions of different nature between the molecule and the studied surfaces. Interactions between AA and DEZ molecules on Cu_2O (111) were also investigated. To understand the character of these interactions we studied the charge transfer between the formed molecule-surface bonds and the non-covalent interactions (NCI).

Keywords
Area selective ALD, Self-assembled monolayers, adsorption, density functional theory, interactions

Reference

D. Bobb-Semple, K.L. Nardi, N. Draeger, D.M. Hausmann, S.F. Bent, Area-Selective Atomic Layer Deposition Assisted by Self-Assembled Monolayers: A Comparison of Cu, Co, W, and Ru, Chemistry of Materials. 31 (2019) 1635–1645. https://doi.org/10.1021/acs.chemmater.8b04926.

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[TSM-19] ASSESSING THE EFFECTS OF SURFACE FUNCTIONAL GROUPS ON THE Li STORAGE CAPACITIES OF Ti2Ta2C3 MXENE ANODE MATERIALS

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First-principles studies on Ti/Ta-based ordered alloy MXenes have demonstrated their viability as anode material in Li-ion batteries due to their promising electrochemical properties. However, the effect of surface functional groups on the lithiation and delithiation processes at atomic scale is currently unknown. Here we use first-principles DFT calculations to study the thermodynamic stability and the structural and electrochemical properties of O-, F-, Cl-, and OH-functionalized Ti2Ta2C3 ordered alloy MXenes in the Li intercalation process. Calculations show that surface functionalization with O, F, Cl, and OH is thermodynamically stable. Also, we demonstrate that the H3 high symmetry site is the most favorable configuration for the Li intercalation process. Electrochemical characterization is carried out employing Open Circuit Voltage (OCV) curves. Our results demonstrate changes in storage capacities depending on the functional group, with O-functionalized MXenes exhibiting larger storage capacities compared to other functional groups in Ti2Ta2C3 MXene anode materials. These results show how the functional groups affect the potential performance of Ti2Ta2C3 MXene materials in energy storage applications and provide insights for correctly selecting the functional group of the host material.

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Keywords
MXene, Li-ion Battery, Carbide MXene, Ordered Alloy MXene
This work was supported by
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[TSM-80] MXENE HETEROSTRUCTURES BASED ON Cr2C AND Cr2N: EVIDENCE OF STRONG INTERFACIAL INTERACTIONS THAT INDUCE AN ANTIFERROMAGNETIC ALIGNMENT

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2D heterostructures with Cr2C and Cr2N stacked were created. The structural, electronic, and magnetic properties. Two stacking cases were treated: Cr2C on top of Cr2N and Cr2N on top of Cr2C. The most favorable configuration is Cr2C/Cr2N, with a vertical distance of 2.35 Å. The antiferromagnetic alignment evidences a possible exchange bias effect. Cr2C MXene preserves its ferromagnetic behavior and changes the top Cr layer polarization of Cr2N to form the antiferromagnetic alignment with Cr2C. The bottom Cr layer of Cr2N conserves the intrinsic polarization as antiparallel. Electronic properties evidence a metallic behavior. Although the vertical distance in the MXene heterostructure is comparable with a van der Waals interaction, the 2D charge density maps and Electron Local Function (ELF) indicate a metallic interaction at the interface. The new 2D heterostructure and the properties that emerge from it could attract the interest of the spintronics community due to their applications in information storage devices.

Keywords
2D heterostructures, MXene, spintronic, DFT, spin polarization
This work was supported by
DGAPA-UNAM-IA100822 and -IN101523 projects. Calculations were performed in the DGCTIC-UNAM Supercomputing Center, project no. LANCAD-UNAM-DGTIC-150, LANCAD-UNAM-DGTIC-368 and LANCAD-UNAM- DGTIC-422. We thank E. Murillo, Aldo Rodriguez-Guerrero, J.I. Paez-Ornelas for technical support and useful discussions. S.J.G.O. acknowledges DGAPA-UNAM for the postdoctoral position.

[TSM-268] STUDY OF THE POSSIBLE ADSORPTION MECHANISM OF A CO2 MOLECULE ON THE SURFACE OF GRAPHENE AND GRAPHENE OXIDE STRUCTURES, VIA DENSITY FUNCTIONAL THEORY

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This research performed a theoretical interpretation of the molecular and electronic properties of graphene and graphene oxide (GO) nanoflakes through the density functional theory. Here, a pristine armchair graphene system (C100H26) was passivated by hydrogen atoms at its edges and then coated the surface with hydroxyl and epoxy groups to obtain the GO at 5%, 9%, 13%, and 16% of oxidation coverage. Computational calculations were carried out employing the generalized gradient approximation (GGA) functional PBE. The proposed molecular structures were brought to a stable minimum. The adsorption energies (Eads), the molecular electrostatic potential (MEP), and non-covalent indexes (NCI) were determined, to analyze the type of CO2 adsorption on the surface of graphene and GO. The obtained results suggest a possible physisorption mechanism between the graphene and CO2, that describes Van Der Waals interaction between the GO and CO2, making these materials excellent candidates for the carbon capture and decontamination of the air.

Keywords
graphene oxide, DFT, NCI, CO2.

Reference

N. Osouleddini and S. F. Rastegar, “DFT study of the CO2 and CH4 assisted adsorption on the surface of graphene,” J Electron Spectros Relat Phenomena, vol. 232, pp. 105–110, 2019, doi: 10.1016/j.elspec.2018.11.006.

This work was supported by

This work was funded in part by Universidad del Quindío and MinCiencias project SGR BPIN2020000100600 internal code 1112. We also acknowledge DGAPA-UNAM projects IA100822. Calculations were performed in the Supercomputing Center projects LANCAD-UNAM-DGTIC-368.

[TSM-241] ASSESSING THE STABILITY OF KAGOME D019-Mn3Ga (0001) SURFACES: A FIRST-PRINCIPLES STUDY

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Using non-collinear spin-polarized first-principles calculations, we have investigated the properties of the hexagonal $D0_{19}$ (0001) Mn_3Ga surface. Two different surface terminations were considered: type-1 and type-2, with opposite chiralities. In the case of pristine surfaces, the Kagome triangular AFM character remains on the surface and in inner layers, with a slight increase in the surface magnetic moments due to the low coordination of the surface atoms. An increase in the remnant out-of-plane FM character compared to the bulk is also noticed. The effect of Ga or Mn vacancies on both surfaces was also investigated. Ga vacancies in the 2nd monolayer are more stable than in other layers. Such vacancies distort the triangular AFM configuration of the neighboring layers. Despite this, the AFM layer-by-layer nature remains. Conversely, Mn vacancies stabilize in the most exposed layer. In this case, the neighboring layers completely lose the triangular alignment. However, Mn atoms rearrange to preserve the AFM layer-by-layer character. Upon evaluating the thermodynamic stability of these surfaces, we observe that the pristine Kagome AFM magnetic surfaces are the most stable. Ga vacancies are the least stable configurations because they break down the super-exchange interaction that holds the Kagome magnetic arrangement. Finally, our calculations show that the Kagome magnetic arrangement at the surface is stabilized by both the magnetic (Mn) and non-magnetic (Ga) atoms. Therefore, it is expected that $D0_{19}$-Mn3Ga will not present low-index reconstructions induced by vacancies.

Keywords
Non-collinear magnetism, hexagonal D019 Mn3Ga, (0001) surface, vacancies, Kagome lattice
This work was supported by
We thank DGAPA-UNAM projects IN105722, IN101523 and IA100822, and CONACyT grant A1-S-9070 and grant A1-S-17539 for partial financial support. Calculations were performed in the DGTIC-UNAM Supercomputing Center projects LANCAD-UNAM-DGTIC-051, LANCAD-UNAM-DGTIC-368, LANCAD-UNAM-DGTIC-422. JMGH acknowledges a postdoctoral fellowship from DGAPA-UNAM.

[TSM-362] GALLIUM DIFFUSION CHANNELS BOOST THE OXYGEN ACTIVATION FOR THE CO TO CO2 CONVERSION IN CeO2

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In this talk, we will elucidate gallium's key role in boosting oxygen activation to oxidize CO to CO2 in the presence and absence of oxygen. First, the Ga effect in the CO to CO2 conversion is evaluated at different Ga/Ce ratios. Its incorporation improves oxygen activation. Low Ga content generates efficient conversion rates. Atomic scale calculations demonstrate that diffusion channels appear in the 0.25 Ga/Ce ratio, facilitating the Ga diffusion toward the surface. Ga also incorporates at the CeO2 subsurface, inducing Ce-O bonds weakening, thus improving the CO oxidation ability through oxygen vacancy formation. The vacancies can be occupied once more by either O2 from the environment or O from the bulk, thus renovating the catalyst for further CO oxidation.

We thank DGAPA-UNAM project IN112922, IN101523 and IG101124. Thanks to project CONACYT-F003 117373 for their partial financial support. Calculations were performed in the DGCTIC-UNAM Supercomputing Center projects LANCAD-UNAM-DGTIC-422 and 36fabrication. JGS acknowledges LNS-BUAP project 202201042N and THUBAT KAAL IPICYT supercomputing center project TKII-JGSA001 for their computational resources. The authors thank Francisco Ruiz, David Dominguez, Eric Flores, J. Mendoza, Israel Gradilla, Eloisa Aparicio, and Aldo Rodriguez for technical assistance.

Keywords
Boosting, Ga diffusion channels, CeO2

THIN FILMS

CHAIRMEN

Dr. José Alberto Duarte Moller (Universidad de Sonora, URS), josealberto.duarte@unison.mx
Dra. Adriana Alvídrez Lechuga (Universidad Tecnológica de Chihuahua)

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-49] RESEARCH OF MULTILAYERS OF BiFeO3/SrTiO3 FOR ENERGY STORAGE AND BIOSENSORS

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New lead-free materials, with piezoelectric coefficients equal to or greater than Lead Zirconate Titanate (PZT), are necessary to replace this compound in power generator devices such as defibrillators or pacemakers; also, in applications such as spintronics and magnetoelectronic. Among the materials investigated, Bismuth Ferrite ($BiFeO_3$) stands out, generally known as BFO, it has a high polarization, which has been theoretically calculated by means of the density functional, of 103.3 microcoulomb/cm^2 (1),and which is equivalent to that of the piezoelectric PZT, and a very strong piezoelectric response of 70 pm/V (2). However, the BFO has high leakage currents and a large coercive electric field that limits its applications in industry.To overcome this obstacle, it has been shown that multilayers of ($SrTiO_3$/$BiFeO_3$/$SrTiO_3$)present piezoelectric coefficients equal to or even higher than PZT. Therefore, in this work we will seek to optimize the growth process of multilayers of($SrTiO_3$/$BiFeO_3$/$SrTiO_3$) on silicon substrates by pulsed laser deposition method to achieve piezoelectric coefficients d_{33}> 300 pm/V and currents densities lower than 10^{-8} A/cm^2.Nb doped $SrTiO_3$ were used as a layer between the silicon substrate and the BFO thin films to be used as conductive electrode and as buffer layer.Through UV-Visible spectroscopy, we found that BFO has a direct band gap of 2.8 eV which agrees with the theoretical value obtained for this material by calculating of the density functional. These indicated that the high-power conversion efficiency may be obtained in BFO-based devices.

Keywords
Piezoelectricity, Bismuth Ferrite, Leakage Currents.

Reference

(1) Z. Zhang, P. Wu, L. Chen, and J. Wang, “Density functional theory plus U study of vacancy formations in bismuth ferrite,” Appl. Phys. Lett., vol. 96, no. 23, 2010, doi: 10.1063/1.3447369.

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Conahcyt.

[THF-65] NON-DESTRUCTIVE THERMAL STUDY OF THIN FILMS THERMAL DIFFUSIVITY USING THE LOCK-IN THERMOGRAPHY TECHNIQUE

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In this work, a methodology for a thermographic procedure is developed with the aim to determine the thermal diffusivity of metal and organic-based thin films. Thin films were built by dipping the nanoparticles growth substrate into a bath solution. The in-plane thermal diffusivity was obtained by monitoring the temporal evolution of the spatial temperature distribution on the surface by an infrared camera. For this experiment, a single pulse from a diode laser source was used to generate a thermal contrast on the surface of the sample to be analyzed. An infrared thermal camera employed to acquire the temperature gradient of the sample surface, which was processed by an algorithm developed in MATLAB by our research group in order to calculate the thermal diffusivity. For this methodology, a 454 nm blue laser with a power of 300 mW was used. From these results it was demonstrated that this technique is useful for the measurement of thermal diffusivity in Cu and Fe_3O_4 thin films. Moreover, the thin films were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM) and Raman spectroscopy.

Keywords
thermography, thermal properties, diffusivity.

Reference

C.M. Basheer, C.V. Krishnamurthy, and K. Balasubramaniam, Hot-rod thermography for in-plane thermal diffusivity measurement, Measurement 103 (2017), 235-240. https://doi.org/10.1016/j.measurement.2017.02.022.

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[THF-125] NANOSTRUCTURES CORE-SHELL Si/SiOx EMBEDDED IN A ZnO MATRIX PRODUCED BY RF SPUTTERING

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Nanostructures were produced by sequential deposit of ZnO/Si/ZnO fims employing RF sputtering at room temperatute, 200 °C and 300 °C; using glass and silicon as substrates. In order to evaluate the effect of each film in the core shell nanostructure, films of ZnO, ZnO/Si and ZnO/Si/ZnO were produced. Chemical, structural and electronic characterization results were obtained for the films employing AFM, SEM, EDX, UV-Vis, Raman and PL spectroscopies. IvsV characteristics and spectral response were obtained.
Results are discussed in terms of the characteristics of core-shell nanostructures determined by substrate temperature.

Keywords
Thin films, semiconductors, nanostructures, optical spectroscopies, sputtering.

Reference

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. Journal Electronic Materials, 47, 6607-6612.

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[THF-165] TEMPERATURE CONTROL DEVICE FOR CHEMICAL BATH DEPOSITION METHOD

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Chemical bath deposition (CBD) is a method commonly used in the preparation of electronic devices and coatings. In this process, temperature is an important factor in CBD that allows obtaining coatings with uniform properties of thin films using temperatures close to 20 to 80°C, which allows us to obtain films from 20 to 1000 nm thick from a material immersed in a chemical solution. Lack of temperature control can cause coating variations, negatively affecting product performance and reliability. For which a PID (Proportional-Integral-Derivative) control system was designed and developed that continuously calculates and adjusts the signal, provides a continuous variation of the output within a control loop feedback mechanism to precisely control the process. , eliminating the oscillation and increasing the efficiency, much faster and more precise of the controller based on the data that allows us to collect the ensor Lm35 sensor, used to measure precise and stable temperature variations in transient states using a heat transfer model in combination with a tec115710 Peltier module that uses the thermoelectric effect is the direct conversion of the temperature difference to electrical voltage and vice versa, generated through two metals which have a temperature difference between the junctions, that is, one cools while that the other is heated, the temperature variation is from -50 to 150 °C to obtain and maintain the desired temperature during the process[3].

Keywords
temperature control, peltier module, PID control.

Reference

[1] De, F., & Mecánica, I. ESCUELA POLITÉCNICA NACIONAL. Edu.ec. Recuperado el 1 de julio de 2023
[2] Org.co. Recuperado el 1 de julio de 2023
[3] Termoeléctrico, Trabajo Fin de Grado. Unican.es. Recuperado el 1 de julio de 2023

[THF-171] ALUMINUM-DOPED ZINC OXIDE POLYCRYSTALLINE THIN FILMS PREPARED BY CO-SPUTTERING FROM A ZnO–Al TARGET

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Aluminum-doped Zinc oxide polycrystalline thin films (AZO) were grown on 7059 Corning glass substrates at room temperature by co-sputtering from a ZnO-Al target. The target was designed as follows, high purity elemental Aluminum was evaporated onto a ZnO target covering small areas. The structural, optical, and electrical properties were analyzed as a function of Al content. The Al doped ZnO polycrystalline films showed an n-type conductivity. It was found that the electrical resistivity drops and the carrier concentration increases as a consequence of Al incorporation within the ZnO lattice. In both cases the changes are of several orders of magnitude. From the results, we conclude that, using this ZnO-Al targets n-type Al doped ZnO polycrystalline films with high transmittance and low resistivity can be obtained.

Keywords
II-VI compounds, semiconductors, low resistivity, ZnO-Al films.

Reference

Kousik Sivakumar; S. M. Rossnagel. Journal of Vacuum Science & Technology A 28, 515–522 (2010) doi: https://doi.org/10.1116/1.3425640.
Tadatsugu Minami, Semicond. Sci. Technol. 20 (2005) S35–S44. DOI 10.1088/0268-1242/20/4/004.

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[THF-209] MANUFACTURE OF A SEMICONDUCTOR DEPOSIT DEVICE BY NEBULIZARÍAN, AS AN ALTERNATIVE TO SPRAY PYROLYSIS

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The chemical deposition of semiconductors by an alternative to spray pyrolysis method is performed due to the control of growth with a nebulizer [1]. The accessibility of the method makes it affordable in terms of scaling and costs, however, commercial robotic system to execute the process are expensive since the price range is usually around $10500.00 USD. up to $16000.00 USD. With this in mind, an automation low-cost system was developed to carry out the chemical deposition (DC) by spray pyrolysis. A devise developed at the Autonomous University of Zacatecas that includes a microcontroller, a user interface that allows interact with the system, a power driver circuit, and a heating system attached to the structure as an optimization for portability of the system. The microcontroller is programmed with a series of different menus in which the user selects the compound to deposit, adjust the number of cycles, temperatures and series of sprays. A thin film of MnS (manganese sulfide) will be deposited and characterized crystallographically, morphologically and electrically as control test.

Keywords
Automation, spray pyrolysis, synthesis.

Reference

[1] M. Shkir “Impact of ND doping in BI2S3 thin films coated by nebulizer spray pyrolysis technique for photodetector applications,”2023. doi:10.1016/j.optmat.2023.113837.

[THF-229] SYNTHESIS AND CHARACTERIZATION OF ZnO THIN FILMS BY THE sol-gel METHOD WITH ADITTION OF WATERMELON QUANTUM DOTS

André Zamora Arellano Bachelor's degree[1], Gerardo Hernández Reyes Bachelor's degree[2], Ángel Yamil Lomelí Félix Bachelor's degree[3], Ricardo Yael Mata Hernández Bachelor's degree[3], José Guadalupe Quiñones Galván Doctoral degree[4]

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The present work focuses on the synthesis and characterization of ZnO thin films incorporating carbon quantum dots (CQDs) derived from watermelon rind. The objective is to develop thin films that can capture a wide range in the electromagnetic spectrum, to take advantage of their optical and electronic properties. Zinc oxide (ZnO) is a semiconductor material with a wide bandgap, being able to absorb UV light and emit light in different regions of the electromagnetic spectrum, this makes ZnO films attractive for applications related to optoelectronics, such as solar cells, LED devices, lasers, among others. CQDs are nanostructures that exhibit interesting optical and electronic properties, making them attractive for various applications. Unlike conventional quantum dots, CQDs are composed of organic materials, synthesized from organic compounds or biomass by-products.

For the synthesis, two solutions of 20 mL of methanol were made with 0.005 g of watermelon rind powder thermally treated at 100 and 200°C for 3 hours. Then, 0.5 g of zinc acetate was added to 10 mL of each solution. The films were deposited on glass substrates via the sol-gel method. The substrates were immersed into the CQDs solution for a few seconds and then subjected to a temperature of 120°C for 2 minutes. This process was repeated 5 times for each film. Two films were prepared for each CQDs solution and were annealed at 200 and 400°C for three hours, resulting in a total of four films.

The resulting films were characterized by UV-Visible spectroscopy and photoluminescence methods. Through these methods, valuable information about the optical and electronic properties performance of the ZnO films incorporating CQDs was obtained.

Keywords
Zinc oxide, thin films, quantum dots, semiconductor, sol-gel.

Reference

Rodwihok, C. et al. (2022). Preparation and Characterization of Photoluminescent Graphene Quantum Dots from Watermelon Rind Waste for the Detection of Ferric Ions and Cellular Bio-Imaging Applications. Nanomaterials (Basel, Switzerland), 12(4), 702.

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Universidad de La Ciénega del Estado de Michoacán de Ocampo.

[THF-231] SYNTHESIS AND CHARACTERIZATION OF CdS THIN FILMS WITH THE ADDITION OF CARBON QUANTUM DOTS BY THE CHEMICAL BATH DEPOSITION METHOD (DBQ)

Gerardo Hernández Reyes Bachelor's Degree[1], Andre Zamora Arellano Bachelor's Degree[2], Ricardo Yael Mata Hernández Bachelor's Degree[3], Angel Yamil Lomeli Felix Bachelor's Degree[3], Jose Guadalupe Quiñones Galvan Doctorate Degree[4]

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One of the most common elements present in the organic residues is carbon, which due to its properties at a nanometric scale is suitable for the creation of nanostructures known as quantum dots, particles with striking electronic and optical properties that can be used in photovoltaic devices. The addition of quantum dots into semiconductor films has been shown to optimize the collection of solar energy since the wide range of light absorption of these nanostructures allows them to capture photons at UV wavelengths and emission in the visible range, so their implementation in the path of chemical bath synthesis claims to be beneficial for optoelectronics applications.

For the creation of the carbon nanostructures in the present work, 0.005 gr of sieved powder of dehydrated watermelon peel was diluted in 20 ml of bidistilled water, with 4 different samples of powder: one without thermal treatment and another 3 with a treatment at 100, 200 and 400C for 3 hours, obtaining 4 solutions that were later divided into 8 solutions to apply a microwave treatment to four of these. The properties of these solutions were analyzed using the UV-Vis and PL spectroscopies.

As a synthesis technique for the deposition of cadmium sulfide thin films, the chemical bath method was chosen due to its easy availability, starting with 10 ml of water, this was mixed with 2 ml of cadmium chloride (CdCl2) solution, 1 ml of hydroxide of ammonium(NH_4OH), 2 ml of ammonium chloride(NH4Cl) and 2 ml of thiourea(SC(NH2)2)under constant agitation for 5 minutes for the deposition of 2 substrates, one with microwave treatment and the other with ultraviolet radiation. This procedure was repeated substituting the water for the solution containing quantum dots. Finally, these films were characterized using the UV-Vis and PL spectroscopies as well.

Keywords

Thin films, semiconductors, Quantum Dots, Chemical Bath depositation.

Reference

Rodwihok, C, et.al (2022). Preparation and characterization of photoluminescent graphene quantum dots from watermelon rind waste for the detection of ferric ions and cellular bio-imaging applications. Nanomaterials, 12(4), 702.

This work was supported by

Universidad de la Cienega del Estado de Michoacan de Ocampo.

[THF-32] EFFECT OF THE SUBSTRATE AND TEMPERATURE VARIATION ON THE PHYSICAL PROPERTIES IN MnS THIN FILMS SYNTHETIZED BY SILAR METHOD

Brandon Lauro Martinez Lopez BCE[1], Jesus Octavio Sigala Valdez MSc[1], Harumi Moreno García PhD[2], Ismailia Leilani Escalante García PhD[1], Edgar Lopez Luna PhD[3], Sergio Miguel Duron Torres PhD[1], Antonio Del Rio De Santiago PhD[1]

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The use of metal sulfides (MSs) for the synthetization of semiconductor materials with the objective of thin films growth, a topic that has taken on importance in recent years as it is constantly sought to generate alternative energies. The production of photovoltaic solar cells from MSs is feasible because of the abundance in these reagents and the various techniques for the production of MSs thin films. In this work, we will use the SILAR method, to synthesize manganese sulfide (MnS) thin films from room Temperature ( ) up to 80 °C on glass, ITO and FTO as substrates, with the SILAR technique, the formation of a thin film is sought in different cycles where aspects such as: rinse, transfer and immersion time between cationic and anionic precursor to be deposited. A reaction mechanism is then proposed to understand how the substrate interacts with the cationic and anionic precursors, in order to understand how thin films of MSs are synthetized. For the study of the film morphology, scanning electron microscopy images were taken. Optical transmittance and reflectance data were measured from an UV-Vis spectrophotometer in 250-1400 nm wavelength range, with the obtained data we observe the variation in transmittance as a dependent variable of the substrate used, having the highest transmittance was identified in the glass substrate with 90% and the lowest in the ITO substrate with 60% as well as identifying the reflection in the near infrared (NIR) on the ITO. Also, we determinate the bandgap which are in the range of 4.05 to 3.84 eV respectively to the substrates used and is specific for the MnS compound1. The aforementioned characterizations open a window to investigate the photovoltaic use for the thin films of MnS.

Keywords
synthetization, semiconductor, substrates y thin films.

Reference

Yıldırım, M. A., Yıldırım, S. T., Cavanmirza, İ. & Ateş, A. Chemically synthesis and characterization of MnS thin films by SILAR method. Chem Phys Lett 647, 73–78 (2016).

[THF-40] COMPARISON, DEVELOPMENT AND IMPLEMENTATION OF PID CONTROLLER BY CHEMICAL BATH DEPOSITION METHOD

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There are several types of methods to synthesize thin films at atmospheric pressure and low temperature, such as Chemical Spray Pyrolysis (CSP), Successive Ionic Layer Absorption and Reaction (SILAR), and Chemical Bath Deposition (CBD). In this project, the chemical bath deposition (CBD) method was selected, this consists in having a substrate immersed of a dissolution contained in a reactor at a controlled temperature. The advantages of CBD compared with the aforementioned methods are: the simplification in the synthesis of thin films due to the implementation of simple equipment and the reduction of control variables in the process. The general components of the equipment are: PID controller, a beaker of 100ml, a tray, and a thermal panel [1]. One disadvantage is the time required in reach the desired temperature value, caused by the programming of the system such as the relay installed in the device. Also, the given temperature values vary every time the equipment was turned on. For the optimization of this equipment, the behavior of the temperature was observed after several tests with common water both in the beaker and in the tray. Also, a movement of the hysteresis from 0 to 1, followed by an analysis of the variation of the temperature over time by taking data every 10 minutes to generate a graph. Subsequently analyzing the results obtained, a PID control system will be carried out on the Arduino nano board, based on the equipment previously used at Universidad Autónoma de Zacatecas, replacing the mechanical relay with a solid-state one, optimizing steady-state and transition times, making it possible to vary temperature continuously and smoothly, unlike commercial devices that use a mechanical relay that only opens and closes the heater circuit.

Keywords
PID Controller, Arduino, CBD.

Reference

[1] A. Kherkhar, Y. Chiba, A. Tlemçani, y H. Mamur, «Thermal investigation of a thermoelectric cooler based on Arduino and PID control approach», Case Stud. Therm. Eng., vol. 36, p. 102249, ago. 2022, doi: 10.1016/j.csite.2022.102249.

[THF-42] STUDY OF ELECTRICAL PROPERTIES BALL MILLING WITH ZINC ACETATE FOR FZO FILMS DEPOSITED BY ULTRASONIC SPRAY

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In this paper, the results of the study of ZnO:F films deposited on glass substrates using the ultrasonic chemical spraytechnique are reported. For the preparation of the films, starting solutions were used at a concentration of 0.2 M of zinc acetate dihydrate. [Zn(CH3COO)2.2H2O]dissolved in a mixture of deionized water:methanol:acetic acid. The precursorwas previously ground in a planetary ball milling at 300 rpm and different times. For the addition of the dopant, a 1.6 M solution of ammoniumfluoride in deionized water was prepared[NH4F]. The atomic ratio of[F]/[F+Zn] remained constant at 30 at%. Structural characterizations by X-ray diffraction, morphological by scanning electronmicroscopy, optical by UV-Vis spectroscopy, and electrical by Hall effect wereperformed on all deposited films. From the analysis of results, the hexagonalwurtzite phase was confirmed. In general, the films presented high optical transmittance in the visible region and high n-type conductivity.

Keywords
Zinc oxide, Fluorine doping, Ball milling.

Reference

RAMIREDDY, Thrinath Reddy, et al. Effect of the milling time of the precursors on the physical properties of sprayed aluminum-doped zinc oxide (ZnO: Al) thin films. Materials, 2012, vol. 5, no 8, p. 1404-1412.

This work was supported by

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[THF-90] THIN FILMS FABRICATION OF COBALT ANTIMONATE (CoSb2O6) BY RF SPUTTERING TECHNIQUE

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Currently, air pollution is one of the most severe problems worldwide. Every year, hundreds of millions of people suffer from respiratory diseases and other health issues associated with air pollution, both indoors and outdoors. As a result, intensive research is being conducted in the field of gas sensors, with great interest in semiconductor materials such as SnO2, ZnO, TiO2, and WO3, as well as ternary oxides with trirutile-type structure, such as ZnSb2O6 and CoSb2O6 [1]. These materials exhibit good sensing properties while remaining chemically stable in the presence of polluting gases. In this study, we aimed to obtain thin films of the semiconductor oxide CoSb2O6 to explore their potential applications as gas sensors. The films were deposited on single-crystal alumina substrates (A-plane) using the RF magnetron sputtering technique at high oxygen pressures [2]. The following conditions were used for the film deposition in an oxygen atmosphere: a gas flow of 10 SCCM, pressure of 1.5x10-1 T, a target-to-substrate distance of 5 cm, and a working power of 90 Watts. The deposited films were characterized using the X-ray fluorescence (XRF) technique, confirming the formation of CoSb2O6 films with an approximate Co: Sb composition of 25:75 and thicknesses ranging from 25 nm to 30 nm. Furthermore, the crystalline structure was analyzed by X-ray diffraction (XRD). The obtained films will be tested in the presence of different gases using the thermal impedance analysis technique to evaluate their potential application in sensing devices.

Keywords
Sensor, trirutile, RF cathodic erosion, thin films.

Reference

A. Guillén-Bonilla et al, “Synthesis and characterization of cobalt antimonate nanostructures and their study as potential CO and CO2 sensor at low temperatures,” Journal of Materials Science: Materials in Electronics, vol. 29, no.18, pp. 15632–15642, Sep. 2018, doi: 10.1007/s10854-018-9157-2.

This work was supported by
Consejo Nacional de Humanidades Ciencias y Tecnologías (CONAHCYT).

[THF-92] ELECTRICAL, OPTICAL AND MORPHOLOGICAL PROPERTIES OF NiOx THIN FILMS GROWN BY Sol-Gel METHOD FOR APPLICATION IN OPTOELECTRONIC DEVICES

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Non-stoichiometric nickel oxide (NiO_x) is a transparent conductive oxide (TCO) with interesting properties for many optoelectronic applications, among them light sensors. It has a band gap of 3.8 eV, a transmittance of almost 90%, a resistivity can be less than ~103 Ω·cm, and an excellent chemical stability. Moreover, in contrast to the most TCOs used in optoelectronic and electronic devices, it is a p-type semiconductor.

NiO_x thin films have been deposited using various techniques, including Atomic Layer Deposition, Chemical Vapor Deposition, Sputtering, Pulsed Laser Deposition and e-beam evaporation. However, these techniques require high vacuum and expensive equipment. In this work, we present a simple and low-cost method for the synthesis and deposition of NiO_x thin films by Sol-Gel process. As an example for application of these films in optoelectronic devices we study photosensors based of NiO_x layers deposited by spin-coating technique.

Keywords
NiOx thin films, Sol-Gel method, optical sensors, low cost process.

Reference

Ivanova, T.; Harizanova, A.; Shipochka, M.; Vitanov, P.Materials 2022, 15, 1742.
J.R. Castillo-Saenz, N. Nedev, B. Valdez-Salas, M. Bernechea, E. Martínez-Guerra, I. Mendivil-Palma, M. Curiel-Alvarez, D. Mateos, O. Perez-Landeros, Thin Solid Films 734, 138849 (2021).

This work was supported by

Conahcyt

[THF-142] STUDY OF THE FORMATION OF NANOGRANULAR SILVER DEPOSITS BY THERMAL EVAPORATION

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In this study the formation of silver nanogranular deposits by thermal evaporation is examined in detail. An Intercovamex T12 thermal evaporation system equipped with a glass hood was used for the deposits. Silver powder of 99.99% purity and molybdenum boats were used. For all deposits the vacuum pressure was maintained at 10-6 Torr. Deposit formation was monitored by in situ measurement of the change in electrical resistance of the deposit. During evaporation, resistance change curves as a function of time were obtained. Resistance was measurement on 1 x 2.5cm glass substrates. It is observed that the curves of resistance versus evaporation time show several stages that depend on electric power used for heating and the initial mass of silver. Which determines the stage of nanoparticle formation, agglomerated nanoparticles, and continuum formation. The electrical measurements coincide with the visual observations of the evolution of the deposit due to its plasmonic characteristics.

Keywords
Silver, Nanogranular deposits, Thermal evaporation, Electrical resistance, Plasmonic characteristics

Reference

The evolution and analysis of electrical percolation threshold in nanometer scale thin films deposited by electroless plating V. Sabayev, N. Croitoru, A. Inberg, Y. Shacham-Diamand, Materials Chemistry and Physics, Volume 127, Issues 1–2, 214- 219, (2011)

This work was supported by

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[THF-150] DDA NUMERICAL SIMULATION OF OPTICAL PROPERTIES OF NbN/Nb AND TIN/TI NANOSTRUCTURED BILAYERS: EFFECT OF ROUGHNESS

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The study of optical properties of thin films has been and is currently of considerable scientific interest, due in part to the many potential applications that these materials can present to current technological development. Many of these applications and research are directly related to the development of nanostructures. It is known that in thin films the response obtained when characterizing the material is considerably different from that of bulk material. The study of the morphology and roughness effect on optical properties of thin films has been rarely explored, since it is difficult to synthesize and characterize samples with the required characteristics. In the case of thin films, the combination of two factors, thickness decrease and roughness, generates a local (roughness) and global (thin film) confinement of free or conduction electrons. This confinement influences a change in the dielectric function, which in turn drastically modifies the optical properties of the material: reflection, transmission and absorption. In this work, the effect of roughness on the optical response of Nb, NbN, Ti and TiN nanofilms, and in a bilayer arrangement of NbN/Nb and/or TiN/Ti type, is studied using the discrete dipole approximation (DDA). Different real roughness patterns, obtained from AFM topography images of Nb thin films, were used for the calculations. We show the changes in the intensity and shape of the optical spectral lines due to the roughness patterns. In addition, we also present the electric field intensity on the rough surfaces.

Keywords
Bilayer, Surface Roughness Pattern, Optical Properties, Nanofilms.

Reference

[1] Draine B.T., Flatau P.J., J. Opt. Soc. Am. A, 25 (11), 2693, (2008).
[2] Weaver J.H., Lynch D.W., Olson C.G., Phys. Rev. B, 7 (10), 4311–4318, (1973).

This work was supported by

[1] VIEP-BUAP, Project 100504244-VIEP 2023
[2] (JAPL) CONACYT scholarship #861219.

[THF-168] STUDY OF EDIBLE GOLD IMITATION SHEETS USING FRAUNHOFER DIFFRACTION

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The optical behavior of imitation gold edible sheets is analyzed by Fraunhofer diffraction. Due to the demand that arose because of the massive dissemination through social networks, there is a wide catalog of edible sheets that imitate the optical properties of genuine gold sheets. However, in the characterization of the sheets carried out by means of x-rays, no gold particles were found. The majority component of the sheets is dukeite Bi243+Cr86+O57(OH)6 3H2O with a trigonal crystallization system, resinous in appearance, yellow or dirty yellowish brown. Its structure is based on irregular layers of Biφ n polyhedral, φ being O, OH and H2O; the layers are parallel to (001), linked together by chromate tetrahedrons. Edible gold sheets is prepared to pass through the human body without leaving a trace, so it does not provide any nutrients to the body, as it is only an ornament to add extra visual value to dishes or drinks.

Keywords
Fraunhofer diffraction, gold edible sheets, x-rays, dukeite.

Reference

Bragg, W. Lawrence, Ewald, P. Peter (ed.) (1962). “The growing power of X-ray analysis” (PDF). Fifty Years of X-Ray Diffraction. International Union of Crystallography. pp. 120-135.

This work was supported by
Instituto Politécnico Nacional

[THF-180] WATERBORNE ANTIFOULING PAINTS CONTAINING NANOMETRIC COPPER AND SILVER AGAINST MARINE BACILLUS SPECIES

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Due to the concern to find an alternative to reduce the colonization (microfouling and macrofouling) or the biocorrosion of surfaces submerged for long periods in water, we evaluated the antifouling activity of a commercial paint added with silver nanoparticles (AgNP's) and copper nanoparticles (CuNP's), beside copper-soybean chelate, by electrolytic synthesis, using them in low concentrations (6.94E − 04 mg Ag g−1 paint, 9.07E − 03 mg Cu g−1 paint, and 1.14E − 02 mg Cu g−1 paint, respectively). The test for paint samples was carried out by JIS Z2801-ISO 22196 for periods of initial time, 6 months, and 12 months, against three bacterial strains of marine origin, Bacillus subtilis, Bacillus pumilus, and Bacillus altitudinis. It was possible to demonstrate, according to the standard, that the sample with the greatest antimicrobial activity was the copper-soybean chelate against two of the three strains studied (B. pumilus with R = 2.11 and B. subtilis with R = 2.41), which represents more than 99% of bacterial inhibition. Therefore, we considered a novel option for inhibiting bacterial growth with nanoparticles as antifouling additives.

Keywords
Silver and Copper Nanoparticles, Antifouling Paints, Biocorrosion.

Reference

DeAlba-Montero, I., Guajardo-Pacheco, J., Morales-Sánchez, E., Araujo-Martínez, R., Loredo-Becerra, G. M., Martínez-Castañón, G. A., ... & Compeán Jasso, M. E. (2017). Antimicrobial properties of copper nanoparticles and amino acid chelated copper nanoparticles produced by using a soya extract. Bioinorganic chemistry and applications.

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[THF-288] NON-ENZYMATIC GLUCOSE SENSOR BASED ON METAL ELECTRODES MODIFIED WITH 2D MATERIALS

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In this research, we present a non-enzymatic glucose sensor employing metal electrodes modified with two-dimensional (2D) materials, notably graphene oxide (GO) and molybdenum disulfide (MoS2). Our findings substantiate that metal electrodes, specifically modified with GO and GO/MoS2, manifest superior glucose responsiveness.

Our study further identified gold (Au) substrates as offering the most effective linear fit for limit of detection (LD) and sensitivity, thereby indicating their promising potential for glucose detection applications.

Further characterization of these electrodes through cyclic voltammetry and chronoamperometry provided results that are consistent with previously reported findings. These results were reflected in both the linear form of the voltammograms and the location of the peak maxima associated with glucose oxidation processes.

Our findings reveal promising prospects for the development of high sensitivity and selectivity non-enzymatic glucose sensors based on metal electrodes modified with 2D materials. The potential advantages of these sensors include greater stability, the ability to operate across a broad range of conditions, and rapid response, which may have significant implications for glucose monitoring in medical and biotechnological applications.

Keywords
Non-enzymatic glucose sensor, Graphene oxide (GO), Molybdenum disulfide (MoS2).

Reference

Onur Parlak, Anıl İncel, Lokman Uzun, Anthony P.F. Turner, Ashutosh Tiwari, “Structuring Au nanoparticles on two-dimensional MoS2 nanosheets for electrochemical glucose biosensors”, Biosensors and Bioelectronics, Volume 89, Part 1, 2017, Pages 545-550.

This work was supported by

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[THF-290] STUDY OF THE TOPOGRAPHY, OPTICS, AND ELECTRIC PROPERTIES OF SELF-ASSEMBLED NANOMATERIAL THIN FILMS FOR THE DEVELOPMENT OF THZ DEVICES

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We present an experimental study of thin films of Graphene Oxide (GO), Reduced Graphene Oxide (rGO), and rGO decorated with Titanium (Ti) nanoparticles deposited onto solid substrates such as glass and Al2O3 (Sapphire) through the Langmuir-Blodgett technique (LB). We did the optical characterization of the thin film with the substrate using Terahertz Time-Domain Spectroscopy (THz-TDS) and RAMAN spectroscopy techniques. The structural characterization we carried out by X-Ray Diffraction Analysis (XRD), the topographic and morphological characterization was carried out by Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM), respectively. As a result, we obtained a uniform and homogeneous thin film transfer with a controlled distribution of the nanomaterials on the substrates. Through AFM measurements, we report an average thickness of approximately 2 nm for three self-assembled thin films. In addition, the optical characterization by THZ-TDS and RAMAN reveals that the deposited films have specific absorption and transmission properties depending on the wavelength of the incident radiation indicating optical properties of the deposited nanomaterials are particularly interesting for applications in THz devices.

Keywords
Thin film, 2D materials, Optical properties, Terahertz, Langmuir-Blodgett technique.

Reference

D. Kaplan, R. Fullon, and N. A. Simonson, “Characterization of two-dimensional materials,” in Synthesis, Modelling and Characterization of 2D Materials and their Heterostructures, Elsevier, 2020, pp. 289–322. doi: 10.1016/B978-0-12-818475-2.00014-3.

This work was supported by

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Sesión Oral

[THF-7] EFFECT OF THE TRISODIUM CITRATE AS A COMPLEXING AGENT IN THE DEPOSITION OF ZnS BY SILAR.

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Zinc sulfide thin films were deposited on glass substrates using the Successive Ionic Layer Adsorption and Reaction (SILAR) method. The effect of tri-sodium citrate (TSC) as a complexing agent and their concentrations on optical properties, morphology, structure, and chemical mechanism of ZnS thin films were investigated. The results indicated that the SILAR-deposited ZnS thin films exhibit an average transmittance of 16% in the range of visible light and a zinc blend structure. The ZnS films synthesize using TSC as a complexing agent, present a smaller average particle size, an average transmittance of 85%, and a sharper adsorption edge at 300-340 nm. Based on our experimental observation and analysis, we conclude that the contribution of the oxychloride species, a subproduct in the chemical deposition, is suggested to be related to impurity level formers in the formation of ZnS thin films. TSC as a complexing agent in the SILAR technique is a non-toxic option to reduce the generation of the oxychloride species and synthesize a wide band gap semiconductor. Moreover, the use of complexing agents could be extended to other types of semiconductors deposited by SILAR.

Keywords
SILAR, thin films, wide bandgap semiconductors, complexing agent, zinc sulfide.

Reference

S. J. Pearton et al., “Recent advances in wide bandgap semiconductor biological and gas sensors,” Progress in Materials Science, vol. 55, no. 1. pp. 1–59, Jan. 2010. doi: 10.1016/j.pmatsci.2009.08.003.

[THF-27] GLUCOSE AND pH RELATION IN A NON-ENZYMATIC GLUCOSE SENSOR

Pablo Tirado Ph.D., Iker Chávez Ph.D., Gilberto Martínez Ph.D., Alexis Cruz Ph.D., Joselyn Alvarado Ph.D., Jesús Alcantar Ph.D., Daniela Díaz Ph.D.

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According to the World Health Organization (WHO), diabetes is one of the main causes of death in the world. With more than 537 million people affected worldwide and the number of diabetic patients is expected to double in 20 years. Therefore, is significant to develop accurate, fast, and reliable technology for blood glucose detection. One drawback of non-enzymatic sensors is that it requires a basic medium to work. The basic medium was satisfied by incorporating a pH-boasting microfluidic medium on the sensor, which consisted of a cellulose layer with NaOH crystals embedded which are dissolved in the blood sample, increasing the pH to the necessary value for glucose detection. However, the glucose sensor doesn't count with an integrated pH sensor, making it difficult to accurately predict the pH of the sample after it passes through the microfluidic medium. Therefore, a real-time integration of pH sensing significantly improves the accuracy of glucose measurements as a correction variable, since the amperometric signal produced during glucose sensing is heavily dependent on the sample's pH. In this work, we presented the relationship between pH with non-enzymatic glucose sensing and how pH levels impact on glucose calibration plot. A 3-electrode system was used: Cu/CuO working electrode, Ag/AgCl reference electrode, and a graphite counter electrode. Glucose detection was evaluated by CV and CA measurements at different glucose concentrations (0-8 mM) and pH values (12-13.5), while pH sensing was done by measuring the open-circuit potential in the 11-13.5 pH range. A minimum pH of 12.5 was determined for glucose sensing, and the maximum glucose sensitivity of 304 μA/mMcm2 was obtained (pH=13).

Keywords
Electrochemical sensor, Glucose Detection, pH measurements, non-enzymatic sensor, amperometry.

Reference

G. Martinez-Saucedo, F.M. Cuevas-Muñiz, M. Sanchez-Fraga, I. Mejia, J.J. Alcantar-Peña, I.R. Chavez-Urbiola, Cellulose microfluidic pH boosting on copper oxide non-enzymatic glucose sensor strip for neutral pH samples, Talanta. 253 (2023) 123926–123933.

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[THF-28] NOVEL METHOD FOR THE NON-ENZYMATIC DETECTION OF GLUCOSE IN BLOOD

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Centro de ingeniería y desarrollo industrial, Querétaro, Mexico.

Diabetes mellitus is a worldwide public health problem caused by high blood glucose levels. According to the WHO, diabetes is one of the main causes of death in Mexico and in the world, it is estimated that there are approximately 422 million people affected and 1.5 million deaths due to direct complications derived from it. Therefore, it is necessary to have glucose detection and control systems for the general population. Glucometers are a very useful control tool for this condition, however, since most of the test strips use working electrodes with enzymatic methods, their useful life (shelf) is a problem, requiring the development of new ones methods with longer usefulness. This work describes a novel non-enzymatic methodology for in vitro detection of blood glucose by means of a 3-electrode electrochemical sensor using an AgCl electrode as a reference, copper oxide (Cu_2O) as a working electrode, and graphite as a counter electrode. The operating stages of the system are divided into 4 stages; i) alkalinization of blood pH (pH 12-13.5) by paper microfluidics modified with NaOH/KOH crystals ii) pH measurement by potential changes between the electrodes iii) current measurements by electrochemical techniques and iv) correlation of the measured current with the concentration of glucose present in an analyte sample to obtain a value in units of mg/dL. According to the preliminary tests, the electrochemical tests carried out in the laboratory allowed confirming the modification of the pH up to sufficiently alkaline values, in addition, it was possible to reliably detect glucose in concentration ranges from 0 to 180 mg/dL (0 to 10 mmol/L).

Keywords
Glucose, electrochemical sensor, non-enzymatic, chronoamperometry, potential, copper oxide, alkaline, microfluidics.

Reference

G. Martinez-Saucedo, F.M. Cuevas-Muñiz, R. Sanchez-Fraga, I. Mejia, J.J. Alcantar-Peña, I.R. Chavez-Urbiola, Cellulose microfluidic pH boosting on copper oxide non-enzymatic glucose sensor strip for neutral pH samples, Talanta, Volume 253, 2023, 123926, ISSN 0039-9140, https://doi.org/10.1016/j.talanta.2022.123926.

This work was supported by

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[THF-33] AUTOMATION OF ROBOTIC DEVICE FOR CHEMICAL DEPOSITION. BY SUCCESIVE IONIC LAYER ADSORPTION AND REACTION(SILAR)

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The chemical deposition of semiconductors by succesive ionic layer adsorption and reaction (SILAR) is practiced due to the control of growth layer-by-layer, the separation of adsorption and reaction simplify the understanding of the process. To perfom the process a mechanism is implemented in which the user controls manually the time between the beakers [1]. The accesibility of the method makes it affordable in terms of scaling and costs, however, comercial robotic system for carrying out the process are expensive since the price range is usually around $2958.00 USD up to $7,875.00 USD [2]. With this in mind, an automation low cost system between $80.00 up to $100.00 USD was developed to effectuate the chemical deposition(DC) by SILAR method. A Printed circuit board developed at the Autonomous University of Zacatecas that includes a microcontroller, an user interface that allows user interact with the system, a power driver circuit, and a heating system attached to the structure. The microcontroller is programmed with a series of different menus in which the user selects the compound to deposit, the user can adjust the number of cycles, immersion Depth, transfer time and modify the immersion time in reagents as in rinses. A control anylisis through a dinamic model is performed in order to reduce errors in the positioning of the reail, increasing the reproducibility of the depositions and the posibility of implementation in a larger scale system. A thin film of MnS (manganese sulfide) will be deposited and characterized crystallographically, morphologically and electrically as control test.

Keywords
Automation, SILAR, synthesis,thin films,semiconductos.

Reference

1. Y. F. Nicolau, «SOLUTION DEPOSITION OF THIN SOLID COMPOUND FILMS BY A SUCCESSIVE IONIC-LAYER ADSORPTION AND REACTION PROCESS», p. 14.
2. «SILAR Coating System». https://www.holmarc.com/silar_controller.php (accedido 31 de mayo de 2022).

[THF-83] SYNTHESIS OF ZnO-Ag NANOCOMPOSITES BY COMBINING Sol-Gel AND LASER ABLATION OF SOLIDS IN LIQUIDS

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This project aimed to develop a composite material with a zinc matrix and silver nanoparticles. The composite material was deposited on a glass substrate in the form of a thin film. Two techniques were used to integrate the silver nanoparticles into the zinc oxide matrix: Sol-Gel and laser ablation of solid-in-liquid.
In the Sol-Gel technique, a precursor solution composed of dihydrated zinc acetate, methanol and polyvinylpyrrolidone as stabilizing agent was obtained. Next, for the laser ablation technique of solids in liquids, we ablated a 99.99% pure silver target immersed in the precursor solution where the target will expel nanometer scale particles into the solution.
A glass substrate was introduced into the solution to form a xerogel film on the glass surface. Next, the film was dried at 120°C and different samples were subjected to a heat treatment of 100°C, 200°C and 400°C for 3 times with and without silver, also without heat treatment.
Characterization of thin films was performed using UV-Vis spectroscopy, X-ray diffraction, electrochemical impedance spectroscopy, and fluorescence. The UV-Vis absorbance spectra of the zinc acetate solution with silver nanoparticles showed surface plasmon sound at 400 nm. Plasmon resonance absorption was found on the ZnO films, however it seems to be temperature sensitive.

Keywords
zinc oxide, silver nanoparticles, thin films, solid-in-liquid laser ablation.

Reference

Arif, A., Belahssen, O., Gareh, S., & Benramache, S. (2015). The calculation of band gap energy in zinc oxide films. Journal of semiconductors, 36(1), 013001.

This work was supported by
Conahcyt and the University of Guadalajara.

[THF-87] FABRICATION OF PRESSURE SENSORS FOR APPLICATIONS IN MEDIUM TO HIGH PRESSURE ENVIRONMENTS

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At present, for the manufacture and design of pressure sensors used as MEMS, high care and high complexity are required in the process and design of each of the thin films of its components. Among the most important parts, that compound the pressure sensors, the piezoresistors and diaphragm stand out, whose materials used to manufacture them are currently widely studied (e.g. silicon, polysilicon, silicon carbide, etc.) so to seek innovation when manufacturing new pressure sensors, special emphasis must be placed on process variation and changes in the design to obtain the highest possible efficiency (sensitivity, voltage outputs, etc). This investigation presents the design, manufacturing and packaging of a sensor for medium and high pressures, as well as its characterization at different pressure ranges to obtain its variation of voltage outputs (Vout). The design was made based on the modeling of the structure by finite element method (COMSOL) and its manufacture was based on a Silicon on Insulator wafer (SOI). On the SOI's surface 4 piezoresistors were deposited to the edges of a circular diaphragm and these were connected in a Wheatstone bridge form. The geometry transference was made using different phases of photolithography. The variation of the Vout was evaluated in a test station with pressure control and supplying air pressures from 0 cm H2O to 200 cm H2O. The maximum Vout was 2.87 V at room temperature. The results obtained give rise to its possible use for applications that require of medium to high pressures.

Keywords
Thin Films, Pressure sensor, piezoresistors, photolithography.

Reference

B. Sheeparamatti, K. Balavalad, "Fabrication and characterization of PolySOI and a-SOI based micro piezoresistive pressure sensor for harsh environment applications". Microsyst. Technol, pp. 1-15, 2019.

This work was supported by

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[THF-127] "MODULACIÓN ESPACIAL DE MICROCAVIDADES ÓPTICAS CON PATRONES METÁLICOS EMBEBIDOS"

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En el presente trabajo se muestra el proceso de estudio, desarrollo y fabricación de microcavidades basadas en espejos dieléctricos, las cuales contienen depósitos metálicos con el fin de modular espacialmente la luz dentro de dichas microcavidades. Este trabajo es una prueba de concepto para demostrar y caracterizar el confinamiento fotonico en el plano que que será usado posteriormente para modular polaritones en microcavidades a base de semiconductores. La motivación de este trabajo es la de estudiar fenómenos de interacción luz-materia para desarrollar dispositivos optoelectrónicos de estado sólido con capacidades superiores o diferentes a los ya existentes, por ejemplo, simuladores cuánticos o aislantes topológicos fotónicos.
Otra de las motivaciones del presente trabajo es la de proveer una alternativa a los métodos utilizados en otros trabajos para modular polaritones en el plano. Por ejemplo, en el trabajo realizado en [1] se hicieron depósitos metálicos periódicos en la superficie de una microcavidad, de esta manera cambiando el potencial y por lo tanto la dispersión de, por ejemplo, la parte fotonica de polaritones dentro de la microcavidad.

Keywords
Microcavidad(MC), Depositos metalicos, Dispersion, Modulacion, Potenciales periodicos, Polaritones.

Reference

[1] Lai, C., Kim, N., Utsunomiya, S., Roumpos, G., Deng, H., Fraser, M., Byrnes, T., Recher, P., Kumada, N., Fujisawa, T., & Yamamoto, Y. (2007). Coherent zero-state and π-state in an exciton–polariton condensate array. Nature, 450(7169), 529–532. https://doi.org/10.1038/nature06334.

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[THF-144] STRONG LIGHT-MATTER COUPLING IN HYBRID MICROCAVITIES

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Optical microcavities (MC) constitute an attractive system for the study of light-matter interaction. In a high-quality MC with embedded quantum wells (QW) placed at the antinodes of the confined electromagnetic field, a photon can be coherently absorbed and reemitted by the direct excitons confined in the QW, yielding hybrid light-matter bosonic quasiparticles named exciton-polaritons. A light effective mass, strong inter-particle interaction and nonlinearity are some of the properties of polaritons which can produce remarkable phenomena such as Bose-Einstein condensation, superfluidity, soliton formation, among others. To achieve the strong light-matter coupling, MCs with high Q-factors are required. These high-quality samples are typically obtained through molecular beam epitaxy (MBE) using semiconductor materials from the III-V groups. While MBE provides a precise thickness control and low interfacial roughness, its long fabrication times due to slow growth rates, and its high technological complexity, allow for little flexibility in the fabrication of polaritonic devices. In this work, we demonstrate the strong light-matter coupling in a hybrid MC in which one half of the sample is fabricated through MBE while the other half is made of porous silicon. This methodology reduces the complexity and the fabrication time of high-quality samples and represents a novel and promising technique for the modulation of exciton-polaritons in deep potentials, which can be produced, for example, by embedding a metallic layer between the two halves of the MC.

Keywords
microcavities, exciton-polaritons, porous silicon.

Reference

E. A. Cerda-Méndez et al, Quantum fluids of light in acoustic lattices, J. Phys. D: Appl. Phys. 51 (2018). https://doi.org/10.1088/1361-6463/aa9ec7.

This work was supported by
CONACYT PhD grant.

[THF-162] 2D MATERIAL TRANSFER METHODS AND DETERMINISTIC ASSEMBLY OF VAN DER WAALS HETEROSTRUCTURES

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Two-dimensional (2D) materials derived from van der Waals (vdW) crystals, such as graphene, which was the first material isolated in a single layer, have opened a new area of research dedicated to the study of 2D crystals. These materials are characterized by their atomically thin structures and numerous electronic, optical, and mechanical properties, leading to novel devices and technological innovations. Among the diversity of these materials, there are 2D semiconductors like transition metal dichalcogenides (TMDCs). In recent years, fabrication techniques have been developed with the aim of obtaining single-layer materials on a large scale and with high quality, such as mechanical exfoliation, liquid-phase exfoliation, physical vapor deposition, chemical vapor deposition, among others. However, it is often necessary to transfer them onto arbitrary substrates for further investigation. In this work, we will focus on the deterministic transfer assisted by various polymer methods. We aim to transfer TMDCs flakes onto different substrates, such as silicon dioxide, metallic surfaces, and one-dimensional photonic crystals based on porous silicon, for the study of light-matter interaction. Furthermore, the transfer enables the design of vdW heterostructures by assembling different materials layer by layer, leading to the fabrication of new devices with unique properties.

Keywords
2D materials, semiconductors, deterministic transfer and vdW heterostructures.

Reference

Fan, Sidi, et al. "Transfer assembly for two-dimensional van der Waals heterostructures." 2D Materials 7.2 (2020): 022005. https://doi.org/10.1088/2053-1583/ab7629.

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National scholarships CONAHCYT phd thesis.

[THF-233] SELENIZATION OF NIOBIUM THIN FILMS BY ELECTRODEPOSITION AND RAPID THERMAL PROCESSING FOR THE OBTENTION OF NbSe2 FILMS

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Transition-metal dichalcogenides are of great interest due to their exotic electronic properties, such as charge density wave states and superconductivity, that they can show, especially in two dimensions. Among the dichalcogenides (WS2, WSe2, MoSe2, NbS2, NbSe2, etc.), NbSe2, a metal, has been one of the least explored experimentally.[1] Reports indicate that techniques such as CVT, APCVD, VDWE, and PLD, give niobium selenide in many stoichiometric forms. However, reducing the thickness looking for the sheet configuration, only structures of micrometer spatial size are usually formed. Here, we explore an alternate route to obtain bulk NbSe2 to search for a layer structure later. For this work, the objective was the incorporation of selenium into niobium thin films previously prepared by sputtering. Selenization of niobium film was carried out by electrodeposit and resulted in a morphological change regarding niobium films and the emergence of the characteristic band corresponding to selenium. Afterward, the film was treated by rapid thermal processing (RTP), and the resulting film was studied by AFM, Raman, and DRX. AFM micrographs showed a change in morphology and the formation of niobium diselenide (NbSe2), as revealed by Raman modes at 228 y 243 cm-1 assigned the reported bulk NbSe2.1 XRD patterns showed preferential growth in the (103) plane (COD-9016023) at an angle 2q of 36.6°. These results shed light on a practical route to obtain transition metal dichalcogenides in bulk and possibly in two dimensions.

Keywords
Thin film, niobium, dichalcogenide, electrodeposit, rapid thermal processing.

Reference

Hill, H. M.; Rigosi, A. F.; Krylyuk, S.; Tian, J.; Nguyen, N. V.; Davydov, A. V.; Newell, D. B.; Hight Walker, A. R. Comprehensive Optical Characterization of Atomically Thin NbSe2. Phys Rev B 2018, 98 (16), 165109. https://doi.org/10.1103/PHYSREVB.98.165109/FIGURES/4/MEDIUM.

[THF-293] SPUTTERING YIELD AMPLIFICATION STUDY OF Si DOPED WITH W, Cu, Ag, OR Mo

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In the DC magnetron sputtering technique there is a phenomenon called Sputtering Yield Amplification, SYA [1], which is related to the doping of a sputtering target with atoms of different atomic mass than the target material. This doping changes the collision cascade on the surface of the target. Consequently increases the number of atoms ejected from the target. In this work, we present a way of generating SYA by increasing the working gas pressure, i.e., the number of collisions in the gas phase, when small pieces of W, Cu, Ag, and Mo, were added, as dopants, on the Si target. We studied the physical phenomena necessary to generate the SYA, such as the surface binding energy and the atomic mass of the dopant elements, etc,. As well as, we calculated the number of W atoms returning to the target surface, in order to determine their effect on the cascade of collisions. In addition, calculations with the SIMTRA code were developed to determine the spatial distribution of the returning atoms on the target surface. By analyzing reference samples placed on the racetrack, via XPS, and RBS. We found that the percentage of SYA, measured with the Co-Sputtering Simulation software, depends on the number of dopant atoms redeposited. The results showed SYA of Si doped with W, where the sputtering yield increased almost linearly, as a function of the number of redeposited atoms. Somewhat similar results have been reported earlier. These results may be particularly interesting for those materials which have lower sputtering yield and have important applications in the thin films industry.

Keywords
Sputtering Yield Amplification, Sputtering, Si doped, SiW.

Reference

[1] S. Berg. Atom assisted sputtering yield amplification. J. of Vac. Sci. & Tech. A 10, 1592–1596 (1992).

This work was supported by
J. Cruz wants to thank the CONACyT postdoctoral fellowship.

[THF-301] THE 2P PHOTOEMISSION SPECTRA FOR THE FOURTH PERIOD OF METAL OXIDES BASED ON TRANSITION METALS

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Peak fitting the 2*p* corelevel from oxides of 4th-period (Sc to Zn) transition metals is challenging because of the presence of complex background, multiplet structure, and satellite peaks. In this work we present the peak-fitting analysis of the XPS spectra for these oxides.

Except for Sc and Ti, which were obtained from databases, the spectra was acquired from pure metallic films thermally oxidized. The films were characterized with an XPS instrument using 1486.7 eV monochromatic source (XR5, ThermoFisher), and a 7-channeltron hemispherical spectrometer (Alpha110, ThermoFisher).

Advanced tools were used to robustly fit the 2*p* and O 1*s* core levels. Similarities between the 2*p* spectra allow applying similar criteria during the peak fitting. Spectra are analyzed using the Voigt line shapes for the main photoemission peak and satellites. The background was modeled as a combination of the Shirley type (SVSC) background, the baseline, and, in some cases, the slope background. The SVSC parameter of the metallic 2*p* spectra goes from 0.0015 eV^{-1} (for scandium oxide) to 0.011 eV^{-1} (for zinc oxide) with a local maximum of 0.075 eV^{-1} (for manganese oxide). The parameter of the Shirley-type background is larger for Mn, Cr and Fe, which are elements with half filled *d*-band.

The intensities of the photoemission peaks of the core 2*p* and the O 1*s* for each metal oxide are employed for calculating chemical composition through the Multilayer Model (MLM).[1,2] The MLM is a self-consistent analysis method for multilayer films and systems with protrusions.

Keywords
Active Fitting Approach, Multilayer Model, transition metal oxides, XPS spectra.

Reference

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

[2] A. Herrera-Gomez, et. al, ARXPS assessment of the structure and composition of nanofilms including uncertainties through the MultiLayer Model, (submitted) (2023).

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SCIENCE OUTREACH

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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. 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 y Tecnología** que cada año tiene lugar dentro del marco del Congreso anual de esta sociedad científica.

[SCD-44] TÉCNICAS FOTOGRÁFICAS Y ESPECTROSCÓPICAS EN LA AGRICULTURA DE PRECISIÓN

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La agricultura de precisión hace uso de herramientas tecnológicas para monitorear campos de cultivo con el fin de mantenerlos en buen estado fitosanitario; lo cual, se ve afectado por diversos desastres naturales o provocados. El uso de tales herramientas permitiría tomar acciones más acertadas en el manejo agronómico, y así evitar pérdidas económicas debido a la fitosanidad por presencia de microorganismos o plagas; o por estrés hídrico, salinidad, contaminantes en el suelo, carencia de nutrientes; e incluso, para calcular daños ocasionados por fenómenos hidrometeorológicos como sequías, granizo, heladas. Gracias a los sensores de las cámaras multiespectrales e hiperespectrales, las técnicas espectroscópicas usadas en ciencia de materiales, se han visto escaladas porque dichas técnicas sólo sirven para caracterizar muestras muy pequeñas. La fotografía convencional permite captar la luz dispersada desde un objeto iluminado en el rango óptico. Sin embargo, el espectro de radiación electromagnética es muy amplio y abarca desde las ondas electromagnéticas hasta la radiación gamma. Por lo cual, obtener imágenes producidas dentro de un rango del espectro electromagnético nos lleva a la fotografía multiespectral o la hiperespectral. Sin embargo, las imágenes en el rango óptico, solamente tienen una resolución de alrededor la longitud de onda de la luz, por lo que explorar en el mundo más pequeño, ha llevado a técnicas de microscopía electrónica que pueden discernir imágenes muy cercanas al tamaño de los átomos. En esta ponencia expondremos diversas imágenes en el rango óptico, multiespectral y de microscopía electrónica aplicadas a la agricultura; cuya belleza es comparable estéticamente con imágenes de algunas corrientes artísticas a lo largo de la historia de la pintura. Aparte de ser, fuente para obtener información científica para el conocimiento profundo de los campos agrícolas.

Keywords
cámara multispectral, enfermedad foliar, índice de vegetación, agricultura de precision.

Reference

J. Cotton-Martin, HYPERSPECTRAL AND MULTISPECTRAL IMAGING, Photonics Spectra 54 (4), 36 (2020).

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Instituto Politécnico Nacional, “Proyectos de Desarrollo Tecnológico o Innovación en el IPN 2022”, Project No. 20227041.

[SCD-118] CELDAS SOLARES DE PELÍCULA DELGADA: "AÚN UNA GENERACIÓN PROMETEDORA"

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La creciente demanda de energía eléctrica en la sociedad moderna ha impulsado la búsqueda de fuentes alternativas de energía. Entre estas, la energía solar destaca por ser accesible, global y amigable con el medio ambiente. El aprovechamiento de esta energía a través de celdas solares ha prometido beneficios económicos, sociales y ambientales. Sin embargo, hasta la fecha, el uso masivo de esta tecnología y el efecto de los beneficios deseados han sido limitados. Esta plática proporcionará una visión general de los antecedentes y desarrollos en celdas solares, con un enfoque especial en su segunda generación que comprende a las celdas solares de película delgada. Desde el punto de vista de la Ciencia e Ingeniería de Materiales, se destacarán sus aplicaciones, versatilidad y la rentabilidad en términos de costo. Además, se presentarán algunos de los esfuerzos realizados en México por el grupo de investigación interinstitucional "Diseño y Optimización de Recubrimientos Avanzados (DORA-Lab)" del CIMAV-Mty/TECNL-CIIT, en cuanto al desarrollo de semiconductores utilizados en estos dispositivos, con la finalidad de fomentar el interés en la investigación de temas relacionados con celdas solares de película delgada.

Keywords
Energía solar; Celdas solares de película delgada; Semiconductores.
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Proyecto interno CIMAV: 23025-2021 y 25024-2023.

[SCD-167] MATERIALES COMPUESTOS DE MATRIZ EPÓXICA REFORZADOS CON MICROFIBRA DE CARBONO ESTABILIZADA: EVALUACIÓN MECÁNICA

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Los materiales compuestos de matriz polimérica reforzados con fibra de carbono son materiales de nueva generación empleados en industrias como aeronáutica, automotriz, espacial, deportiva y médica debido a sus excelentes propiedades mecánicas y la alta relación resistencia/peso [1]. Las fibras de carbono (FC) son excelentes materiales para reforzar materiales poliméricos por su alta resistencia mecánica. Una de las principales desventajas en el uso de FC como refuerzo es su elevado costo de procesamiento, lo cual hace a este tipo de materiales poco accesibles. El desarrollo de nuevos materiales de refuerzo de bajo costo, representa una excelente alternativa para la elaboración de materiales compuestos (MCs) que no comprometan su calidad mecánica y que sean accesibles en térmicos de costos, además de que puedan ampliar los campos de aplicación. Este estudio se centra en la evaluación de las propiedades mecánicas de MCs de resina epoxi reforzados con fibras de carbono de baja pureza. Tres tipos de fibras base de acrilonitrilo (F1, F2 y F3) fueron estabilizadas térmicamente a diferentes temperaturas y se utilizaron para elaborar MCs con resina epóxica. Los MCs con diferentes concentraciones de refuerzo de fibra (10% y 30% en volumen) se evaluaron mecánicamente para conocer la resistencia a la tracción, el alargamiento a la rotura y el módulo de Young. La resistencia a la tracción de la resina epóxica mejoró en un 3%, el alargamiento mejoró en un 10% y el módulo de Young mejoró en un 5%. Las propiedades de tracción y el módulo de Young de los compuestos mejoran con la cantidad de refuerzo, excepto la resistencia a la tracción de los materiales reforzados con fibra F3. Los resultados proporcionan un medio para el diseño de nuevos materiales con buenas propiedades mecánicas y con bajo costo de fabricación.

Keywords
fibras estabilizadas, materiales compuestos, fibra de carbono, estabilización.

Reference

[1] K. Yu, M. Wang, J. Wu, K. Qian, J. Sun and X. Lu, Modification of the interfacial interaction between carbon fiber and epoxy with carbon hybrid materials, Nanomaterials, 6 (2016) 6050089. https://doi.org/10.3390/nano6050089.

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[SCD-175] LA EVOLUCIÓN DEL SER HUMANO CON LOS SEMICONDUCTORES Y LA TECNOLOGÍA DE CHIPS

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En la actualidad la Electrónica se desarrolla con base en la tecnología de los circuitos integrados o chips (Microelectrónica). La gran mayoría de los instrumentos electrónicos de uso actual, sistemas de comunicación o artefactos personales, se ensamblan combinando algún tipo de chip con programas de computadora, o software. A esta combinación se le llama sistema electrónico, por lo que actualmente gracias a la tecnología de Microelectrónica, diversos tipos de sistemas están presentes en nuestro entorno. Algunos ejemplos de ellos son los sistemas de localización (GPS), tabletas, pantallas inteligentes, los hornos de microondas y los teléfonos celulares, por mencionar algunos. Ahora los chips se usan con gran impacto en el sector salud, no sólo en sistemas de diagnóstico como los ultrasonidos, también en nuevos sensores de tipo biomédico. Pero, ¿cómo es esto posible?, pues con base en la ciencia de materiales, biología, química, principalmente, evolucionando 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 dispositivos electrónicos son recubiertos con algún tipo de polímero, logrando que el organismo no rechace el sistema electrónico implantado. Esta nueva funcionalidad de los circuitos en el cuerpo humano se llama biocompatibilidad. Es importante señalar que la mayoría de los materiales de uso común en los chips, son tóxicos para el tejido biológico. En esta charla se abordan conceptos de la Microelectrónica y sus aplicaciones.

Keywords
Chips, Circuitos integrados, Microelectrónica, Sensores, Electrónica.
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Conacyt.

[SCD-177] SEMICONDUCTORES: COADYUVANTES EN LA MITIGACIÓN DEL CALENTAMIENTO GLOBAL

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El calentamiento global es un grave problema que pone en riesgo la viabilidad de la humanidad. A partir de la revolución industrial se ha producido un incremento sistemático de la temperatura promedio del mundo y recientemente se ha llegado a un consenso sobre su influencia en fenómenos naturales catastróficos.
Desde el siglo pasado durante la crisis del petróleo se puso en relieve la necesidad de contar con fuentes de energía renovable. El sol es la fuente de energía de la tierra y su principal aprovechamiento ha sido mediante dispositivos fotovoltaicos fabricados empleando semiconductores.
Los semiconductores además de ser útiles para generar energía pueden coadyuvar en la reducción del calentamiento global al ser empleados como fotocatalizadores artificiales, medidores de gases de efecto invernadero y elementos pasivos para manejar el calentamiento térmico asociado con la radiación solar.
En la plática se presentará una visión general de aplicaciones de la física en la mitigación de problemas que contribuyen al calentamiento global.
Finalmente se describirá trabajo realizado en mis laboratorios relacionados con la síntesis de materiales semiconductores en forma de película delgada y su aplicación potencial en el desarrollo de materiales fotovoltaicos y fotocatálisis. También presentaremos algunos resultados obtenidos con sistemas pasivos para aprovechar la energía térmica solar hechos con materiales compositos producidos por la técnica de electrohilado.

Keywords
Semiconductores, Calentamiento global, Fotovoltaicos, Termoelectricos, Energia renovable.

Reference

Gurevich, Y. y Melendez-Lira ;M. (2013). Fenómenos de contacto y sus aplicaciones en celdas solares. fondo de cultura económica.

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[SCD-178] ÓXIDOS CONDUCTORES TRANSPARENTES?: ALTERNATIVAS PARA LA FABRICACIÓN DE DISPOSITIVOS ELECTRÓNICOS MODERNOS

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Los óxidos conductores transparentes (mejor conocidos como TCOs por sus siglas en inglés) son materiales versátiles que han revolucionado la tecnología moderna. Aunque todos los días interactuamos de alguna manera con un TCO, para la mayoría de la sociedad son desconocidos. Estos materiales tienen la capacidad de conducir la electricidad y, al mismo tiempo, permitir el paso de la luz (dos propiedades que comúnmente se oponen entre sí) lo que los hace idóneos para su uso en dispositivos como pantallas táctiles, paneles solares y ventanas inteligentes. El ITO, el TCO más utilizado, es un compuesto químico llamado óxido de estaño que tiene impurezas de indio; sin embargo, el indio es un elemento químico con poca abundancia en la corteza terrestre lo que genera cierta preocupación en cuanto a su disponibilidad a largo plazo y su impacto económico en los dispositivos que lo utilicen. Por tal razón, en el campo de la ciencia e ingeniería de materiales existe una corriente que investiga materiales alternativos que puedan ocupar el lugar del ITO. En esta charla se comentarán, por un lado, aspectos generales de los TCOs y su implementación en dispositivos electrónicos. Además, se presentarán los retos enfrentados por el grupo de investigación de Diseño y Optimización de Recubrimientos Avanzados (DORA-Lab) del CIMAV-Mty&TECNL-CIIT en el desarrollo de recubrimientos TCOs basados en óxido de zinc con impurezas de aluminio (AZO) y sus potenciales aplicaciones en edificios inteligentes.

Keywords
óxidos conductores transparentes, TCO, recubrimientos.
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Proyecto interno CIMAV No. 23025-2021: Recubrimientos fotoactivos para combatir la contaminación ambiental y promover el uso eficiente de energía.
Proyecto interno CIMAV No. 23025-2021: Recubrimientos fotoactivos para combatir la contaminación ambiental y promover el uso eficiente de energía II.

[SCD-179] ÓXIDOS METÁLICOS EN FORMA DE RECUBRIMIENTOS Y SU FUNCIÓN EN LA LIMPIEZA DEL AGUA CONTAMINADA

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En la actualidad, el tratamiento de agua residual se ha vuelto imprescindible en varios países del mundo en busca de la reutilización del vital líquido debido a su alto índice de escasez; además, se tiene conciencia de los elevados niveles de contaminación del agua, incluso con algunos contaminantes que son muy difíciles de remover o degradar, lo que disminuye la eficiencia de los tratamientos convencionales de aguas. Para abordar esta problemática, se han tratado de copiar algunos procesos naturales como la fotosíntesis, pero cuando se enfoca en limpiar el agua se le conoce como “fotocatálisis”. Para llevar a cabo este proceso se necesita de un material fotoactivo (fotocatalizador, típicamente un semiconductor) que con la acción de la luz (solar, idealmente) promueven reacciones químicas específicas que provocan la degradación de los contaminantes. En la búsqueda del fotocatalizador ideal se han utilizado una gran variedad de materiales, pero aún se trabaja en mejorar el rendimiento fotocatalítico con métodos alternativos que incluyan su funcionamiento con luz solar y fotocatalizadores en forma de recubrimientos. De esta manera, algunos óxidos metálicos, por ejemplo el óxido de hierro y el óxido de zinc, juegan un papel importante en esta área. En esta charla se comentarán las propiedades de interés más relevantes de estos óxidos que pueden aprovecharse en el proceso fotocatalítico, brindando así un panorama general de las áreas de oportunidad que se tienen para maximizar la degradación de contaminantes presentes en el agua. Además de mostrar las investigaciones realizadas por el grupo DORA-Lab en torno a su desarrollo con el objetivo de mejorar los procesos de tratamiento del agua residual y contribuir a la preservación de nuestros recursos hídricos para un futuro sostenible.

Keywords
fotocatálisis, semiconductor, óxidos metálicos, recubrimientos.

Reference

A. L. Martínez-García, Z. Montiel-González, O. Y. Ramírez-Esquivel and D. A. Mazón-Montijo, ¡A limpiar agua con óxidos! Química de materiales al servicio del ambiente. Revista Digital Universitaria, 23(5), 9. https://doi.org/http://doi.org/10.22201/cuaieed.16076079e.2022.23.5.7.

This work was supported by

CONAHCYT-Beca.
Proyecto interno CIMAV No. 23025-2021: Recubrimientos fotoactivos para combatir la contaminación ambiental y promover el uso eficiente de energía.
Proyecto interno CIMAV No. 25024-2023: Recubrimientos fotoactivos para combatir la contaminación ambiental y promover el uso eficiente de energía II.

[SCD-193] NANOTECNOLOGÍA Y EL DESARROLLO SOSTENIBLE EN MÉXICO: UNA ALIANZA CON VISIÓN HACIA UN MEJOR FUTURO

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Con el objetivo de erradicar la pobreza, proteger el planeta y asegurar la prosperidad de las futuras generaciones, los Estados Miembros de la Organización de las Naciones Unidas (ONU) aprobaron la Agenda 2030 para el desarrollo sostenible. Esta agenda establece "los 17 Objetivos de Desarrollo Sostenible (ODS)" como una ruta para abordar los desafíos socioeconómicos y ambientales a nivel mundial. En México se creó el Consejo Nacional de la Agenda 2030 para el Desarrollo Sostenible, entidad encargada de la coordinación de las acciones necesarias para el cumplimiento de los ODS. Las acciones que ha tomado esta entidad respecto a problemas ambientales abordan el acceso a agua purificada, atendiendo el objetivo 6 (agua limpia y saneamiento), fomentar el uso de fuentes de energía renovables, lo cual impacta en el objetivo 7 (energía asequible y no contaminante) y el objetivo 13 (acciones para combatir el cambio climático). Sin embargo, es necesario seguir trabajando en cumplimiento de estos objetivos. Es aquí donde la innovación y desarrollo de nuevas tecnologías, como la nanotecnología, desempeña un papel fundamental para el cumplimiento de estos ODS. En los últimos años ha habido un aumento significativo en el estudio de la nanotecnología debido a su potencial para el desarrollo de soluciones enfocadas a problemáticas ambientales. En esta charla se proporcionará una visión general de la nanotecnología, sus principios y como es empleada en cuestiones ambientales, asimismo se presentarán algunos ejemplos de recubrimientos nanoestructurados sintetizados por el grupo de investigación "Diseño y Optimización de Recubrimientos Avanzados (DORA-Lab)" y potencial de aplicación en remediación ambiental. De esta manera, se pretende dar a conocer la importancia y relevancia de la incorporación de la nanotecnología a favor de un desarrollo sostenible.

Keywords
Nanotecnología, desarrollo sostenible, Agenda 2030.
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[SCD-196] COSECHANDO ENERGÍA DE NUESTRO ENTORNO

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En la actualidad, la humanidad en su conjunto requiere una gran cantidad de Energía para sus actividades diarias. La Energía, en sus diferentes formas, nos permite realizar Trabajo, desplazarnos, transformar materias primas, y así producir bienes y dar servicios.
En nuestro entorno tenemos disponibles fuentes de Energía en muy diversas formas. Por ejemplo en el petróleo y los derivados que producimos, los cuáles quemamos, para mover diversos tipos de máquinas, para generar electricidad, para desplazarnos, para realizar otros procesos de producción. De forma muy similar utilizamos la quema de carbón. También en las últimas décadas se ha explotado la producción de biodiesel, con el mismo enfoque de obtener energía a partir de un combustible.
Sin embargo, algo que encontramos en común entre las diversas actividades humanas, es el uso de la electricidad, la cual puede producirse a partir de otro tipo de fuentes de energía, sin la necesidad de combustibles. Este sería el esquema de energías renovables por el que vale la pena apostar; la energía del viento (eólica), de las mareas (mareomotriz), de la luz solar que recibimos (fotovoltaica y termosolar), del movimiento (triboeléctrica) y, más recientemente, de la humedad en el ambiente.
En esta charla te platico algunos de los detalles importantes, en los que un día podrías profundizar profesionalmente, para dedicarte a cosechar energía de nuestro entorno.

Keywords
Energía, Entorno, Renovables.
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Universidad de Guadalajara.

[SCD-199] TRIBOLOGÍA: CIENCIA APLICADA EN EL DEPORTE

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La tribología es la ciencia que estudia los fenómenos presentes cuando dos superficies se encuentran en contacto y movimiento relativo, como son la fuerza de fricción, desgaste y lubricación. Es por ello que toda clase de movimiento de un cuerpo que eta en contacto con otro presentan los fenómenos tribológicos y más cuando el resultado de este movimiento debe de ser preciso, como pasa en todos los deportes. Es por ello que en esta presentación se mostrara algunos ejemplos de cómo la ciencia de la tribología es aplicada en diferentes de portes, como son: Futbol soccer, básquetbol, béisbol y futbol americano, destacando la ropa utilizada para los uniformes, contacto del cuerpo con el balón (lanzar y/o patear) y la forma de correr durante un partido.

Keywords
Tribología, Deportes, Movimiento, Fuerza, Precisión.

Reference

Carré, M., & Lewis, R. (2012). Special issue on tribology of sport. Proceedings of the Institution of Mechanical Engineers, Part J: Journal of Engineering Tribology, 226(7), 587-587.

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[SCD-238] ¿DÓNDE HAS ESCUCHADO LOS TÉRMINOS: NANOROBOTS, NANOFORMAS, NANOMITES, NANODOTS, NANOHORMIGAS, NANOSURFERS?

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El título de la plática parece examen, o reto, o tal vez oportunidad para que demuestres tu experiencia en las películas, tu espíritu cinéfilo. Y de hecho es de todo un poco. Algo que la Ciencia de Frontera puede agradecer al cine, televisión y series de streaming, es la difusión de la nanotecnología a través de los términos que leíste en el título: todos con el prefijo "nano" [1]. Como podrías haber constatado en las películas, es realmente fantástico el mundo de posibilidades que se le han adjudicado a la Nanotecnología: maquinas minúsculas reparadoras de órganos humano, restauradores del medio ambiente, combate de plagas, establecen batallas contra células cancerígenas y otras enfermedades, combaten el envejecimiento con radicales antioxidantes, son minúsculos mensajeros de entrega de medicina nano local, habilitan el intercambio de información ultrarrápida y de encriptación ultra-segura, son entes minúsculos pero demasiado fuertes en relación a su tamaño, hábiles surfeadores en torrentes sanguíneos, entre otras propiedades. El protagonista en esta plática serás tú como asistente activo, imaginando escenarios de posibilidades de las anteriores aplicaciones, compartiendo tus críticas y planteando escenarios reales, futuristas y/o imaginarios. Te invito a debatir en equipos si Hollywood sueña o enseña. Yo como guía te expondré únicamente la dimensión de las cosas que pretendemos dominar en esta nueva área de la Ciencia, hablaré de las posibilidades para manipular la materia a esta escala y de algunos de los hallazgos y avances científicos reales.

Keywords
Nanotecnología, cine, nanomáquina, divulgación, nano medicina.

Reference

https://www.imdb.com/search/keyword/?keywords=nanotechnology.

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[SCD-248] NUESTRO CEREBRO: UNA MAQUINARIA CELULAR Y MOLECULAR FASCINANTE

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El cerebro es un órgano fascinante de nuestro cuerpo. Nos permite percibir las condiciones del medio ambiente a través de nuestros sentidos (vista, olfato, oído, gusto, tacto) as cómo reaccionar ante situaciones favorables para la vida y evitar peligros. También nos permite interactuar y comunicarnos con nuestros congéneres por medio del lenguaje oral, escrito o corporal. Nos hace capaces de amar a otros seres humanos, lo cual es crucial para asegurar la supervivencia de nuestra especie. Además, nos permite estar conscientes de nuestro propio ser y de nuestra ubicación en el universo. Nos sirve para preservar en la memoria información necesaria para nuestras vidas. Pero: ¿Cómo es posible que este órgano pueda realizar tantas funciones tan especializadas como sorprendentes? Después de todo, está hecho con átomos similares a los que conforman toda la materia…
En esta plática exploraremos cómo funciona el cerebro y en general el sistema nervioso central desde el punto de vista de la ciencia de materiales: su composición química y las interacciones físicas entre los átomos y las moléculas que lo conforman. Hablaremos de las neuronas y de otras células especializadas, así como de algunas moléculas que hacen posibles las funciones cerebrales: neurotransmisores, receptores, proteínas, etc. Hablaremos también brevemente del problema de la conciencia humana. ¿Cómo se puede definir? ¿Cómo se puede estudiar? ¿Cuál es su función biológica? Finalmente, haremos comentarios breves sobre algunas de las grandes incógnitas y enigmas científicos que continúan sin respuesta hasta el momento. ¡Todavía hay mucha investigación por realizar para comprender mejor nuestro cerebro!

Keywords
Cerebro, Neurociencia, Conciencia, Biofísica.

Reference

Fundamental neuroscience, Squire et al, Academic press, 4th edition, 2012.

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[SCD-261] FOTONES COMESTIBLES

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Probablemente, en algún curso de física hemos escuchado hablar acerca de los “fotones”, pero para aquellos que desconocemos el significado de la palabra, estos se definen de manera concisa, como partículas que componen la luz (cuantos).
Pero ¿por qué son tan importantes los fotones?, descubriremos que estas partículas son las responsables de transportar energía, la cual nos permite observar diversos fenómenos físicos.
Y a todo esto ¿qué relación tienen los fotones con la comida?, la respuesta a esta pregunta no es sencilla, sin embargo, tiene relación directa con la energía que se obtiene de forma directa de la luz solar. Se ha observado que muchos desechos comestibles como cáscaras frutales o vegetales y residuos orgánicos como el café o sargazo pueden ser utilizados como bio-marcadores en aplicaciones de detección y tratamiento de enfermedades.
El contenido de esta plática se centrará en mencionar generalidades de emisión luminosa de infusiones comestibles.

Keywords
Fotones, Comestibles, Desechos-orgánicos.
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[SCD-269] SENSORES, EXTENDIENDO LA CAPACIDAD DE NUESTROS SENTIDOS

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Nuestra percepción de la realidad está limitada por los sentidos humanos. Dependemos de nuestros sentidos, como la vista, el oído y el tacto. Ellos nos suministran de información con el fin de interpretar y comprender el mundo que nos rodea. Sin embargo, a medida que avanzamos en el conocimiento y la comprensión de la realidad, hemos descubierto que nuestras percepciones sensoriales son solo una parte de la ecuación.

Las matemáticas, la física y la tecnología han desempeñado un papel fundamental en la disminución de las limitaciones de nuestra percepción. A través de estas disciplinas, hemos logrado desarrollar herramientas y tecnologías que nos permiten captar y comprender aspectos de la realidad que van más allá de lo que nuestros sentidos pueden percibir directamente.

Un ejemplo destacado de esto es el desarrollo de sensores y biosensores. Estos dispositivos han revolucionado nuestra

capacidad para medir y cuantificar fenómenos biológicos, químicos y físicos. Los sensores nos permiten ampliar nuestra percepción al captar señales y datos que no son detectables por nuestros sentidos naturales.

Por ejemplo, los biosensores pueden analizar muestras biológicas y proporcionar información detallada sobre la salud y el funcionamiento del cuerpo humano. Nos ayudan a ampliar el entendimiento de la complejidad de las interacciones que el hombre tiene con su medio ambiente, permitiéndonos cuantificar factores como la contaminación por metales pesados en el aire o en el agua, la acidificación de los mares, la proliferación de agentes patógenos en alimentos, entre otros.

Estos avances tecnológicos tienen un impacto significativo en diversas áreas, como la medicina, la industria alimentaria y la protección ambiental. Gracias a los sensores y biosensores, podemos obtener datos precisos y en tiempo real, lo que facilita la toma de decisiones informadas y la implementación de medidas correctivas oportunas.

Keywords
Sensores, percepción, limitaciones, tecnología, ciencia.

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[SCD-283] EL PEQUEÑO GRAN AVANCE DE LOS NANOMATERIALES

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Hoy en día, una parte de los científicos en el mundo se han propuesto resolver problemas medioambientales, para ello los dispositivos como los paneles solares, los generadores de hidrógeno o la conversión y/o captura de gases tóxicos son sumamente importantes. Lo anterior puede ser posible gracias a la nanoestructuración de los materiales, que en palabras simples es acomodar los átomos de cierta forma para potenciar sus propiedades o inclusive darle nuevos usos. Sin embargo, esto no es una tarea sencilla ya que involucra manipular átomos, y sabemos que son diminutos. Para darte una idea de lo que es la nanoescala, puedes tomar una cinta métrica y a uno de sus centímetros marcados trata de dividirlo en diez millones de partes iguales, ahora, un buen ejemplo de la nanoestructuración es el grafito, que es un material que podemos encontrar en nuestros lápices, pero al reordenar los átomos podemos tener el famoso grafeno, que es una fina capa de grafito con 1 átomo de espesor.

Como ya se ha mencionado, las áreas de aplicación de las nanoestructuras no se limitan a aplicaciones medioambientales, también pueden ser aplicadas en medicina, sensores, computación cuántica entre otros, además pueden servir para mejorar propiedades de los materiales como la dureza, conductividad térmica o la electroluminiscencia. En México, se desarrolla investigación sobre estos interesantes temas y a lo largo de esta platica mencionaremos lo que investiga dentro del IPN, particularmente en el grupo de investigación de nanociencias en donde estudiamos todo lo anteriormente mencionado con un enfoque teórico, empleando recursos computacionales de alto nivel, y conocimientos de física, química entre otras áreas.

Keywords
Divulgación, Ciencia, Nanomateriales, Nanoestructuras, Grafeno, Teoría.

Reference

Materials 2022, 15(3), 1012; https://doi.org/10.3390/ma15031012.

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[SCD-295] GOTAS DE VIDA: PRESERVANDO EL RECURSO VITAL PARA UN FUTURO SOSTENIBLE

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El agua es uno de los recursos vitales y fundamentales para la existencia y el funcionamiento de la Tierra. Es esencial para todos los seres vivos y desempeña un papel importante en diversos procesos naturales, desde el mantenimiento de la salud humana hasta el funcionamiento de los ecosistemas y el desarrollo económico. En primer lugar, el agua es esencial para la supervivencia de los seres humanos. Es necesaria para mantener la hidratación, regular la temperatura corporal, transportar nutrientes y facilitar el buen funcionamiento de los órganos y sistemas del cuerpo humano. Además es esencial para la producción de alimentos,la agricultura y desempeña un papel crucial en los ecosistemas terrestres. Los ríos, lagos, océanos y humedales proporcionan hábitats para las especies y son el hogar de una gran diversidad biológica. Los ecosistemas acuáticos actúan como reguladores del clima, ya que el agua absorbe y almacena el calor solar, ayudando a mantener la estabilidad térmica en las regiones costeras y mitiga los efectos del cambio climático. Además, el agua es un recurso clave para el desarrollo económico y la actividad industrial. Muchas industrias dependen del agua como parte de sus procesos de producción, como la generación de energía hidroeléctrica, la fabricación de productos químicos y la producción de alimentos. Además, el agua es fundamental para el transporte y el comercio marítimo, ya que proporciona una vía de navegación para el intercambio de bienes y servicios a nivel global.Sin embargo, a pesar de la importancia vital del agua, enfrentamos desafíos significativos en la gestión y conservación de este recurso. La sobreexplotación, la contaminación y el cambio climático afectan la disponibilidad y calidad del agua. Por tanto, es crucial adoptar medidas para promover la conservación del agua, la gestión sostenible de los recursos hídricos, la protección y recuperación de los ecosistemas acuáticos.

Keywords
Contaminantes emergentes, remediación ambiental, sistemas acuáticos, agua.

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[SCD-299] LA SUSTANCIA MÁS EXTRAORDINARIA

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Seguramente muchos se sorprenderán al tratar de relacionar lo de extraordinario con el agua, la sustancia a la que nos referiremos en esta plática. Esto indica que sabemos poco de este increíble líquido, con propiedades que permiten desde la existencia de nuestra vida hasta la del planeta tal cual lo conocemos. En esta plática comentaremos cuantos tipos de agua hay y como una sustancia tan sencilla y común tiene propiedades tan increíbles. Se resaltarán algunas propiedades termodinámicas del agua que explican, por ejemplo, por qué los hielos flotan y el impacto que esto tiene en el planeta. Presentaremos las diferencias entre el agua de mar, de los ríos y de lluvia, y qué características tiene el agua potable. Y por supuesto, comentaremos la importancia del cuidado del agua y de contar con un agua de calidad para tener una buena calidad de vida.

Keywords
Calidad del agua, tipos de agua, propiedades del agua.

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[SCD-303] AGUA DE USO, NO DE ABUSO

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Uno de los principales retos que enfrentamos hoy en día es el abastecimiento y la calidad del agua. En particular en México, CONAGUA prevé períodos críticos de escasez hacia el año 2030. Por tanto, es imperativo tomar acciones para mitigar esta problemática. Esta charla versará sobre el desarrollo y la implementación de una planta piloto sustentable operada con energía solar para el tratamiento de agua pluvial de la CDMX. Esta planta permite el aprovechamiento del agua, el uso de energía solar, la monitorización en tiempo real de diversas variables fisicoquímicas para la determinación de la calidad del agua, así como la implementación de procesos innovadores en un tren de tratamiento de agua. La planta se orienta a fortalecer la investigación aplicada en el tratamiento de agua a través de la síntesis, caracterización y evaluación de diferentes materiales sustentables y tecnologías. La investigación se enfoca a la búsqueda de tratamientos innovadores de diferentes contaminantes presentes en efluentes para la obtención de tres tipos de calidad de agua: 1) uso de agua para riego, 2) agua desionizada tipo 1 y 3) agua potable; mediante la determinación, el análisis, la monitorización y control de los parámetros fisicoquímicos. Se busca que este proyecto beneficie a la población en general en condiciones de vulnerabilidad económica-social con base en el Plan Nacional Hídrico 2020-2024.

Keywords
agua, contaminantes emergentes, energía solar, tratamiento de agua.
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Flores Conde Araceli NSN-360
Flores Daniel RWE-228
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Flores Ian RWE-158
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García Ernesto NSN-255
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Garcia Garduño Olivia-Amanda LPM-350
García Lamont Jair MEM-358
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Garcia Lopez Karla Berenice LPM-111
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García Rafael LPM-70
García Ramírez Sandra Xaxil RWE-332
García Rocha Miguel BIO-109
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García Rodríguez Francisco Javier NSN-151
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García Sánchez Mario Fidel RWE-242
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García Sánchez Mario Fidel RWE-323
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García Serrano Jesús NSN-34
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García Vazquez Valentín RWE-69
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García Vidal Usiel Omar BIO-63
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Garcia-Bustos Ernesto David SIT-216
García-Cruz Miguel Ángel NSN-26
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Gonzalez Silos Benjamin Alejandro THF-127
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Hernandez Hernandez Arturo RWE-122
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Hernández Norberto MEM-280
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Hernández Oliva Noemi CHM-62
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Jiménez Vivanco María del Rayo NSN-343
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Juárez Santacruz Libertad RWE-307
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López Laura LPM-10
Lopez Lazcano Carlos Augusto MEM-81
López López M. SEM-339
López- López Máximo NSN-201
López López Máximo NSN-302
López López Máximo NSN-346
López López Máximo SEM-353
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López Luna Edgar THF-209
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López María MEM-280
Lopez Mena Edgar Rene NSN-160

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Mario Hidrogo ALD-317
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Marquez-Mata Claudia Angelica CHM-68
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Martinez Fuentes Marco Antonio PVL-266
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Martínez José BIO-289
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Martinez Laur PVL-35
Martinez Lopez Brandon Lauro THF-32
Martinez Ma.del Rosario SEM-86
Martinez Marco PVL-123
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Martinez Reyes Alejandro SEM-91
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Mateos Anzaldo Francisco David ALD-73
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Mathew Xavier PVL-246
Mathews Nini Rose RWE-69
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Mazón Montijo Dalia Alejandra SIT-82
Mazón-Montijo D. A. SCD-179
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Mejía Israel RWE-267
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Méndez García V. H. SEM-264
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Méndez García V.H. NSN-239
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Méndez-González María Magdalena BIO-197
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Mendoza Davila Miguel Ángel THF-209
Mendoza Sánchez Alberto Rafael NSN-356
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Mendoza-Álvarez J.G. SEM-226
Mendoza-Alvarez Julio G NSN-211
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Mendoza-Alvarez Julio Gregorio SEM-325
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Miguel Angel Vidal Borbolla ALD-300
Millán-Almaraz J.R. SEM-341
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Molina Joel ALD-364
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Mora Mora Zaira NSN-137
Morales Mendez Jose Guadalupe NSN-275
Morales Ramos César Benjamín CHM-297
Morales Rojas Alfredo BIO-197
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Moreno Araujo Jose Enrique CHM-157
Moreno Armenta Guadalupe TSM-80
Moreno Armenta Maria G. TSM-12
Moreno Armenta Maria Guadalupe TSM-19
Moreno Cabrera Nidia Esther NSN-210
Moreno García Harumi THF-32
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Moreno Hernandez Diana Elienay NSN-286
Moreno Palmerín Joel BIO-113
Moreno Pedro Antonio MUL-348
Moreno Saavedra Victoria NSN-221
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Mota-Paniagua Rafael SEM-146
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Muhl Stephen PVL-266

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Rodriguez García Carlos Eduardo LPM-74
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Romero Ibarra Issis Claudette RWE-282
Romero Ibarra Issis Claudette RWE-322
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