
NANO TECH
Puerto Vallarta 2018

NANOTECH

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14th International Topical Meeting on Nanostructured Materials and Nanotechnology NANOTECH 2018

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EDITORS

Dr. Iván Guillén Escamilla
Dr. Bertha Molina Brito
Dr. Juan Carlos Mixteco sánchez
Dr. Alfredo Tlahuice Flores

PROCEEDINGS OF THE 14th INTERNATIONAL TOPICAL MEETTING ON NANOSTRUCTURED MATERIALS AND NANOTECHNOLOGY (NANOTECH 2018)

Abstracts are the responsibility of the authors

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Consejo Nacional de Ciencia y Tecnología, CONACyT
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Dr. Adalberto Zamudio Ojeda, CUCEI, UDG.
Dr. Stefan Heun, Istituto Nanoscienze-CNR and Scuola Normale Superiore.

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INTRODUCTION

Appreciable participants of the 14th Nanotech congress:

For the organizing committee is a pleasure to welcome you. The congress is the meeting place for the community of scientists dedicated to the area of nanoscience and nanotechnology and is the ideal space for the presentation and discussion of ideas and projects in these fields.

In this edition 144 posters were accepted that were presented in three mural sessions. Additionally, fourteen plenary lectures were delivered on topics of particular interest in the nanoscience and nanotechnolgy fields, thirty-eight short talks; the second Workshop on Molecular Simulation as well as the activities of the fifth symposium of nanomaterials with applications in solar energy, environment and health; the annual meetings of the Nanosciences Division of the Mexican Physics Society and the CONACyT Mexican Nanoscience and Nanotechnology theme network. Finally, four courses were lectured to undergraduate and graduate students.

This congress has certainly favored thematic and interdisciplinary discussions and it has promoted collaborations between several academic groups in the country and abroad. We invite you to join these open spaces of reflection during this forum and encourage you to incorporate young Mexican graduates to nanoscience and nanotechnology industry with the goal of incrementing the impact of this discipline in the field.

We express our sincere gratitude to all of you who have contributed to the successful completion of all activities of this congress; this includes sponsors, and staff members, the UNAM Faculty of Sciences, Centro Universitario de los Valles of the University of Guadalajara, and the Mexican Physics Society.

Organizing Committee of the 14th Nanotech Congress

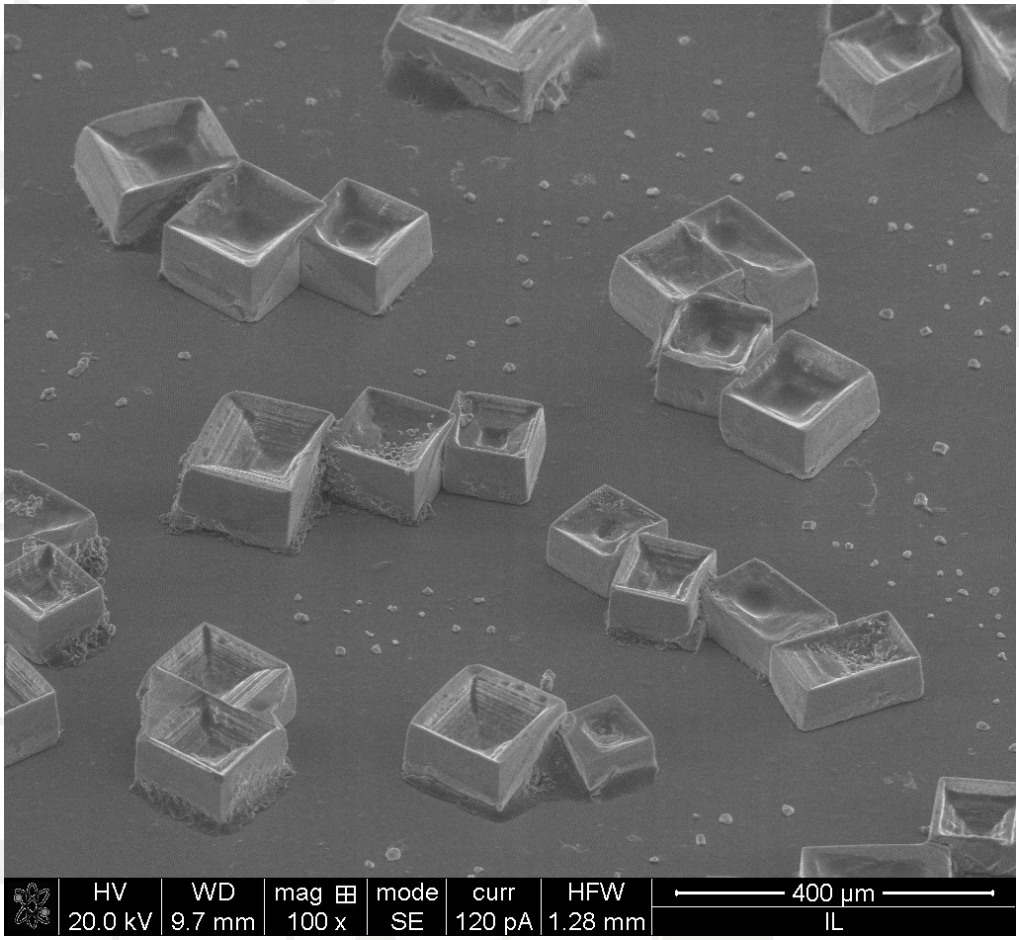
SCIENTIFIC PHOTOGRAPHY CONTEST IN NANOSCIENCE

PHOTOGRAPHY CONTEST

Aarón Israel Díaz Cano[1], Janna Douda[1], Hugo Martínez Gutierrez[2]

[1]Instituto Politécnico Nacional UPIITA-IPN, Av Instituto Politécnico Nacional 2580, La Laguna Ticoman, 07340 Ciudad de México, CDMX.
[2]Instituto Politécnico Nacional CNMN, Unidad Profesional Adolfo López Mateos, s/n, Gustavo A. Madero, C.P. 07738, CDMX.

*aidiaz@ipn.mx



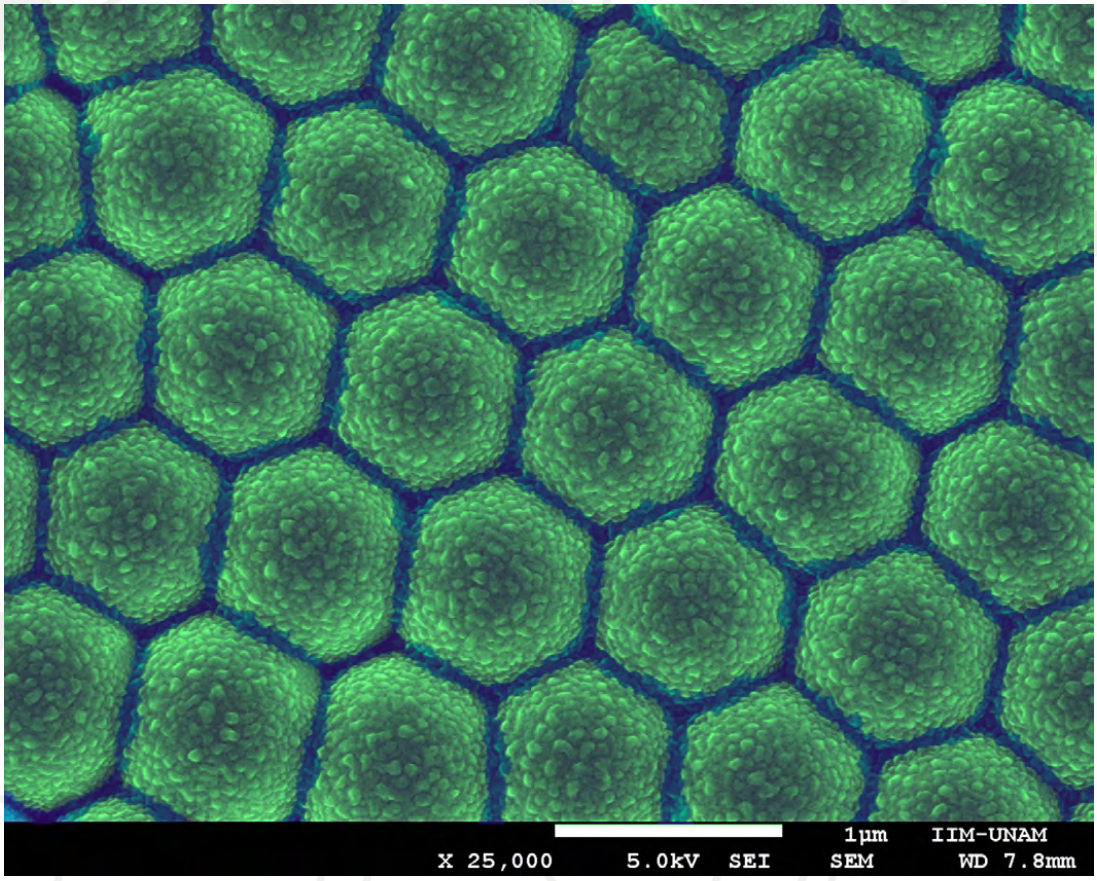
Description
CdSe/ZnS Core Shell quantum dot crystals coated with polyethylene glycol (PEG) bioconjugated with Immunoglobulin G (IgG) antibodies on polycrystalline P-type Silicon substrates.

PHOTOGRAPHY CONTEST

R. González-Campuzano* and D. Mendoza

Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, A. P. 70-360, Ciudad de México 04510, México

*naedra_9999@hotmail.com



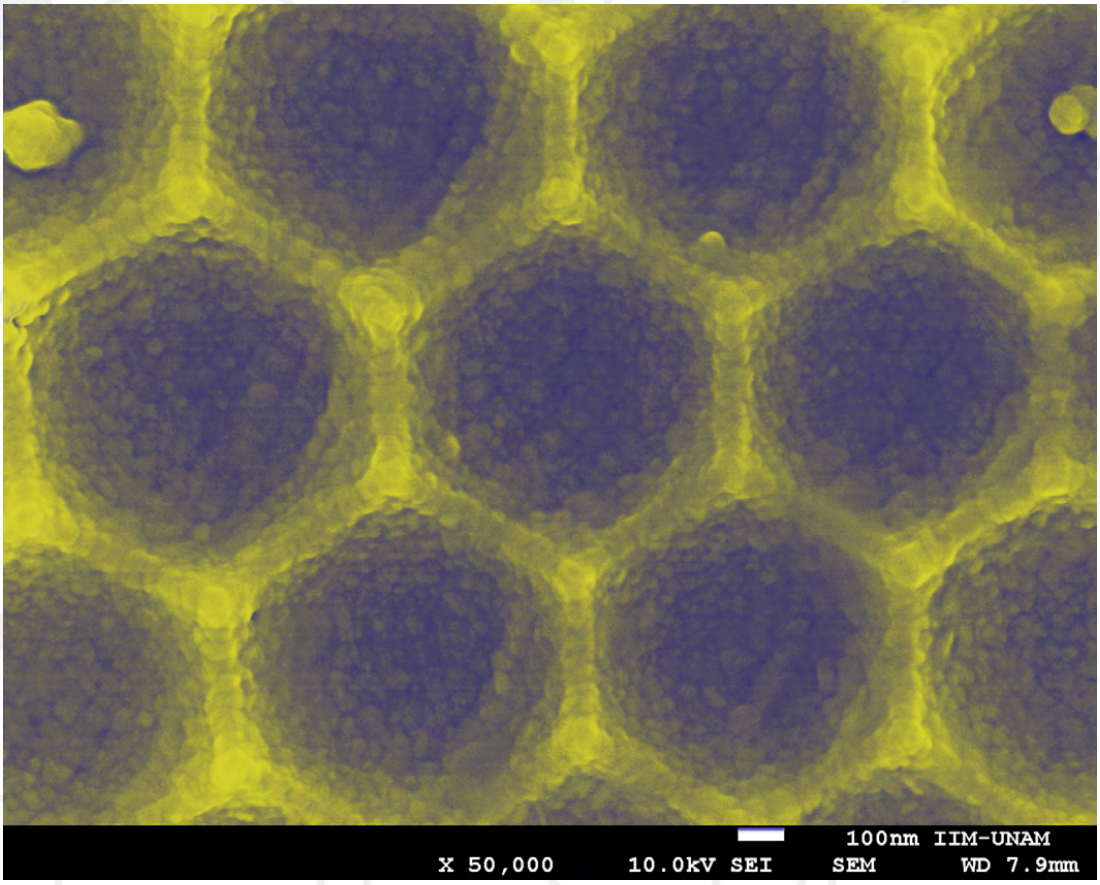
Description
False-colour SEM micrograph of evaporated aluminum nanoparticles on top of a porous anodic alumina film with hexagonal periodic geometry synthesized by electrochemical anodization of aluminum.

PHOTOGRAPHY CONTEST

R. González-Campuzano* and D. Mendoza

Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, A. P. 70-360, Ciudad de México 04510, México

*naedra_9999@hotmail.com



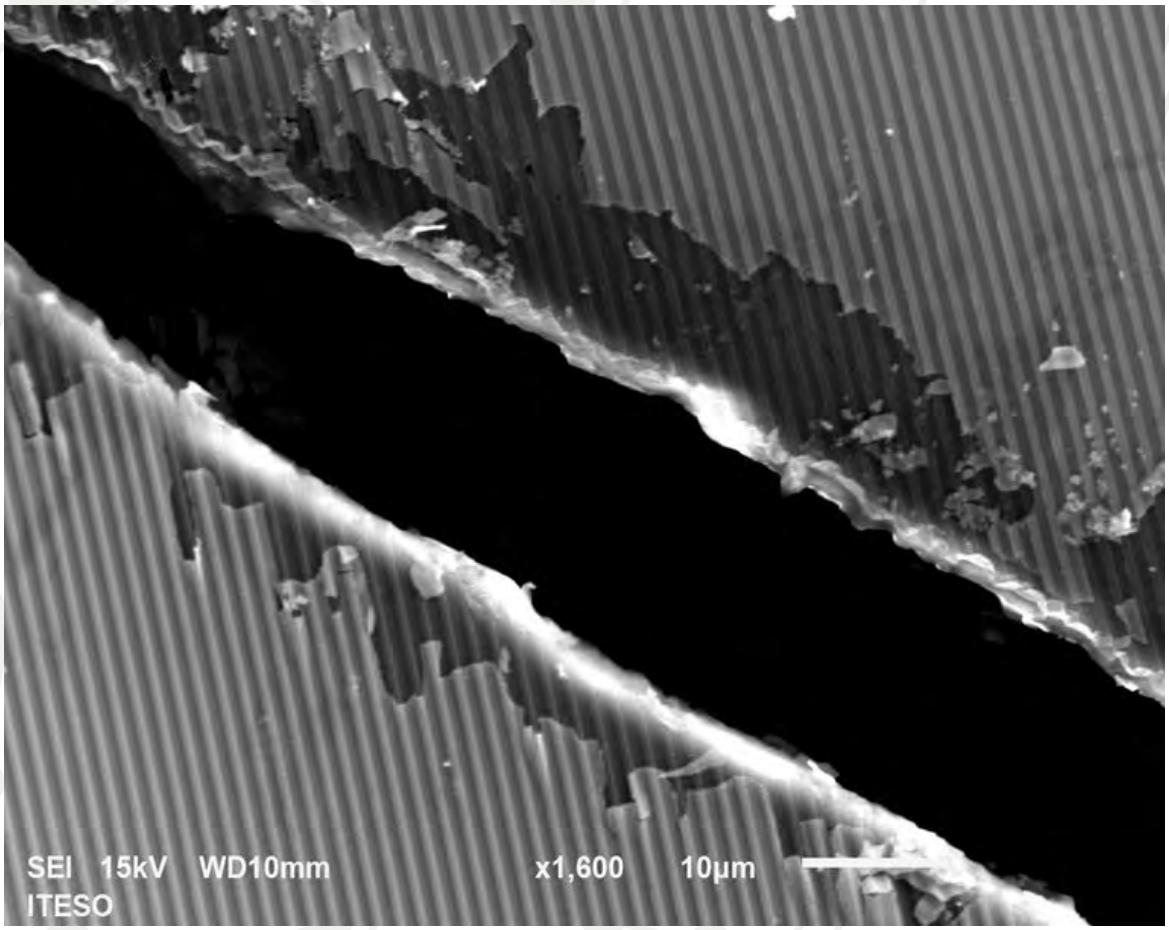
Description
False-colour SEM micrograph of a thin silver film evaporated on top of aluminum hexagonal periodic nanoconcave arrays synthesized by electrochemical anodization of aluminum.

PHOTOGRAPHY CONTEST

Elsie Araujo[1], Dagoberto Cardona[1], Guillermo González[1], Susana Martínez[1*]

[1]ITESO, Anillo Perif. Sur Manuel Gómez Morín 8585, Santa María Tequepexpan, C.P. 45604 San Pedro Tlaquepaque, Jalisco, México

*nt710454@iteso.mx



Description

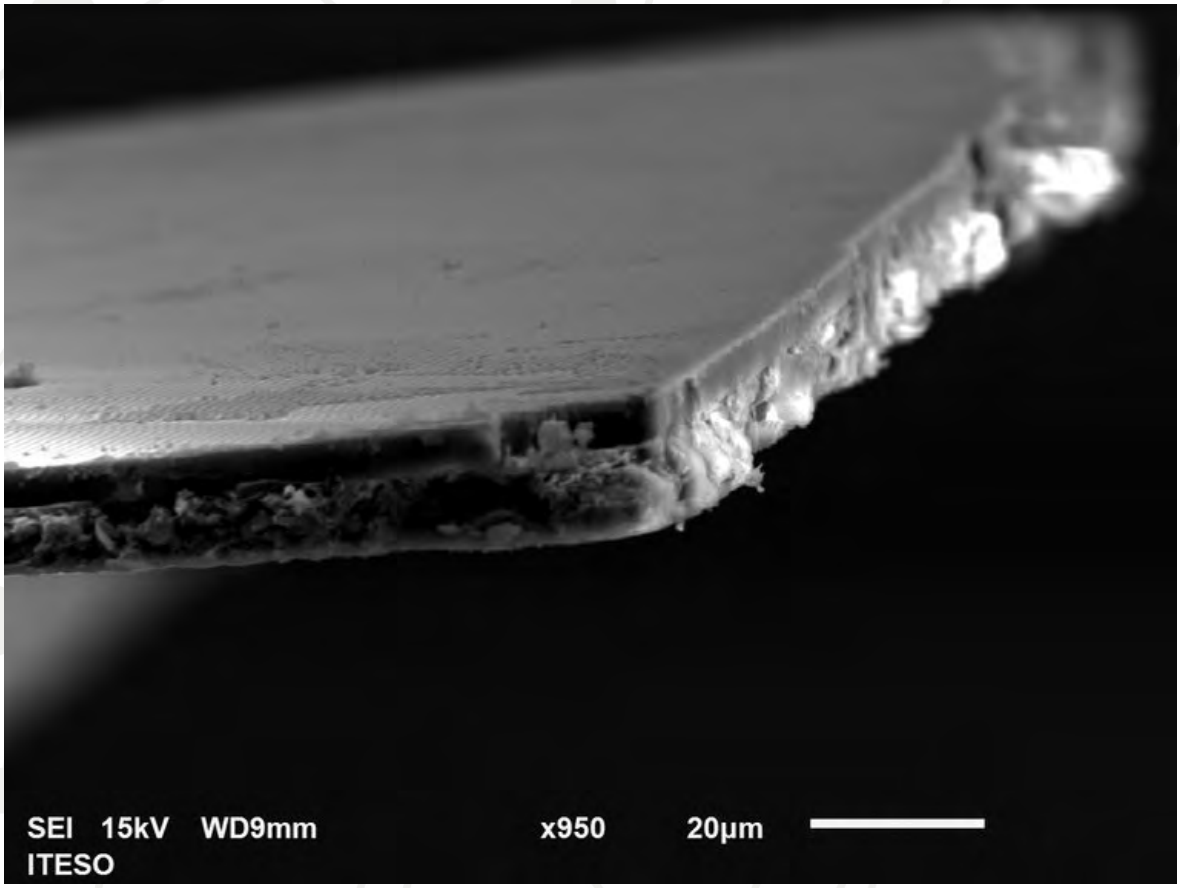
"Between Worlds". A thin film of Ti-Ag in which it is possible to observe wave patterns similar to those of its microstructured substrate used as a template. Elaborated from the magnetron sputtering technique and characterized in a scanning electron microscope.

PHOTOGRAPHY CONTEST

Elsie Araujo[1], Dagoberto Cardona[1], Guillermo González[1], Susana Martínez[1*]

[1]ITESO, Anillo Perif. Sur Manuel Gómez Morín 8585, Santa María Tequepexpan, C.P. 45604 San Pedro Tlaquepaque, Jalisco, México

*nt710454@iteso.mx



Description

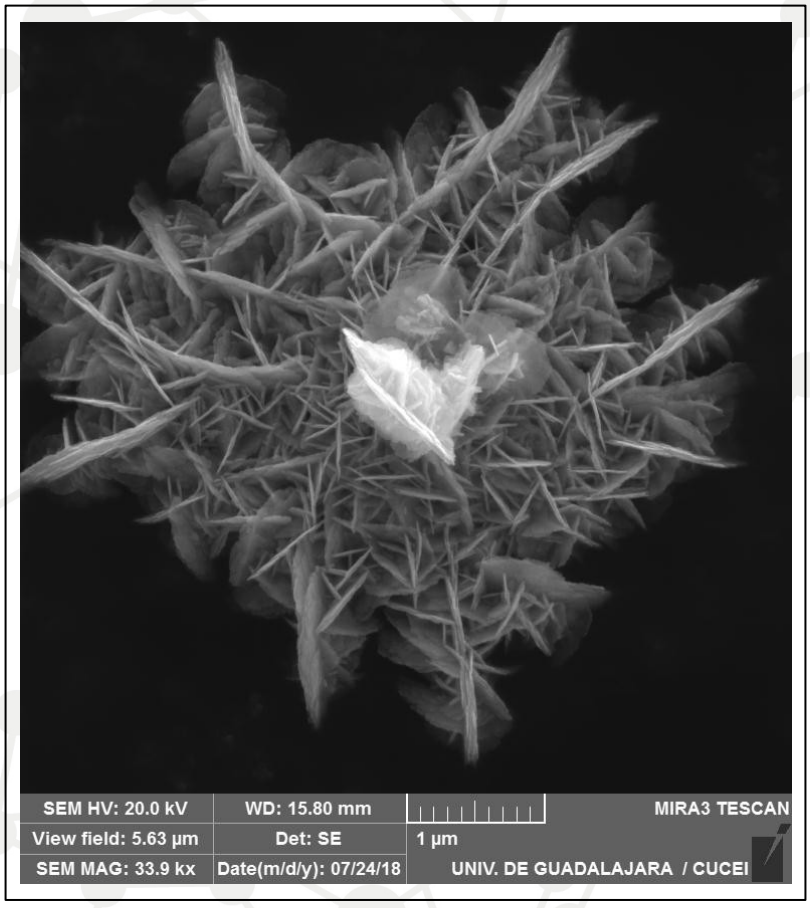
"The coin's best side". It is a transverse view of a thin film of Ti-Cu in which it is possible to observe wave patterns similar to those of its microstructured substrate used as a template. Elaborated from the magnetron sputtering technique and characterized in a scanning electron microscope.

PHOTOGRAPHY CONTEST

Erika HERNANDEZ[1], Susana ROCHA[1] , Leslie MARISCAL[1], Laura MOLINA[1], Hugo RODRÍGUEZ[2], Jose TAPIA[2], Ernesto GARCÍA[3], Lorena GARCÍA[4], and Adalberto ZAMUDIO[1,5]

[1]Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México
[2]Ingeniería de Nanotecnología, Centro Universitario de Tonalá, Tonalá, Jalisco, México.
[3]Cátedras Conacyt, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México.
[4]Departamento de celulosa y papel, Universidad de Guadalajara, Zapopan, Jalisco, México.
[5]Departamento de Física, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México

*erikaf.hernandez@alumnos.udg.mx



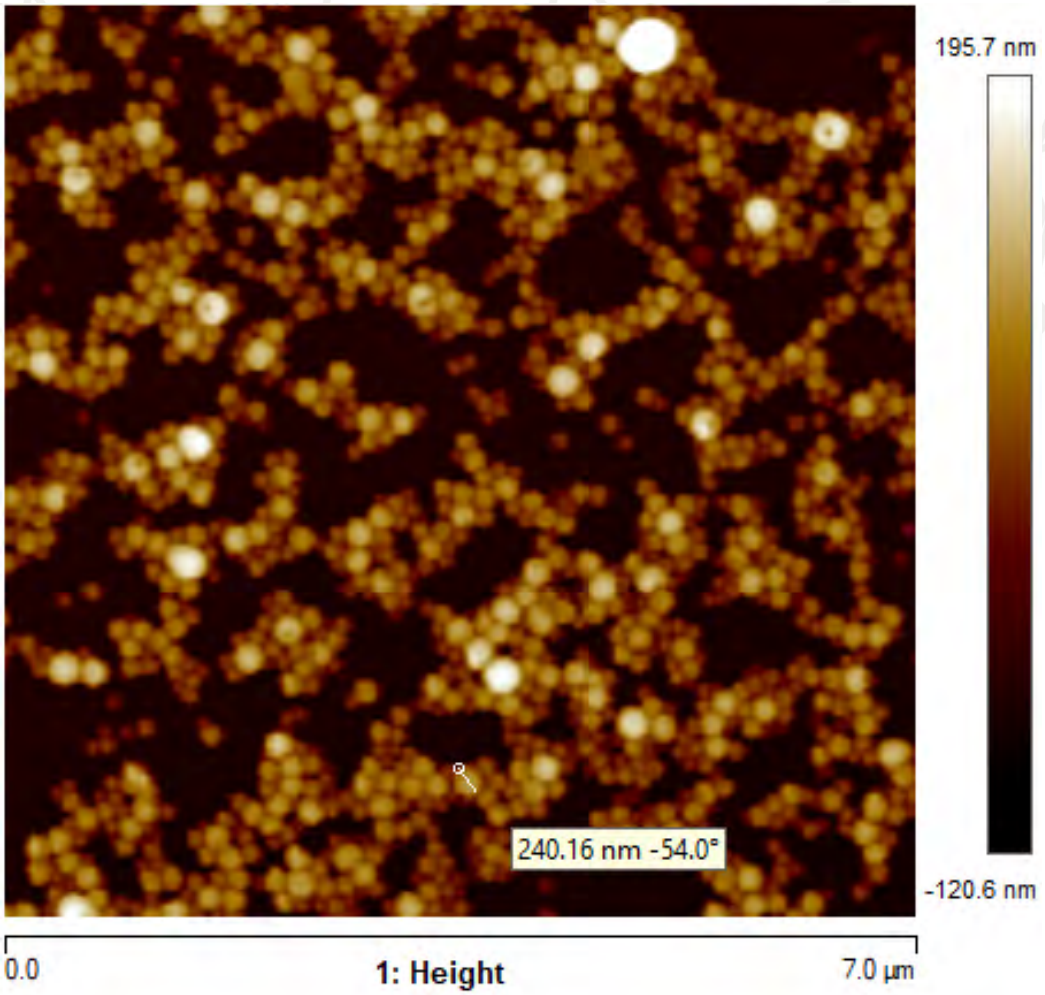
Description
The spiderweb. Set of silver nanowires synthesized in a microwave. Photograph taken from SEM.

PHOTOGRAPHY CONTEST

Martínez-Pérez BEATRIZ[1,2], Cisneros-Tamayo RICARDO[1], Piñón-Segundo ELIZABETH[2]

[1]Universidad Politécnica del Valle de México, Tultitlán, Estado de México , División de Ingeniería en Nanotecnología, Col. Villa Esmeralda, C.P. 54910, Tultitlán, Estado de México.
[2]Laboratorio de Sistemas Farmacéuticos de Liberación Modificada. Facultad de Estudios Superiores Cuautitlán, Universidad Nacional Autónoma de México, Km 2.5 Carretera Cuautitlán–Teoloyucan, San Sebastián Xhala, Cuautitlán Izcalli, Estado de México CP.54714, México.

*betymp21@yahoo.com.mx



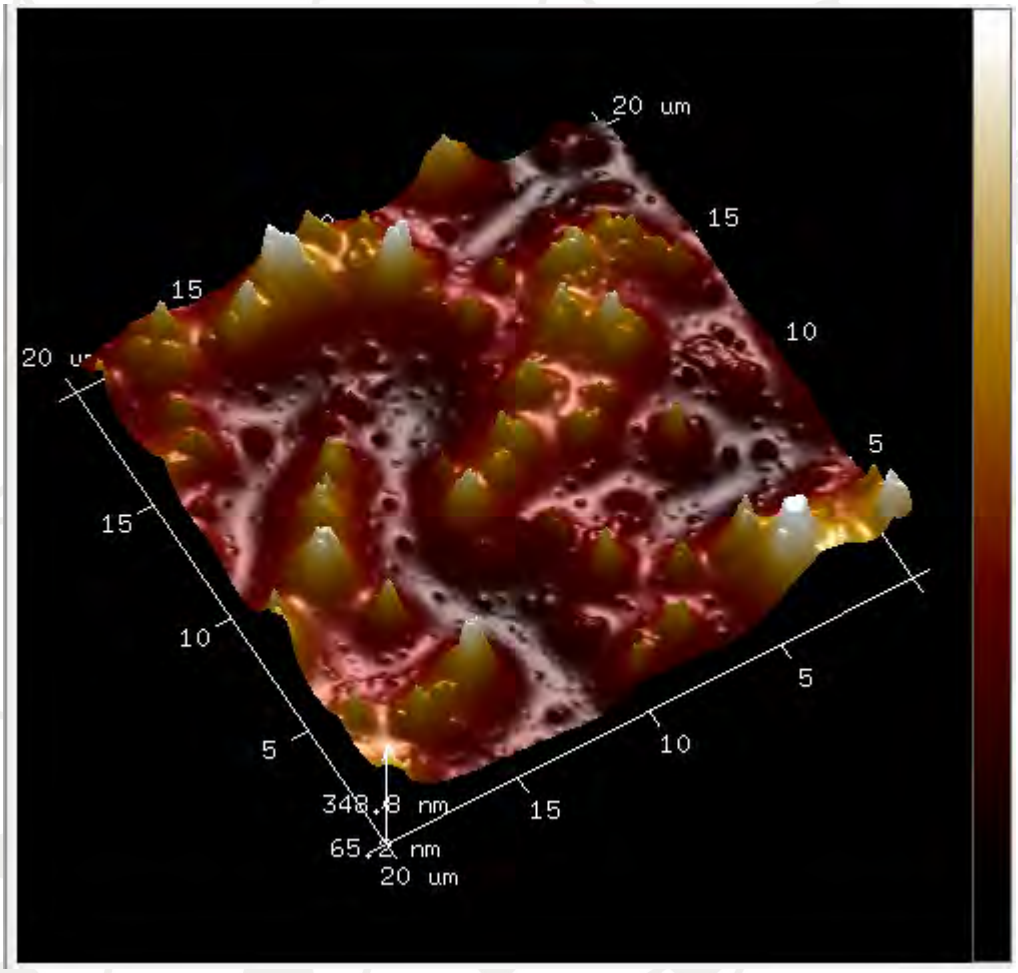
Description
PLGA-CLT-NPs. AFM micrograph of polymeric nanoparticles (NPs) of Poly(lactic-co-glycolic) acid (PLGA) with clotrimazole (CLT) trapped for vaginal applications.

PHOTOGRAPHY CONTEST

Martínez-Pérez BEATRIZ[1,2], Cisneros-Tamayo RICARDO[1], Piñón-Segundo ELIZABETH[2]

[1]Universidad Politécnica del Valle de México, Tultitlán, Estado de México , División de Ingeniería en Nanotecnología, Col. Villa Esmeralda, C.P. 54910, Tultitlán, Estado de México.
[2]Laboratorio de Sistemas Farmacéuticos de Liberación Modificada. Facultad de Estudios Superiores Cuautitlán, Universidad Nacional Autónoma de México, Km 2.5 Carretera Cuautitlán–Teoloyucan, San Sebastián Xhala, Cuautitlán Izcalli, Estado de México CP.54714, México.

*betymp21@yahoo.com.mx



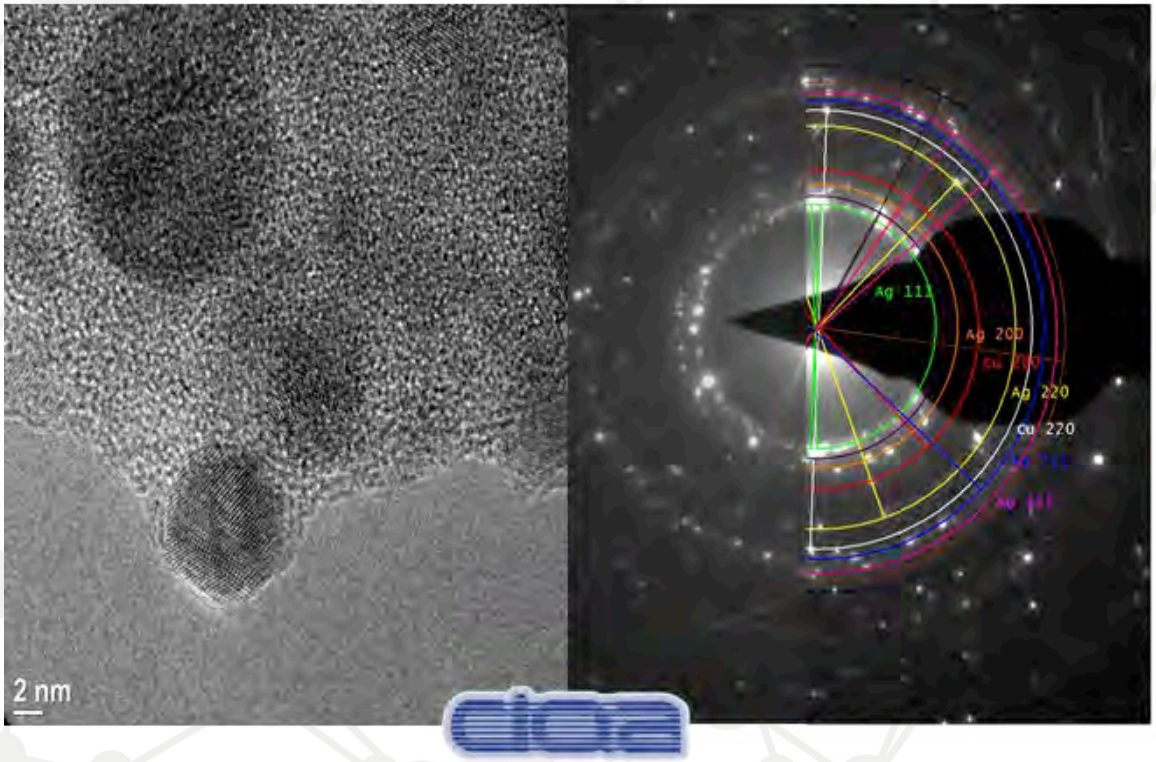
Description
MUCINE FILM WITH PLGA-CLT-NPs. AFM micrograph of mucine film with polymeric nanoparticles (NPs) of Poly(lactic-co-glycolic) acid (PLGA) with clotrimazole (CLT) trapped.

PHOTOGRAPHY CONTEST

DIANA I. Medellín*, DÁMASO Navarro, GREGORIO Cadenas

CIQA Centro de Investigación en Química Aplicada, Blvd. Enrique Reyna Hermosillo 140, C. P. 25294 Saltillo, Coah. México.

*diana.medellin@ciqa.edu.mx



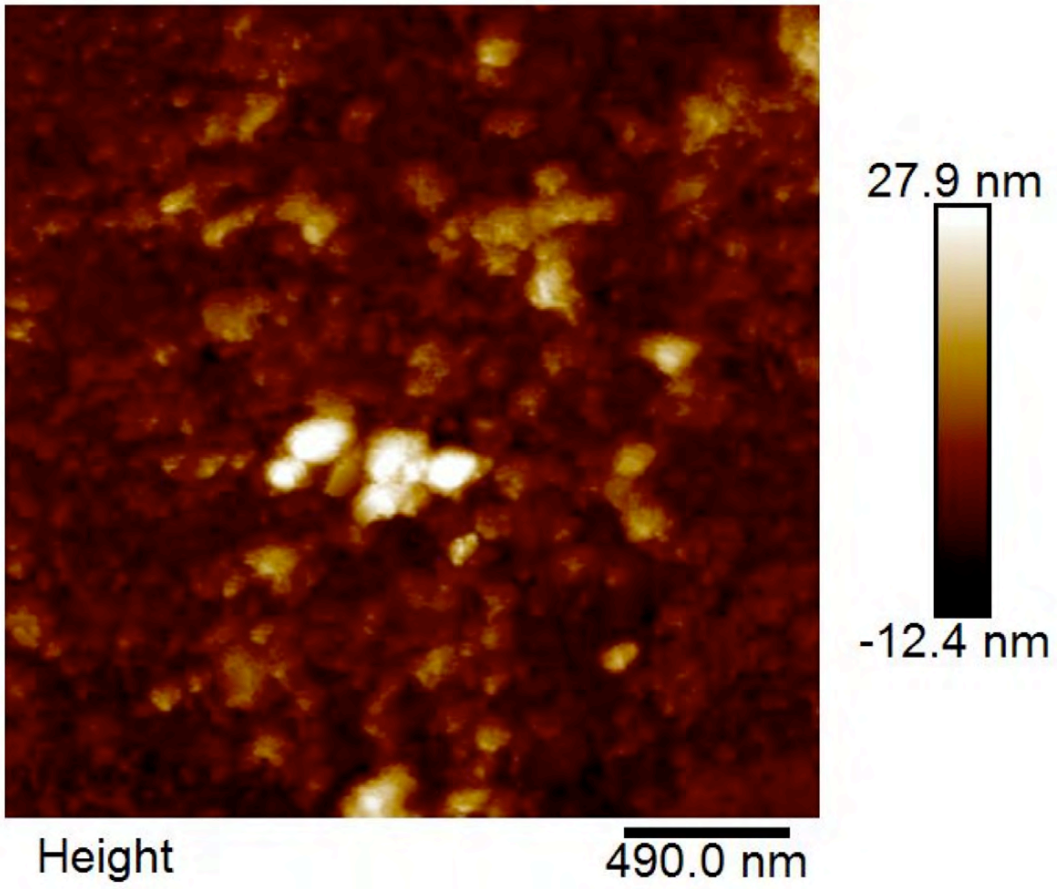
Description
Alloy Cu-Ag synthesized by chemical reduction with different morphologhy. TEM micrography shows cooper and silver nanoparticules, the scale bar corresponds 2 nm. Nanoparticules were used like fillers termo-condcutors for nanocomposites polymer matrix.

PHOTOGRAPHY CONTEST

Cristian B. Palacios-Cabrera, Alan J. Santiago-Cuevas, Jayanthi Narayanan, Ricardo Cisneros-Tamayo

Ingeniería en Nanotecnología, Universidad Politécnica del Valle de México, Av. Mexiquense s/n esquina Av. Universidad Politécnica, Col. Villa Esmeralda, C.P. 54910 Tultitlan Edo de México, México.

*palacios_cabrera@hotmail.com



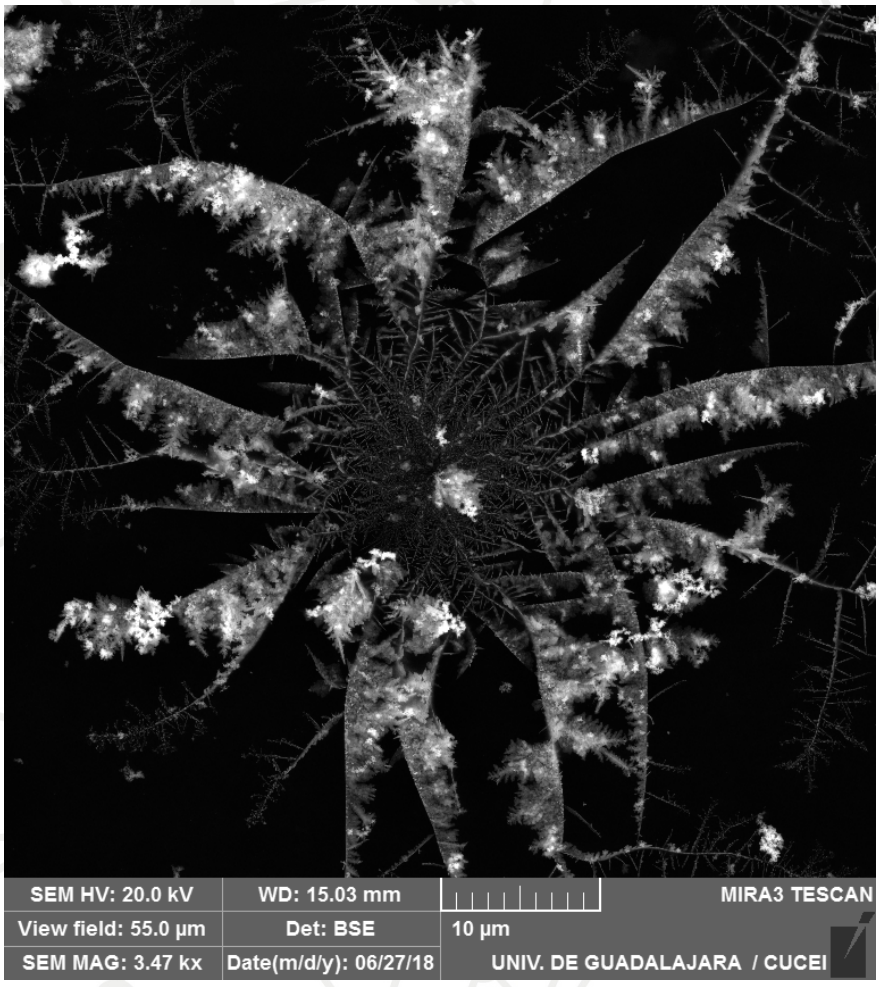
Description
2D image of atomic force microscope of a sample of cobalt ferrite nanoparticles.

PHOTOGRAPHY CONTEST

[1*]Susana Elizabeth Rocha González, [1]Esmeralda Dhamar Rayas Urdiano, [1]Erika Fabiola Hernández Elizarrarás, [2]Hugo Getzael Rodríguez Acosta, [2]José María Tapia Rivera, [4]Adalberto Zamudio Ojeda, [3]Ernesto David García Bustos

[1]Licenciatura en Ciencias de los Materiales, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México
[2]Ingeniería de Nanotecnología, Centro Universitario de Tonalá, Tonalá, Jalisco, México.
[3]Cátedras Conacyt, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México.
[4]Departamento de Física, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México

*Susana.e.r.g.20@hotmail.com



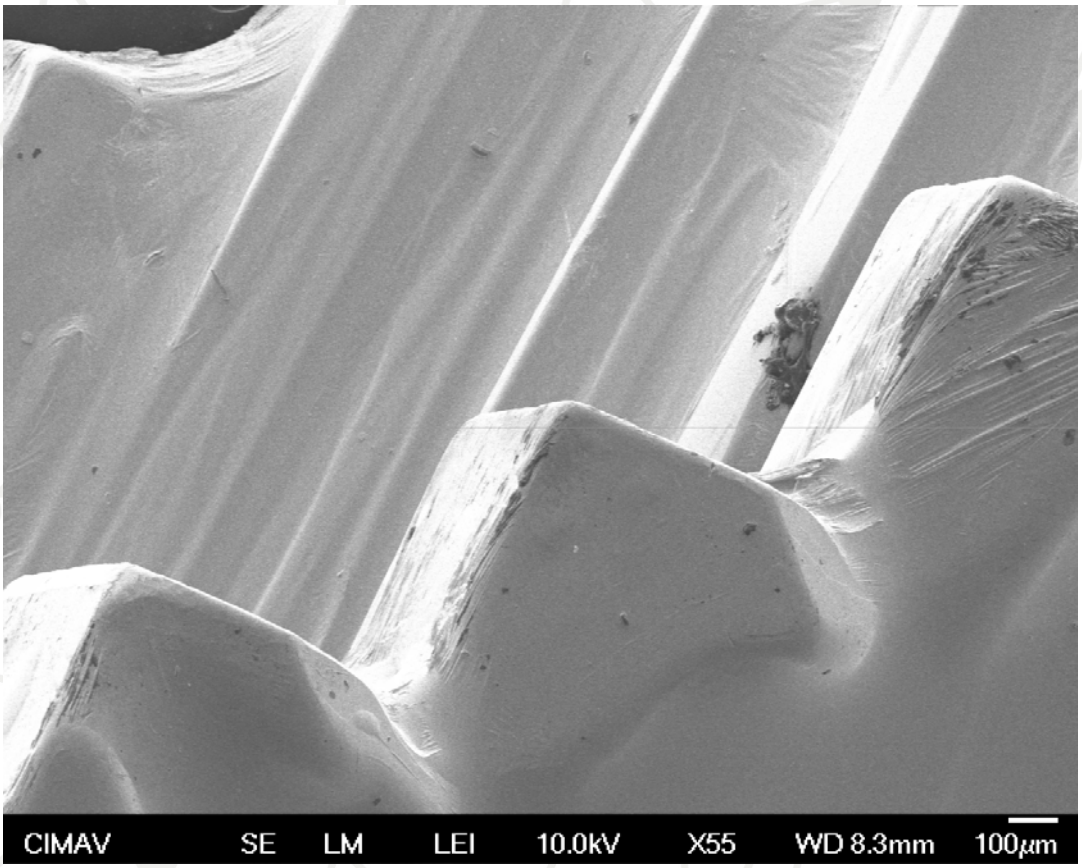
Description
The spiderweb. Set of silver nanowires synthesized in a microwave. Photograph taken from SEM.

PHOTOGRAPHY CONTEST

P. Pizá-Ruiz[1], A. Román-Loya[2], A. Sáenz-Trevizo[3], and M. Miki-Yoshida[3]

[1]Centro de Investigación en Materiales Avanzados, S.C., NANOTECH, Miguel de Cervantes 120, Complejo Industrial Chihuahua, Chihuahua, Chih. México. C.P. 31136.
[2]Universidad Tecnológica de Chihuahua Sur, Km. 3 Carretera Chihuahua a Aldama S/N, Chihuahua, Chih Mexico.
[3]Centro de Investigación en Materiales Avanzados, S.C., Departamento de Física de Materiales, Miguel de Cervantes 120, Complejo Industrial Chihuahua, Chihuahua, Chih. México. C.P. 31136.

*pedro.piza@cimav.edu.mx



Description

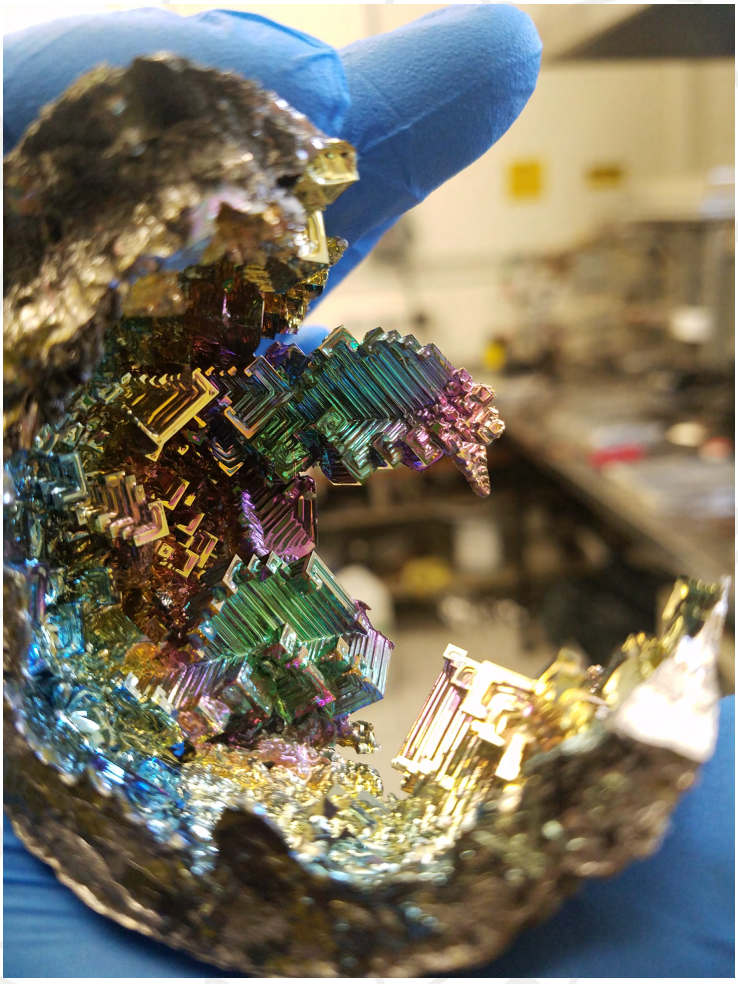
The above secondary electron micrograph was taken using a JEOL Field Emission Scanning Electron Miscroscope FESEM JSM-7401F. The micrograph shows the edges of a bismuth crystal that was formed after rapid cooling. The nature of the almost perfect order of the material while cooling was seen.

PHOTOGRAPHY CONTEST

P. Pizá-Ruiz[1], A. Román-Loya[2], A. Sáenz-Trevizo[3] and, M. Miki-Yoshida[3]

[1]Centro de Investigación en Materiales Avanzados, S.C., NANOTECH, Miguel de Cervantes 120, Complejo Industrial Chihuahua Chihuahua, Chih. México. C.P. 31136.
[2]Universidad Tecnológica de Chihuahua Sur, Km. 3 Carretera Chihuahua a Aldama S/N, Chihuahua, Chih Mexico.
[3]Centro de Investigación en Materiales Avanzados, S.C., Departamento de Física de Materiales, Miguel de Cervantes 120, Complejo Industrial Chihuahua Chihuahua, Chih. México. C.P. 31136.

*pedro.piza@cimav.edu.mx



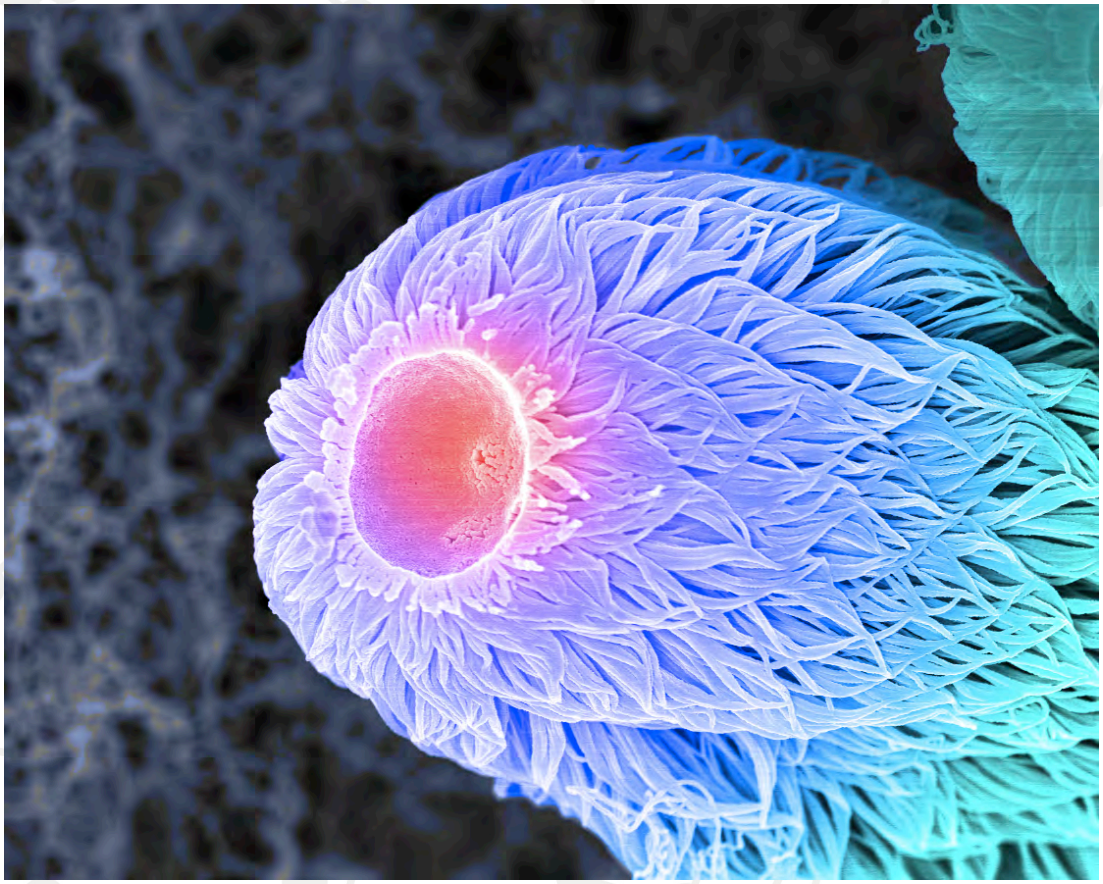
Description
The above photograph is a geode of Bismuth crystals formed after melting and controlling the cooling rate. The rainbow colors observed are a consequence of the oxidation of the crystals after being exposed to atmospheric conditions while cooling. This is a common lab practice for students to show them the solidification process of a crystalline material. It also shows the formation of bismuth oxide thin films at the surface, that have different thicknesses.

PHOTOGRAPHY CONTEST

Francisco Solís Pomar[1*] and Eduardo Pérez Tijerina[1]

[1]Universidad Autónoma de Nuevo León, Centro de Investigación en Ciencias Físico Matemáticas, Facultad de Ciencias Físico Matemáticas, Av. Universidad s/n. Ciudad Universitaria, C.P 66451 San Nicolás de los Garza, Nuevo León, México

*francisco.solispm@uanl.edu.mx



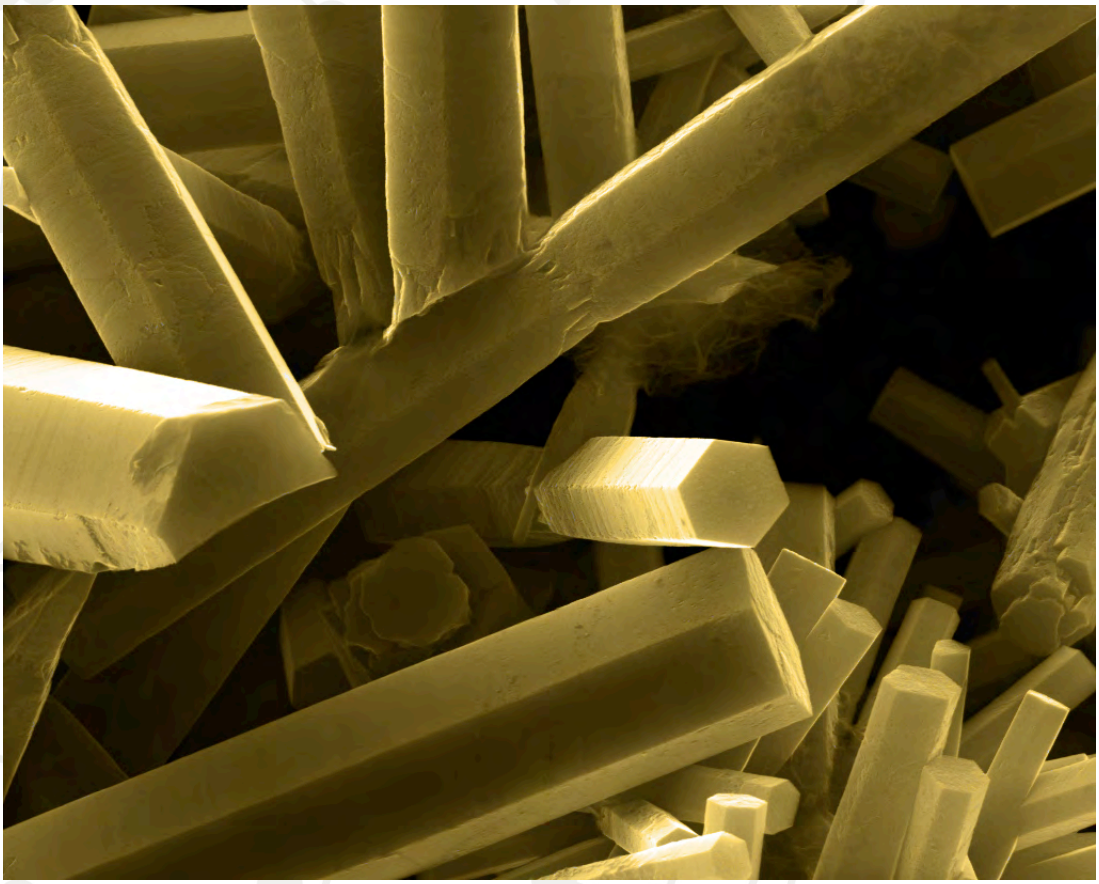
Description
Silicon Oxide Nanowires. Micrograph obtained by Scanning Electron Microscopy FEI - Novananosem 200.

PHOTOGRAPHY CONTEST

Francisco Solís Pomar[1*] and Eduardo Pérez Tijerina[1]

[1]Universidad Autónoma de Nuevo León, Centro de Investigación en Ciencias Físico Matemáticas, Facultad de Ciencias Físico Matemáticas, Av. Universidad s/n. Ciudad Universitaria, C.P 66451 San Nicolás de los Garza, Nuevo León, México

*francisco.solispm@uanl.edu.mx



Description
Zinc Oxide Nanorods. Micrograph obtained by Scanning Electron Microscopy FEI -Novananosem 200.

PLENARY SESSION

MONDAY

Toward Atomic Precision in Nanoscience

Rongchao Jin

Department of Chemistry, Carnegie Mellon University, Pittsburgh, PA 15213

rongchao@andrew.cmu.edu

Recent advances in nanoscience research have marched toward controlling nanoparticles with atomic precision. This talk will present breakthroughs in gold nanoparticle research, including the atomically precise synthesis, total structure determination, and applications in catalysis and sensing. Such perfect gold nanoparticles resemble organic molecules in that they possess definite formulas, $Au_n(SR)_m$ (where SR = thiolate ligand, *n* and *m* refer to the number of gold atoms and surface ligands, respectively). By controlling nanoparticles with atomic precision, one can now reveal the long-sought-after total structures (i.e. metal core plus surface ligands) by X-ray crystallography, as opposed to metal core only in electron microscopy analysis. Significant progress has recently been achieved in determining the total structures, ranging from subnanometer $Au_{18}(SR)_{14}$ to 2.2 nm $Au_{246}(SR)_{80}$. These ultrasmall nanoparticles exhibit interesting electronic and optical properties with manifestations of strong quantum size effects. Many other mysteries at the nanoscale, such as isomerization, chirality and periodicities in nanoparticles, as well as nanoscale self-assembly monolayer (SAM) structure, have now been revealed. Such perfect nanoparticles hold potential in chemical catalysis, energy conversion, optics, and sensing applications.

Probing complex nanostructures one atom at a time using a combination of theory and microscopy

Sokrates T. Pantelides

Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235 USA
Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA
University of the Chinese Academy of Sciences, Beijing, China

pantelides@vanderbilt.edu

Quantum mechanical calculations based on density functional theory using high-performance computers have made enormous strides in describing the atomic-scale properties of complex materials and nanostructures. In parallel, aberration-corrected scanning transmission electron microscopy has reached extraordinary levels of spatial and energy resolution, in both imaging and electron-energy-loss spectroscopy. For two-dimensional materials, scanning tunneling microscopy is equally powerful, as the "surface" is the material. Combining theory and microscopy provides an unparalleled probe to unravel the atomic-scale processes that control vital properties for electronic, optoelectronic, and energy-related applications, and even explore the fabrication of new materials and nanostructures. This talk is a journey through the wide world of complex nanostructures that provides a first-hand experience of the nanoscale using select examples from bulk materials, two-dimensional materials, nanoparticles, and nanowires.

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Quantum Well and Superlattice Solar Cells

Maykel Courel

[1] *CUValles, Universidad de Guadalajara, Carretera Guadalajara-Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México.*

maykel.courel@academicos.udg.mx

Over the last decades, solar cells have received more and more attention from scientific community as one potential candidate to replace fossil fuels, as constitute a more environmentally friendly technology. As an important drawback of the first and second generation of solar cells, about 30% of photons with energy lower than absorber band-gap are lost. In order to reduce these losses, some smart strategies have been proposed in the third generation of solar cells. Among these, the application of nanostructured materials such as quantum wells, superlattices and quantum dots has been found attractive for promoting solar cell efficiency. By using nanostructured materials, improvements to the spectral response of cells in the energy region below the absorption edge of host material are expected. That is, some photons with energies lower than bulk band-gap can be now absorbed, increasing thereby short-circuit current density of solar cell which could improve solar cell efficiency as well. In this talk, it is presented results on the use of quantum wells and superlattices to enhance GaAs and Kesterite solar cell efficiency. In particular, a theoretical work is presented where the impact of quantum well width, barrier width, well depth and well number is evaluated. Besides, conditions that favor the formation of a mini-band (intermediate-band) without and under an electric field are presented, which were studied by the Transfer Matrix Method. As an important result, it is found that solar cell efficiencies higher than 30% can be obtained by using superlattice solar cells. Conditions for optimizing solar cell performance are presented and discussed.

Key Words: Kesterite solar cells, Quantum Wells, Superlattices, Quantum confinement

TUESDAY

The Structural and Electronic Pattern of the Thiolate-Protected Gold Clusters

Yong Pei

Department of Chemistry, Xiangtan University, China

ypei2@xtu.edu.cn

The structure and properties of thiolate-stabilized gold nanoclusters, refer to $Au_n(SR)_m$, received great research interests [1]. The thiolate-stabilized gold nanoclusters show magic-stable sizes in solution synthesis. However, for a long time, the determination of the atomic structures of these nanoclusters was a grand challenge for both experiment and theory. In this talk, I would to like to introduce our recent theoretical works about the structural predictions, optical absorption spectra, dissociation mechanism in mass spectrum (MS) and structure-electronic structure relationships of the thiolate-stabilized gold nanoclusters at smaller size [2-9]. Based on the proposed genetic structure rule of the $Au_n(SR)_m$ clusters, we designed a simple method to avoid the complicated ligand shell in structural search of the most stable cluster structures. Using this method, we have successfully predicted a lot of cluster structures and many of theoretical predictions have been proven by experimental XRD results. Moreover, a genetic structural evolution rule and the structure-electronic structure relationships of the thiolate-stabilized gold clusters is summarized.

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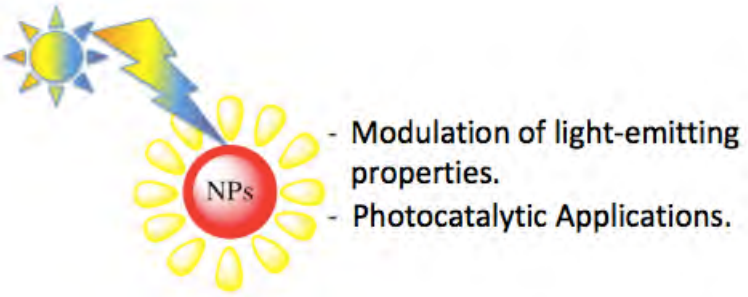
Surface-Functionalized nanoparticles modulated by light

L. C. Schmidt[1]

[1]*INFIQC (CONICET-UNC) Dpto. de Química Orgánica, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba. Ciudad Universitaria, 5000, Córdoba, Argentina*

luciana@fcq.unc.edu.ar

Light-activated systems have attracted attention in the scientific community due to the advantages of triggering reactions in a controllable, efficient and economical approach. In this way, semiconductor nanocrystals (quantum dots, QDs) such as core-QDs (CdSe or CdTe) and core-shell QDs (CdSe/ZnS, CdSe/CdS) are excellent candidates for light-activated systems due to their size-dependent emissive properties. Incorporation of QDs in supramolecular materials such organogels with low molecular weight showed interesting synergic effect that could have potential applications in the preparation of optoelectronic devices and sensors. Moreover, the addition of a photochromic activator/quencher (diarylethene derivatives) to the system was an effective methodology to modulate the light-emitting properties of QDs. Furthermore, light-activated systems have important applications as photocatalysts. The design of the photocatalyst is the key step in the development of a sustainable catalytic reaction. The attachment of specific ligands in the nanocrystal surface strongly affects their properties and colloidal stability in different media.2 In this contribution, examples of photooxidations using different nanoparticles and light sources will be also discussed.



Key Words: light-activated systems, QDs, photocatalysis

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3D Electrocatalytic materials for electrochemical Energy Conversion Systems

Luis Gerardo Arriaga Hurtado

Centro de Investigación y Desarrollo Tecnológico en Electroquímica, Pedro Escobedo, Qro., C. P. 76703, Querétaro, México

larriaga@cideteq.mx

Electrochemical energy conversion systems such as fuel cells, electrolyzers, bateries and others, have received worldwide attention owing to their high energy density, security, low operating temperature, and low pollutant emission. Nonetheless, the commercial application of these systems still faces some critical obstacles: relatively high costs, insufficient performance and inadequate long-term durability of the electrocatalysts. To overcome these issues, various methods have been proposed by tailoring the design of the size, composition, and shape of the electrocatalytic materials. In this sense, 3D materials based on different metals, are an exceptional class of materials which are of interest for several high-performance applications thanks to their extraordinary physical properties such as extremely high porosity, high specific surface area, and extremely low density combined with very versatile synthesis approaches. In this talk, non noble metal 3D-structures, which combine the unique properties of metals such as excellent electrical and thermal conductivity and catalytic performance with the unique properties of common 3D-materials, will be thoroughly reviewed.

WEDNESDAY

Porphyrins A-Π-D-Π-A for bulk heterojunction Solar Cells

Susana Arrechea[12]*, Ana Aljarilla[1], Pilar de la Cruz[3], Ganesh Sharma[3] and Fernando Langa[1]

Universidad de Castilla-La Mancha, Spain
[2]Universidad de San Carlos de Guatemala, Guatemala
[3]LNM Inst. of Information Technology Demed University, India.

arrecheausac@gmail.com

The global challenge of sustainable development, clean energy and climate change needs to be pursued by development of energy technologies. Solar energy is available around the world as radiant light or heat from the sun, using technology such as photovoltaic devices. The new generation of photovoltaics can offer an alternative and complementary approach to the exploitation of solar energy [1]; It offers low manufacturing cost, flexibility and lightweight. The most promising ones for its remarkable progress are: organic, dye sensitized and perovskite solar cells. In this study, twelve families [2,5] of porphyrins with configuration A-π-D-π-A were synthesized and characterized to apply them in bulk heterojunction solar cells (BHJSC) with fullerene derivative PCBM as acceptor. The optical, electrochemical and photovoltaic properties of these systems will be described. After optimizing the processing by a solvent and additive power conversion efficiencies reach values of 7.93%. The e*ff*ects over the film morphology and the device characteristics open circuit voltage (Voc), current (Jsc), fill factor (FF) due to the introduction of additives will be discussed.

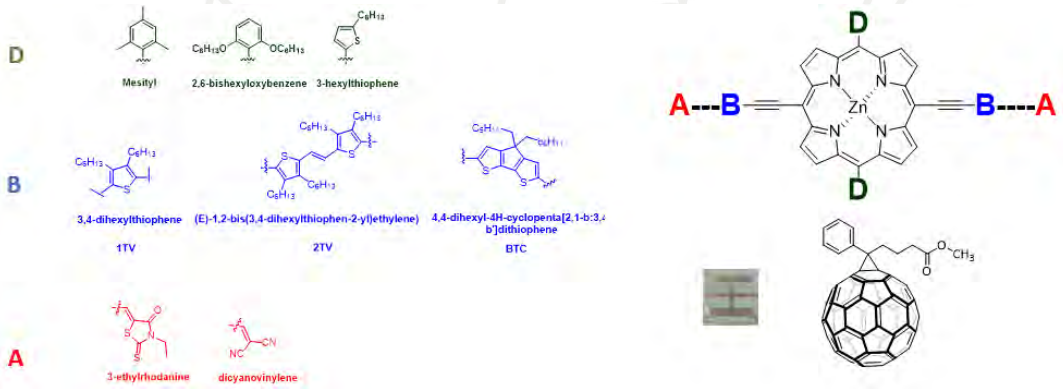

Figure 1 – Structure of porphyrins A-π-D-π-A

Key Words: photovoltaics, porphyrins, bulk heterojunction, nanolayers

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Nanomedicine for functional imaging, image-guided surgery and theranostic. Importance of the characterization of the physico-chemical properties of nano-objects

Nathalie Mignet[1]

[1]*Unité des Technologies Chimiques et Biologiques pour la Santé*
Equipe Vecteurs pour l'Imagerie et la thérapie ciblées
INSERM U1022, CNRS UMR8258, Univ. Paris Descartes,
Chimie ParisTech Centre de Recherche Pharmaceutique de PARIS
4, Avenue de l'Observatoire, 75 270 Paris, Cédex 06.

nathalie.mignet@parisdescartes.fr

Nanoparticles have potentials in imaging in particular as enhanced contrast agent for techniques with low sensitivity, such as MRI or Ultrasound imaging. Thanks to their possible functionalization, various chromophores or contrastophor can be linked to the surface or within the core to provide new properties or to allow obtaining a high number of valuable informations in preclinical studies, while highly reducing the number of animals. Few examples of the interest of functionalized nanomedicine for functional imaging in preclinical evaluation will be shown. First, the conception of a protein scaffold targeting the Asialoglycoprotein receptor (Chaumet-Riffaud et al. 2010.) A radioactive label provide quantitative informations on the liver function while an optical label will provide evidence on the specificity of the targeting. Of main importance for functional imaging is to determine the pharmacokinetic and the stability of the nanomedicine. The aggregation of the nanomedicine will surely disable the functional agent. Characterisation is therefore a main concern of these objects which can also be used for image-guided surgery. A protein fucntionalised with the sialyl Lewis X derivative has been conceived to image tumor margin. Finally, the conception of microbubbles for gene delivery has been proposed, and clearly benefit from ultrasound imaging to fix all parameters and requirement for such interdisciplinary approaches.

Chiral Nanotubes of black phosphorus

Alfredo Tlahuice Flores[1]

[1]*Facultad de Ciencias Físico Matemáticas, Universidad Autónoma de Nuevo León, Nuevo León, México*

tlahuicef@gmail.com

Up to now, the study of phosphorus had been devoted to 2D structures (phosphorene) and to the study of phosporene Nanotubes. In this talk I will deliver an update of our work related to the study of chiral black phosphorus nanotubes. The study of their structure, bonding and electronic (band structure) properties has been carried out based on a periodic plane wave-pseudopotential approach. Chiral phosphorene nanotubes are determined as candidates to be sinthesized given the calculated binding energy, thermal and dynamic stability. Morover, it was found that the bandgap is tuned by varying the chirality of the phosphorus nanotube and it is not related to their diameters. The ultimate goal is to engineer the bandgap to facilitate its applications

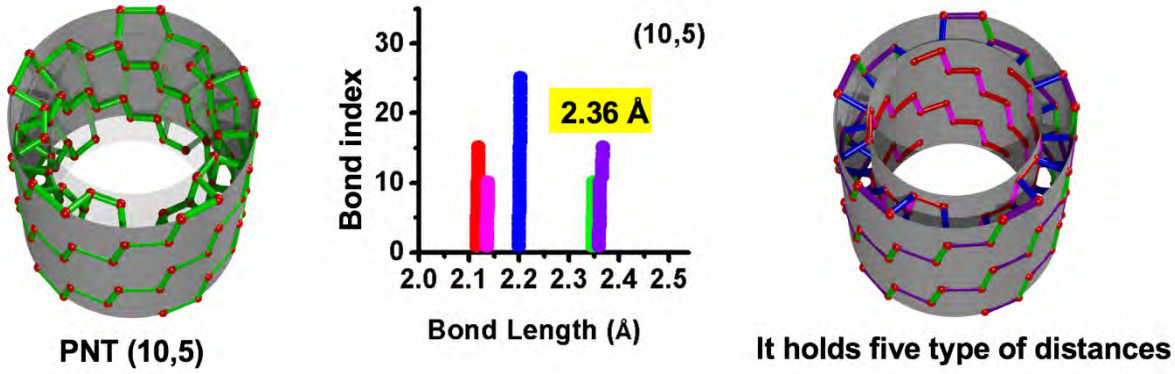

Figure- Bonding displayed by (10,5) black phosphorus nanotube. Colors are used to distinguish between type of bonds.

A novel emissive nanomaterial based on colloidal Perovskites: synthesis and applications

Raquel E. Galian

Institute of Molecular Science (ICMOL), University of Valencia, c/ Cat. José Beltrán 2, Paterna, 46980.

raquel.galian@uv.es

Hybrid lead halide perovskites (PVK) have particular optical and electronic properties with extensive application in photovoltaic and more recently as luminescent materials for light emitting devices (LEDs) [1]. We have reported in 2014 the first example of $CH_3NH_3PbBr_3$ colloidal perovskite nanocrystal (ca. 6 nm) with good luminescence quantum yield (20 %), using medium-long alkylammonium bromide as organic capping [2]. The key role of the organic ligand nature to prepare perovskite emitter with high luminescence properties, stability and dispersibility will be discussed [3]. Different molar ratios between precursors have provided high control on their crystallization, stoichiometry, size, and therefore on their optical performance. A surface engineering on the perovskite nanocrystals enable the formation of host-guest complexes and the preparation of novel nanohybrid [4]. One of the challenge in the development of thin film based on PVK nanoparticles is the use of organic ligand-free nanocrystals to increase the charge transport efficiency between them. The preparation of stable “naked” colloidal nanoparticles to produce conductive thin film with controlled thicknesses and electroluminescent devices will be also discussed [5].

Key Words: colloids, perovskites, photoluminescence, conductive AFM, electroluminescence

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THURSDAY

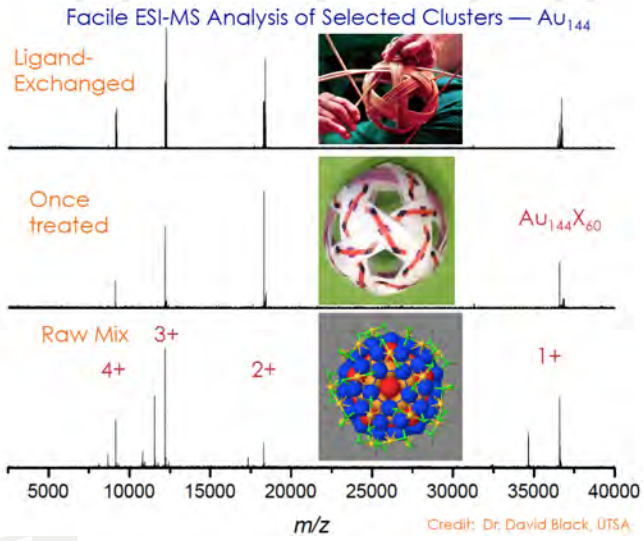
Discovery of Chiral Golden Fullerenes: I–Z60

Robert L. Whetten, David M. Black, Marcos M. Alvarez

Department of Physics & Astronomy, University of Texas, San Antonio, TX, 78249 USA

Robert.Whetten@utsa.edu

The 1990 discovery of molecular solids rich in Ih-C60 clusters was a crucial moment reported first at ISSPIC-5 in Konstanz. Here we report on a development, comparable in several key respects, in cluster-compounds of noble-metal atoms: During experiments aimed at under- standing the geological and microbial origins of metallic gold, aurous-thiolate (AuX) has been reduced and the products analyzed by electrospray volatilization, leading to the accumulation of a remarkably abundant cluster compound comprising precisely 60 anionic ligands (X-) and 144 gold atoms. Concerning the question of what kind of 204-atom structure might give rise to such a ubiquitous species, we suggest a sextuple-strand woven sphere in which the 60 X-sites occupy vertices of the snub-dodecahedron, and are linked in coordinative zig-zag (Z) fashion to 120 Au-sites. This object is commonly encountered as the traditional woven-reed football (cf. Figure below) of Southeast Asia, whose exceptional stability was noted by Fuller & Edmundson and mathematized by Nishiyama. The remaining 24-Au are distributed four to each of the six 5-fold axes, acting to cement the structure. This resulting filled Z60 structure, Z = Au2X, thus has all valences satisfied, has chiral-icosahedral (I) symmetry, and appears to be mechanically resilient as well as maximally compact, accounting for the observed resistance to chemical attack. As will be described in this presentation, key features of this structure were antici-pated in the works of ISSPIC pioneers Farges, Dahl, and Martin; whereas Tsukuda & coworkers advanced the precise determination of composition & structure. New evidence is presented that compounds having this unique structure can account for results from many labs concerned with products, typically described as “~2.0-nm gold nano- particles”, as recent advances in analytical methods have enabled such determinations.



Catalysis and Electrocatalysis: Ex Situ and In Situ/Operando Studies of Nanoalloy Catalysts

Chuan-Jian Zhong

Department of Chemistry, State University of New York at Binghamton, Binghamton, New York 13902, USA

cjzhong@binghamton.edu

Nanoscale alloying in metal nanoparticle catalysts play a critical role in catalytic and electrocatalytic synergies for many reactions, understanding of which constitutes an important front of research and development in sustainable energy and environment. The highly-dynamic nature of nanoalloys in catalytic and electrocatalytic reactions requires probing the detailed surface sites and nanocrystal structures of the catalysts through characterizations of the catalysts as prepared and under the reaction conditions or during the reactions. This presentation will discuss some of the recent results of ex-situ and in-situ/operando studies of several types of nanoalloy (nanoparticles and nanowires) catalysts in catalytic oxidation of carbon monoxide and hydrocarbons, and in electrocatalytic oxygen reduction and alcohol oxidation reactions. Examples will highlight the use of diffuse reflectance infrared Fourier transform spectroscopy and high energy x-ray diffraction coupled with atomic pair distribution function analysis for in situ/operando characterizations of platinum and palladium based binary and ternary nanoalloys, core-shell nanoparticles and nanowires in the reactions. Insights into the correlation of the catalytic or electrocatalytic synergies with the size, shape, composition, and surface sites will be also discussed.

FRIDAY

Controlling molecular transport and confinement in Mesoporous Materials: towards intelligent perm-selective membranes

Galo J. A. A. Soler-Illia

Instituto de Nanosistemas, Universidad Nacional de San Martín, Buenos Aires, Argentina

gsoler-illia@unsam.edu.ar

The combination of nanomaterials synthesis with self-assembly processes led to a significant advance in the production of hybrid inorganic-organic Mesoporous Materials (MM) with controllable pore structures and localized functions. Our ability to produce these precise architectures with well-defined localized functions opens the path to create “intelligent materials” that can change their physical or chemical properties in response to the environment. Programmable nanosystems can be envisaged, in which confinement effects, responsivity, or collaborative functionality can be imparted into the structure through the control of positional chemistry of different chemical building blocks. In this presentation, we will present recent results in the design and perm-selective performance of MM-based systems made up through the incorporation of molecular, biomolecular or polymeric nanobuilding blocks. A variety of MM thin films or colloidal particles can be produced through the self-assembly of inorganic nanobuilding blocks in the presence of supramolecular templates. MM can then be decorated by small molecular species, biomolecules, polymers or nanoparticles. The final functionality is attained through the combined control of the pore size and shape, the contents of the pore interior, and the interactions at the pore surface level. We will discuss in detail the chemical toolbox to incorporate molecular fragments and polyelectrolytes within the mesopores in order to design and produce perm-selective electrodes or membranes. In addition to synthetic and characterization tools, theoretical models and simulations are essential to understand the complexity of the synthesis paths and the final properties. This in-depth knowledge is key to ultimate nanosystems design. A potentially infinite variety of nanosystems with externally controllable behavior is at our disposal, opening the path to design intelligent matter.

Effect of the Protecting Ligands on the Properties of Molecular Gold Nanoclusters

Flavio Maran

[1] *Department of Chemistry, University of Padova, Padova, Italy*
[2] *Department of Chemistry, University of Connecticut, Storrs, Connecticut, U.S.A*

flavio.maran@unipd.it

Thiolate-protected gold clusters are of continuously growing fundamental and applied interests. These molecular systems can be defined as *soft-hard* molecules, *i.e.*, molecules in which a hard gold core is protected by a soft interface of flexible ligands that form a quite unique nanoenvironment. A typical example is provided by $Au_{25}(SR)_{18}$, which is the most studied of the nanoclusters displaying molecular properties. In applications, assessing the dynamic behavior of the thiolate monolayer is crucial as it determines, *e.g.*, the cluster's effective size and electron-transfer (ET) properties. Topics addressed in this talk will include: (i) The effect of the monolayer thickness and its dynamics on the ET between molecular nanoclusters in films and solution; (ii) In redox catalysis, the monolayer can be penetrated by molecular species: what kind of environment do they experience during the activation processes? (iii) Understanding the fine interactions between the cluster metal core and the thiolate monolayer is especially important because the latter interfaces the former to the surrounding medium: nuclear and electron magnetic methods can be used to understand orbital distribution outside the metal core; (iv) Ligand exchange in clusters and interactions between the ligands of two clusters are instrumental to modify the cluster monolayer, cause polymerization in the solid state, and make two clusters fuse to form different clusters; (v) Techniques such as nuclear magnetic resonance and electrochemistry are especially valuable to assess the thiolate-protected cluster structure in solution.

SHORT TALKS

MONDAY

Vibrations of Atomically Defined Metal Clusters: From Nano to Molecular-Size*

Ignacio L. Garzón

Instituto de Física, Universidad Nacional Autónoma de México, 01000, CDMX, México

garzon@fisica.unam.mx

The elastic behavior at lower sizes (<1−2 nm), where nanoparticles become molecular clusters made by few tens to few atoms, is still little explored. The question remains to which extent the transition from small continuous mass solids to discrete-atom molecular clusters affects their specific low-frequency vibrational modes. Theoretical calculations based on density functional theory (DFT) predict, in the case of bare gold clusters, that vibrational periods corresponding to the breathing and quadrupolar modes scale linearly with size down to diatomic molecules. For ligand-protected gold clusters, it is found a pronounced effect of the ligand molecules, related with mechanical mass-loading effects due to the protecting layer.

We also investigate experimentally by ultrafast time-resolved optical spectroscopy the acoustic response of atomically defined ligand-protected metal clusters Aun(SR)m with a number n of atoms ranging from 10 to 102 (0.5−1.5 nm diameter range). Two periods, corresponding to fundamental breathing- and quadrupolar-like acoustic modes, are detected, with the latter scaling linearly with cluster diameters and the former taking a constant value. This study shows that clusters characteristic vibrational frequencies agree with DFT calculations and are compatible with an extrapolation of continuum mechanics model down to few atoms.

This combined theoretical-experimental study indicates that acoustic vibrations of small nanoparticles are still ruled by continuum mechanics laws down to diameters of a few nanometers whose period is classically expected to linearly scale with diameter. [1]

*In collaboration with: P. Maioli, T. Stoll, H. E. Sauceda, I. Valencia, A. Demessence, F. Bertonelle, A. Crut, F. Vallée, G. Cerullo, N. del Fatti.

Key Words: Acoustic vibrations, density functional theory calculations, ultrafast spectroscopy.

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Structuration of magnetic nanowire arrays assisted by Laser ablation to modify its effective magnetic anisotropy

René Licea Virgen*, Armando Encinas.

División de Materiales Avanzados, Instituto Potosino de Investigación Científica y Tecnológica, Camino a la Presa San José 2055, 78216 San Luis Potosí, SLP, México.

rene.licea09@gmail.com

Magnetic nanowire arrays were synthesized by electrochemical deposition in porous anodic alumina membranes to produce ordered arrays with well-defined geometries. To this end, a computer-controlled XY laser mounted on a table has been used. Two paths were followed, the first consisted in laser irradiation of the nanowires to remove them and generate microstructured arrays. In the second method an organic layer is deposited over the membranes to block the pores and inhibit the growth of wires, afterwards certain areas of this layer were removed assisted by laser ablation, defining paths were the wire growth occurred. The optimal conditions have been studied to perform these processes in a controlled and reproducible way, in addition, the morphologies and magnetic properties of the different assemblies were determined by SEM and magnetometry. The results showed that the nanowires were uniform in size with approximately 200 nm in diameter and 60 µm in length, also, it was found that the total magnetic anisotropy varied when structuration patterns were introduced. These changes were interpreted in accordance to a model of effective demagnetizing field in magnetic nanowire assemblies, which incorporates the combined effects of geometry of the wires and the geometrical arrangement they form.

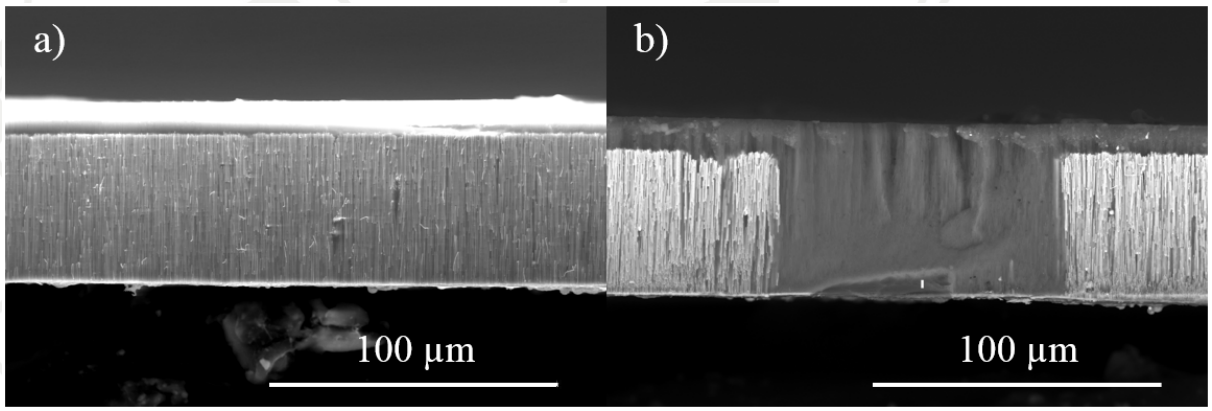

Figure 1. Cross-section SEM images of a) Co wire arrays and b) a design made by the removal of these.

Key Words: Cobalt, nanowires, laser ablation, magnetic anisotropy.

Use of modified carbon Nano-Torus as sensors for magnetoecephalographic imaging

Joel A. Flores-Chávez[1*]

[1]*Tec de Monterrey, Av. Eugenio Garza Sada 2501 Sur, Tecnológico, 64849 Monterrey, N.L., México*

joelantonio@itesm.mx

We propose a carbon-based molecule doped with fluorine atoms to mimic a common Superconducting Quantum Interference Device (SQUID), to be used as a sensor for Magnetoencephalography imaging. To make this possible, we can use the persistent currents that the carbon shows at temperatures close to 5 K [1]. With this, it is expected to reduce the size of the high-precision magnetic sensors that are used nowadays in medical devices from 10000nm^2 [2,3] to 10nm^2, making it possible to augment the density of sensors per unit area and have more precise measurements.

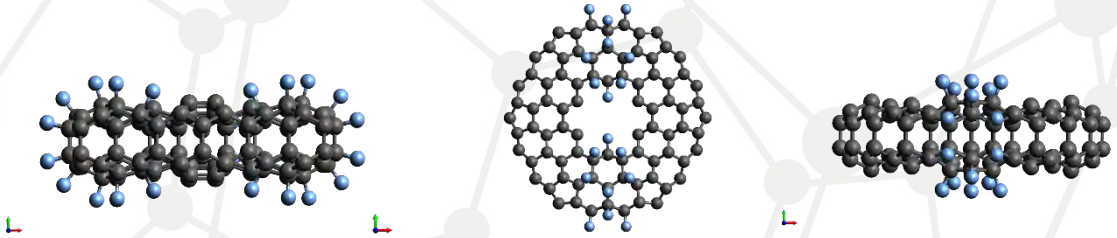

Figure 1 – Proposed carbon structure, seen from three different angles. Gray dots denote carbon atoms and blue dots denote fluorine atoms.

As a consequence of the lack of compatibility of the common algorithms for molecular calculations with the proposed molecule, also we propose a modeling based in differential geometry, making calculations depending on the geometrical space that the structures enclose could require less computer power if used properly. We are opting to use the Compressive Split-Step Fourier Method [4], using the curvilinear Fourier transform on a generalized metric we could generalize this model for any exotic carbon structure, including carbon tubes, knots and coils.

Key Words: Torus, metric, Fourier transform, SQUID

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Macroscopic effects of the Microstructure of magnetic materials: homogenization, advantages and applications

Victor Carrera[1]*, Antonio Capella[2], Armando Encinas[1]

[1] *DMAv-IPICYT, Camino a la Presa San José no. 2055, C.P. 78216, San Luis Potosí, S.L.P., México.*
[2] *IMATE-UNAM, Área de la investigación científica, Ciudad universitaria, 04510, cdmx, México.*

victor.carrera@ipicyt.edu.mx

In this work we study a system of magnetic macrospins laid in a periodic array (figure 1) which posees shape and magnetocrystalline anisotropy. The goal of the study is to better understand the behavior of the magnetization in such systems. To this end, we created a model based in the weak formulation of PDE's and we develop a numerical scheme that allows to find the spatial configuration of the magnetization that corresponds to the minimum of the energy under the right hypothesis. We compute the demagnetization field by means of the magnetostatic scalar potential and the Poisson's equation. We use the homogenization method [1] to acquire the effects of the microscopical structure (figure 2) in the macro quantities that can be measured (as the demagnetization field and the demagnetization factors). Latter, we apply the weak formulation [2] on the maxwell equations to obtain a variational form. Then, using the Lagrange multipliers technique we find the energy minimum. This is represented in a numerical scheme based in the Finite Element Method. Once we have this, we use the Stoner-Wohlfarth [3] particle as a test case, for then use our methods to study particle systems and then we change the geometry to explore the limitations and advantages of our study. Finally we review the advantages of this method as well as the systems that can be modeled with the numerical scheme such as: magnetotactic bacterias (MTB), cellular automatas, and applications for magnetic computational logic (figure 3).

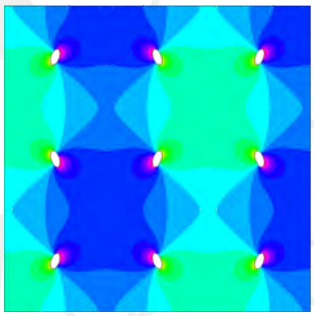

Figure 1 - System of magnetic particles. The magnetic scalar potential is represented in colors.

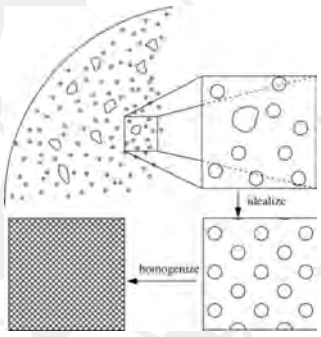

Figure 2 - Scheme of the homogenization concept.

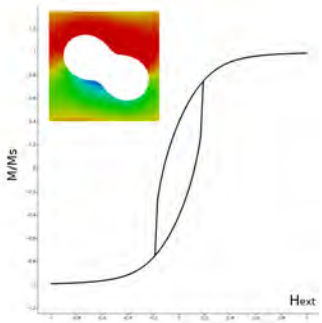

Figure 3 - Peanut shaped particle and its hysteresis curve.

Key Words: Micromagnetics, Simulations, PDE's, Homogenization.

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Polymer nanocomposites thermo-conductors PP and PMMA with nanofillers Cu-Ag and graphene nanoplatelets

D. I. Medellín Banda, D. Navarro Rodríguez, G. Cadenas Pliego, C. Ávila Orta

Centro de Investigación en Química Aplicada, Blvd. Enrique Reyna Hermosillo 140 C. P. 25294, Saltillo, Coahuila. México.

diana.medellin@ciqa.edu.mx

Conformable polymer nanocomposites (NCs) of high thermal conductivity afford significant potential for high-tech materials applications in electronics, transportation, solar and space technologies to name but a few. The present polymer-based thermally conductive nanocomposites were prepared using polypropylene (PP) and polymethylmethacrylate (PMMA) matrices and two different nanofillers; a CuAg alloy and nanoplatelets of graphene (GnP). Nanoparticles of CuAg < 50 nm by transmission electron microscopy were synthesized by reduction of the appropriate salts with hydrazine. Polymers and nanofillers were mixed and extruded in an Xplore M15cc at 200 and 220°C with a rotor speed of 60 rpm for 5 min then compression molded to obtain the composites. The crystallization, thermal stability and mechanical properties of the PP-CuAg-GnP and PMMA-CuAg-GnP nanocomposites were investigated by wide angle X-ray diffraction (XRD), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA) and tensile testing. The thermal conductivity was determined using modulated differential scanning calorimetry and the well-known flash method. Thermal conductivities for the PP-CuAg-GnP NCs at 2.5 and 5.0 wt %, respectively, were 1.56 and 1.75 W/mK while those for the PMMA-CuAg-GnP NCs were 0.96 and 1.14 W/mK, respectively. The nanofillers show good dispersion with an intercalated nanostructure and strong interfacial adhesion with PP and PMMA resulting in good thermal stability and high thermal conductivity. Processing of these new dihybrid NCs provides conformability and scalability.

Key Words: thermal conductivity, nanocomposites, graphene.

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Advances and applications of ultrasound propelled nanomotors

Víctor García-Gradilla*, Adriana García, Keila Correa and Oswaldo Lara.

Centro de Nanociencias y Nanotecnología, UNAM, Km. 107 carretera Tijuana-Ensenada, C.P. 22800, Ensenada B.C., México.

vgg@cnyn.unam.mx

Nanomotors are tiny nanomachines dedicated to transform different type of energy into motion. These nano devices have been designed to perform different advanced tasks like micro-nano cargo transport, target recognition, drug delivery, environmental remediation, nano surgery among many others. Pioneer nanomotors based their propulsion mechanism by converting chemical energy into motion, but the use of chemicals reduce their field of action considerably, making them unable to be used on bioapplications or applications where chemicals are not tolerated. To avoid the use of chemicals, new strategies were developed to produce propulsion at nanoscale. The most successful ones were magnetic and ultrasound propulsion [1,2], the last one has special attention due to its novelty and versatility, and still needs to be fully understand.

In this work we present the advances made by our group in the field of ultrasound nanomotors, from the first nanowire based nanomotor to the design of new generation of ultrasound nanomotors, proposed modelling and the influence of power, density and shape, as long as some proposed and tested applications.

Acknowledgments: This work is financed by SEP-ÇONACYT 239953 project.

Key Words: Nanomotors, ultrasound, nanomachines.

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Effect of power deposition on physical and crystal properties of NiO thin films deposited by the RF sputtering technique

Juan Rubén Abenuz[1], Israel Perez[2], José Elizalde[1]

[1] Department of physics and mathematics Institute of engineering and technology, Universidad Autónoma de Ciudad Juarez, Av. Plutarco Elías Calles #1210 , Fovissste Chamizal, C.P. 32310 Ciudad Juárez, Chihuahua, México.

[2] National Council of Science and Technology (CONACyT), Department of physics and mathematics Institute of engineering and technology, Universidad Autónoma de Ciudad Juarez, Av. Plutarco Elías Calles #1210 , Fovissste Chamizal, C.P. 32310 Ciudad Juárez, Chihuahua, México.

*juan.ruben.abenuz.acuna@gmail.com

This project studies how NiO thin films deposited through the radio frequency sputtering technique at different power deposition affects their morphological, structural, electrical and optical properties. Thin films with different deposition power (60 W, 100 W, 140 W, 180 W and 220 W) with a thickness of 200 nm were manufactured and a heat treatment was carried out at 400°C for 3 hours in ambience. They were characterized by x-ray diffraction and scanning electron microscopy to study the crystalline structure, crystallite size, morphology and average grain size as a function of the sputtering power. Studies of the current-voltage characteristics of the samples were performed by the two-lead technique. The optical transmission and absorption spectra of the films were obtained by UV-VIS spectroscopy and on the basis of these results both the absorption coefficient and the optical band gap were calculated as a function of the deposition power. According to the x-ray diffraction analysis the peaks of the NiO phase were measured and it was found that the grain boundaries of the films decrease as a function of the increase in deposition power. This decrease in grain boundaries affected the differential resistivity. It was found that the films with less grain boundaries possess low differential resistivity than films with higher number of boundaries. Both the optical transmission and the energy band gap decreases as a function of the deposition power.

Key Words: Thin films, Nickel oxide, Sputtering.

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Preparation $NiFe_2O_4$ hollow nanosphere by easy hydrothermal method and application in a hydrogen generation microfluidic system in alkaline medium

A. Matinez-Lazaro[1], E. Ortiz-Ortega[1], J. Ledesma-García[2], L.G. Arriaga[1]

[1]Centro de Investigación y Desarrollo Tecnológico en Electroquímica, Pedro Escobedo, Qro., C.P. 76703, México;
[2]División de Investigación y Posgrado, Facultad de Ingeniería, Universidad Autónoma de Querétaro, 76010, México

eortega@cideteq.mx

The present work shows a simple method to synthesize 3D nickel ferrite hollow spheres by hydrothermal route and its application as catalyst to favor the oxygen evolution reaction (OER) for electrochemical separation of water in alkaline medium. The material NiFe2O4 were developed thanks to a simple mechanism from the urea hydrolisis reaction and later subjected to a hydrothermal process to carry out the synthesis in a single step, showing a simple method of obtaining these 3D materials with surface areas relatively large that showed a catalytic activity comparable to IrO2 and higher than Pt / C which are catalysts commonly used in conventional electrolysers. NiFe2O4 hollow sphere was evaluated in a microfluidic system for H2 production.

Green decoration of MWCNTs with Ag-AuNPs and its application in the remotion of methylene blue dye

D. Mendoza-Cachú[1], J.L. López-Miranda[1], C. Mercado-Zúñiga[2], G. Rosas[1]

[1] *Instituto de Investigación en Metalurgia y Materiales, UMSNH, edificio U., Ciudad Universitaria, C.P. 58000, Morelia, Michoacán, México.*
[2] *Tecnológico de Estudios Superiores de Coacalco, Av. 16 de septiembre # 54, C.P. 55700, Col. Cabecera Municipal, Coacalco de Berriozábal, Edo. de México, México.*

david.mendozach@gmail.com

Carbon nanotubes (CNTs) are used in a wide range of applications, specially due to the possibility to superficially modify them. From this point, the present research aims to the surface treatment of multi-walled CNTs, through its decoration with Ag-Au nanoparticles (NPs), by applying a green, low-temperature process. The first step consists of deagglomerating the nanotubes using sodium dodecyl sulfate (SDS) as surfactant agent, and varying its concentration in distilled water. The results were evaluated by means of UV-Vis spectroscopy and scanning electron microscopy (SEM), observing a considerable reduction in nanotubes agglomeration. Once the better dispersion results were selected, the decoration of MWCNTs proceeded employing a green synthesis process, from the reduction of the AgNO3 and HAuCl4 salts using the A. triphylla plant extract, promoting the formation of the Ag-AuNPs. In order to evaluate the microstructural characteristics of the NPs as well as the final decoration of the MWCNTs, UV-Vis, SEM and transmission electron microscopy (TEM) studies were developed. Finally, the catalytic activity of the composite CNTs/Ag-AuNPs was evaluated in terms of its ability to degrade the methylene blue dye. For this purpose, UV-Vis spectroscopy was helpful to obtain the kinetics of the process.

Key Words: Carbon nanotubes, decoration, green synthesis, nanoparticles, degradation.

Doping impact of IIIA group elements on emission and structure of ZnO nanocrystal films

Tetyana V. Torchynska[1*], Brahim El Filali[2], Jose L. Casas Espinola[1], Chetzyl Ballardo Rodriguez[2] Juan A. Jaramillo Gomez[2] and Lydmula Shcherbyna[3]

[1]Instituto Politécnico Nacional, ESFM, Av. IPN, México D.F.07738, México
[2]Instituto Politécnico Nacional, UPIITA, Av. IPN, México D.F.07320, México
[3]V. Lashkaryov Institute of Semiconductor Physics at NASU, Kyiv, 03028, Ukraine

ttorch@esfm.ipn.mx

The morphology, structure and emission of Al (Ga or In)-doped ZnO nanocrystal (NC) films with the different Al (Ga or In) contents (1-4at%) were studied by means of scanning electronic microscopy (SEM), energy dispersive X ray spectroscopy (EDS), X-ray diffraction (XRD) and photoluminescence (PL) methods. Ultrasonic spray pyrolysis was applied to obtain the ZnO films. To stimulate the crystallization, the ZnO films were annealed at 400 °C for 4h at a constant nitrogen flow (8L/min). It is shown that the Al incorporation in the ZnO films with the concentrations ≥ 2-4at% stimulates: reducing the ZnO grain size, decreasing the film crystallinity owing to disordering the ZnO crystal lattice, as well as the change of surface morphology and increasing the surface roughness.

Meanwhile Al-doping the ZnO film at the concentrations ≤ 2at% enlarges significantly the PL intensity of near band edge (NBE) emission. Last fact testifies to quality improving the ZnO:Al films. Simultaneously, the PL intensities of green and orange PL bands, connected with the native defects: VZn and Oi, respectively, fall down. The ZnO NC films with Al-doping ≤ 2at% still keep the planar surface morphology that is important for their application in electronic device structures.

The Ga or In doping ZnO films demonstrate the similar effects, but for the some different concentration ranges. The shift of optimal concentrations with the IIIA element type varying has been detected and discussed.

Hall effect of carbon nanowalls deposited with different morphology and microstructure

M. Acosta Gentoiu[1*], M. Volmer[2], Re. Betancourt-Riera[3], S. Vizireanu[4], S. Antohe[5], G. Dinescu[4], R. Riera[1]

[1]Departamento de Investigación en Física, Universidad de Sonora, C.P. 83000, Hermosillo, Sonora, México.
[2]Transilvania University Brasov, B-dul Eroilor 29, C.P. 500036, Brasov, Romania
[3]Instituto Tecnológico de Hermosillo, Avenida Tecnológico S/N, Col. Sahuaro, C.P. 83170, Hermosillo, Sonora, México.
[4]National Institute for Lasers, Plasma and Radiation Physics, Atomistilor No.409, PO Box MG-36, C.P. 077125, Magurele-Bucharest, Romania.
[5]Faculty of Physics, University of Bucharest, 405 Atomistilor Street, 077125 Măgurele, C.P. 077125, Romania

macostagen@gmail.com

Hall coefficient reveals variations on three different vertical graphene sheets or carbon nanowalls CNWs samples. The CNWs were synthetized by Plasma Enhanced Chemical Vapor Deposition varying deposition temperature and Ar flux [1, 2]. The morphological and microstructural differences were observed by Scanning Electron Microscopy, Transmission Electron Microscopy, Raman spectroscopy and X-Ray Photoelectron Spectroscopy. The sample with smaller length of walls reveled a change of the Hall coefficient from positive to negative value at high enough temperatures, where the semiconductor characteristic could be turned of p-type to n-type. The landau level vanishes at low temperature due to defects. Our results could be a way towards the use of vertical graphene or CNWs as magnetoelectronic nanodevices.

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Raman spectroscopy study of L-and-D-Cysteine adsorption on gold nanoclusters

Penélope RODRIGUEZ-ZAMORA[1*], Lourdes BAZÁN[2], Benjamín SALAZAR[1], Cristina ZORRILA[1], Ignacio L. GARZÓN[1], Gabriela DÍAZ[1]

[1]*Instituto de Física, Universidad Nacional Autónoma de México, 04510 Ciudad de México, México*
[2]*Department of Physics and Astronomy, University of Texas at San Antonio, Texas 78249, USA*

*penelope.rodriguez.zamora@gmail.com

Understanding the physical mechanisms of adsorption of chiral molecules on metal nanoclusters is highly attractive for practical enantiomeric separation and in view of the transcendence of homochirality on earth [1]. Copious computational work has been done particularly on cysteine-Au systems due to the strong adsorption of this molecule on gold surfaces [2], but experimental results continue being in the curve of improvement in order to be comparable with calculations. Here we present vibrational experimental data of the adsorption of both enantiomers of cysteine on gold nanoclusters by Raman spectroscopy, in order to determine the stabilized conformations of the two amino acids adsorbed on gold surface. Each enantiomer exhibit different polymorphism, while L-cysteine is orthorhombic, D-cysteine has a monoclinic crystal structure. Such difference is reflected in the Raman spectra of the free molecules, but the adsorption on gold nanoclusters homogenizes the vibrational modes, resulting in splicing of the spectra and indicating that, once adsorbed on the gold surface, both polymorphs adopt the same strained conformation. This evidences experimentally that orthorhombic-levorotatory and monoclinic-dextrorotatory cysteine adsorbed on gold nanoclusters share a preferential rotamer out of the three cysteine isomers of different rotable $\chi_1(S-C\alpha-C\beta-C\gamma)$ torsional angle, consequently determining the adsorption sites of the molecule.

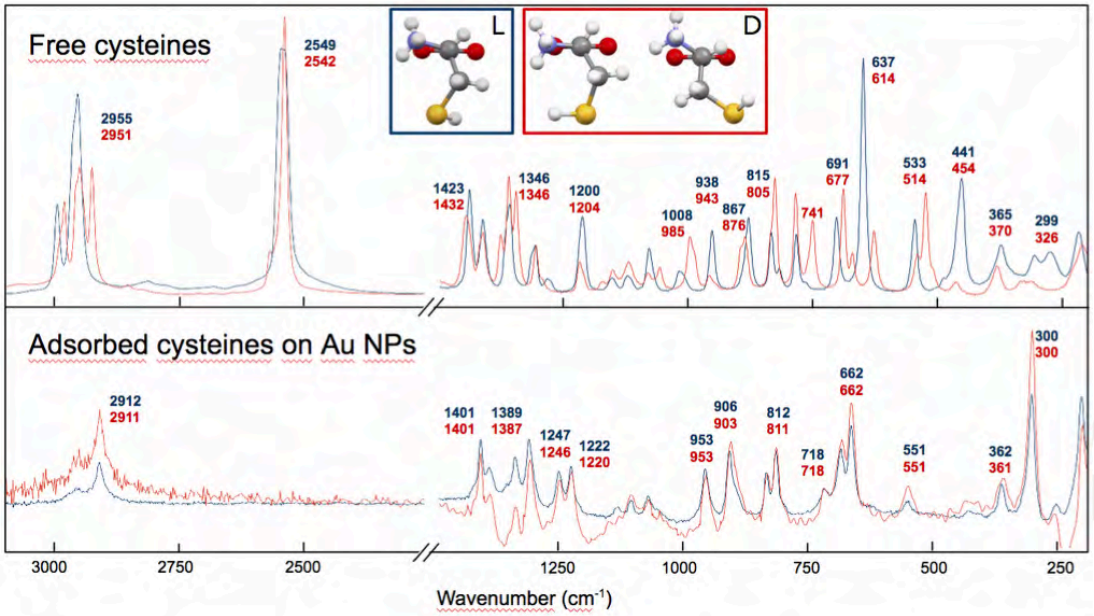

Figure 1 – Raman spectra of free (up) and AuNP-adsorbed (down) orthorhombic L-cysteine (blue) and monoclinic D-cysteine (red), the latter polymorph with two molecules in the asymmetric unit.

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TUESDAY

Development of Ta_2O_5-Based parallel plate Nanocapacitors

Israel Omar Perez Lopez[1]*, Jose Alejandro Gaytan Muñoz [1], Jose Trinidad Elizalde Galindo[1]

[1]*Universidad Autónoma de Ciudad Juárez, Av. Del Charro 450, Col. Romero Partido, C.P. 32340, Juárez Chihuahua, México*

cooguion@yahoo.com

Science and technology go hand by hand with the well-being of a nation. It is for this reason that scientific projects must be fostered to meet the challenges of modern technological developments. For the last 70 years electronics has become one of the most active areas in research and engineering. The evolution of this field demands devices with smaller size, high performance, and enhanced features. Capacitors are some of the most important components in a circuit board and the to meet the requirements of modern electronic circuits, capacitors should increase its capacitance while at the same time reduce its size. According to theory, the capacitance *C* for a parallel-plate capacitor is given by the formula:

$$C = k\varepsilon_0 \frac{A}{d},$$

where *k* is the dielectric constant, e_0 is the permittivity of the vacuum, *A* is the area of the plates and *d* is the dielectric thickness. As can be seen from the expression, the capacitance will increase if *d* is reduced, or *A* and/or *k* are increased. If one wishes to reduce the size and increase the capacitance we have no option but to reduce the dielectric thickness and/or increase *k*. The development of modern deposition techniques and modern materials allow us to meet both of these requirements.

Herein we show the construction and characterization of Ta_2O_5-based parallel plate nanocapacitors using the so-called RF magnetron sputtering technique. Four capacitors, based on amorphous Ta_2O_5 as dielectric, were manufactured. Two of these had a dielectric thickness of 100 nm and the other two of 300 nm. The dielectric was inserted in two 440 nm-thick Au/Pd and Ni plates. To verify their performance, we measured their capacitance and leakage current. Our results are comparable to those reported in the literature. We also discuss the challenges we faced during fabrication and the future perspectives for the improvement of our manufacturing methodology.

Key Words: high dielectric constant, tantalum pentoxide, RF sputtering, capacitor

Life cycle analysis of silver nanoparticles applied to textile fibers

Colín ALFREDO[1]*, García DAYHANA[1], Guzmán JOSÉ[1], Puente JUAN[1], Martínez BEATRIZ[1]

[1]*División de Nanotecnología, Universidad Politécnica del Valle de México, Avenida Mexiquense s/n, 54910, Tultitlán, Estado de México, México.*

alfred.secun@hotmail.com

Introduction. Silver nanoparticles (AgNPs) are one of the most commonly used nanomaterials due to their properties, such as their catalytic and antibacterial activity [1]. AgNPs in textile fibers are used as bactericides, in surgical clothing and to avoid unpleasant odor in clothing. However, there is concern about the release of silver ions to the environment in the washing processes that could have a detrimental effect on the environment [2].

Aim: To elaborate a complete LCA of the AgNPs applied to the textile fibers was carried out to determine their impact on the environment and human health.

Methodology. A comparison was made between two synthesis methods: a conventional chemical synthesis method and a green synthesis method, both following the reduction principle. The ISO 14040-1404 normativities were used to elaborate the LCAs.

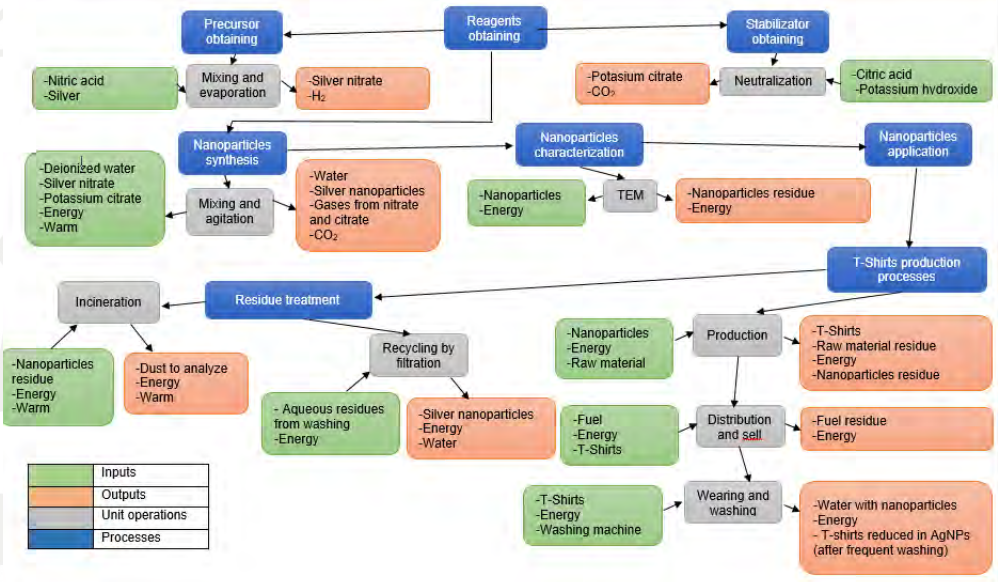

Figure 1: LCA diagram for conventional synthesis method.

Results. The synthesis was identified the part of the LCA that represents the greatest negative impact on the environment and health.

Conclusions. This work demonstrated the importance of using a green synthesis method and the advantages of working with AgNPs in this way.

Key Words: Life Cycle Analysis, textile fibers, silver nanoparticles, environmental impact.

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Synthesis of transition metal oxides mixtures based on NiCo and MoCoW with low Pt content for oxygen reaction reduction in alkaline media

José Béjar[1], L. Álvarez-Contreras[2], J. Ledesma-García[3], L.G. Arriaga[1*] and N. Arjona[1]

[1]Centro de Investigación y Desarrollo Tecnológico en Electroquímica, 76703 Querétaro, México.
[2]Centro de Investigación en Materiales Avanzados S. C., 31136 Chihuahua, México
[3]Facultad de Ingeniería, División de Investigación y Posgrado, Universidad Autónoma de Querétaro, 76010 Querétaro, México

larriaga@cideteq.mx

The oxygen reduction reaction (ORR) remains as the limiting reaction for practical applications of fuel cells as an alternative technology for clean energy. Therefore, new materials with zero Pt loading or with low Pt content must be designed for overcoming the limiting factors. These new materials/catalysts must have high activity and stability towards this reaction. Among the new tendencies in nanomaterials for energy conversion, the transition metal oxides mixtures (TMOMs) have shown excellent electrocatalytic properties and a greater stability compared to platinum. Therefore, in the present work, we present the use of Ni, Co and Mo oxides decorated with platinum as electrocatalysts for the ORR. This study was performed using two combinations: NiCoPt and MoCoWPt (W was used in a low amount as a promoter in the Co oxides formation). The electrocatalytic activity was studied by rotating disc electrode (RDE), from which the kinetic parameters were obtained by Koutecky-Levich an Tafel plots. Small-sized TMOMs based on NiCoPt and MoCoWPt ranging 8-25 nm were obtained. Moreover, these materials presented high stability and excellent activity for ORR. Compared with a commercial Pt/C (30 wt%) catalyst, these TMOMs presented overpotentials lower than 160 mV.

Key Words: Oxygen reaction reduction, Transition metal oxides mixtures, electrocatalysis.

Incorporation of IrO_2 and RuO_2 into Pd nanoparticles for boosting the electrocatalytic activity toward electro-oxidation of crude glycerol from biodiesel

I. Velázquez-Hernández[1], L. Álvarez-Contreras[2], J. Ledesma-García,[3] M. Guerra-Balcázar,[3] L.G. Arriaga[1] and N. Arjona[1*]

[1]Centro de Investigación y Desarrollo Tecnológico en Electroquímica, 76703 Querétaro, México.
[2]Centro de Investigación en Materiales Avanzados S. C., 31136 Chihuahua, México
[3]Facultad de Ingeniería, División de Investigación y Posgrado, Universidad Autónoma de Querétaro, 76010 Querétaro, México

wvelazquez@cideteq.mx

Crude glycerol from biodiesel industries is composed mainly by a mixture of soups, remnants of biodiesel/oils, methanol and glycerol. Moreover, crude glycerol is considered as an undesired byproduct and it is mostly burned or storage, increasing the biodiesel costs. Methanol and glycerol are considered as electro-active species than can be used as fuels for energy conversion applications such as fuel cells. Therefore, the use of crude glycerol as fuel can give it an added-value increasing the renewable aspect of fuel cells technology. Consequently, in this work, we synthesized Pd, $PdIrO_2$ and $PdRuO_2$ (which have shown in literature high affinity for methanol electro-oxidation) electrocatalysts deposited on Vulcan carbon as support. These materials presented according to TEM images, nanoparticulate sizes ranging 8-16 nm. In addition, the elemental composition performed by XRF indicated that both are in a mass ratio of Pd-76% IrO_2-24% and Pd-79% RuO_2-21%. Evaluation of the electrocatalytic activity for crude glycerol electro-oxidation indicated that Pd-RuO_2 presented the most negative onset potential (-0.23 V *vs*. NHE); however, Pd-IrO_2 presented the maximum current density at 2 M crude glycerol (3 and 5-fold higher current density than Pd-RuO_2 and single Pd nanoparticles).

Key Words: crude glycerol, electrocatalysis, energy conversion, Pd-RuO_2, Pd-IrO_2.

Dispersion of carbon nanotubes using commercial surfactants

I. Santos[1], J. Zárate[1], G. Rosas[1]

[1]Instituto de Investigaciones en Metalurgia y Materiales, Universidad Michoacana de San Nicolás de Hidalgo, Av. Gral. Francisco J. Mújica, ciudad universitaria, C.P. 58030, Morelia, Michoacán, México

ismael_3690@hotmail.com

Carbon nanotubes (CNTs) were discovered in 1991 by Sumio Iijima, attracting the attention of researchers thanks to their excellent mechanical properties. However, the use of this material implies a challenge due to its tendency to agglomerate. A good dispersion of carbon nanotubes offers the opportunity to obtain materials with high properties. Deagglomeration and uniform dispersion are necessary stages before final applications. This research presents the dispersion of CNTs in an aqueous medium using two commercial surfactants, such as COFOTAA 44, amino trimethyl phosphonic acid (ATMP) and CONNO 100 nonylphenol 10. The colloidal sols were subjected to ultrasonication to promote deagglomeration and left to stand for 24 hours. Using UV-Vis spectroscopy the stability of the suspension was controlled, and by MEB and TEM the distribution was analyzed. Once a stable suspension, it was left to rest, observing that the suspension after nine months remains stable.

Key Words: carbon nanotubes, dispersion, surfactant, deaglommeration

Nanoparticle deposits formed at driven receding contact lines

Diego Noguera-Marín[1], Miguel Cabrerizo-Vílchez[1], Miguel Ángel Rodríguez-Valverde[1], Carmen Lucía Moraila Martínez[2]

[1]University of Granada, Applied Physics department, Campus de Fuente Nueva s/n ES18071, Granada, Spain.
[2]Universidad Autónoma de Sinaloa, Facultad de Ciencias Físico Matemáticas Av. de las Américas y Blvd. Universitarios 80010 Culiacán, Sinaloa, México

*cmorailam@uas.edu.mx

In order to produce well-ordered structures via evaporation of colloidal suspensions [1], it is essential to control the evaporation flux, solute concentration, interaction between the solute and the substrate, etc. Several authors have reported that the pH of the solution modifies the final deposit pattern [2-4]. Bhardwaj et al. [2] reported different patterns by considering how the electrostatic and van der Waals forces (DLVO forces) alter the particle deposition process. Moraila-Martínez et al. [3] concluded that the morphology of the nanoparticle deposits is modulated to a different extent by the strength of the particle–particle repulsion, the substrate– particle wettability contrast and the substrate receding contact angle. In this work, we compare experimentally the impact of the geometry of the contact line in the nanoparticle deposits using two different configurations: the sessile drop and the meniscus. For both methodologies we examine the role of the DLVO interactions, the nanoparticle and substrate wettability. The set-up used are described in Moraila-Martínez et al. [3] and Bodiguel et al. [5]. We confirmed that the nanoparticle deposits are strongly ruled by the DLVO interactions for both morphologies. In Figure1 the deposits obtained for the different configurations are shown. The results obtained opens up a new method of controlling colloidal deposition patterns by means of DLVO interactions.

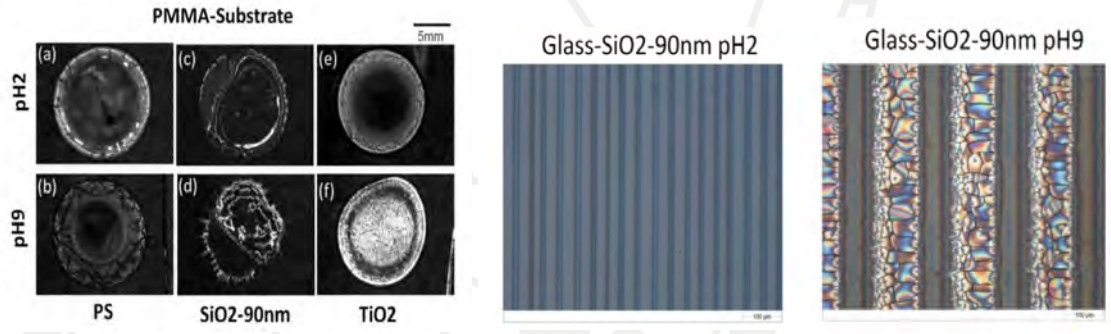

Figure 1 – Nanoparticle deposits obtained at (a)sessile drop and (b) meniscus configuration.

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Metal-organic frameworks (MOFs) as sensitive materials for molecule detection

Arianee Sainz-Vidal[1*]

[1]*Instituto de Ciencias Aplicadas y Tecnología-Universidad Nacional Autónoma de México, Avenida Universidad 3000, C.P. 04510, Ciudad Universitaria, Ciudad de México, México.*

*arianee.sainz@icat.unam.mx

MOFs are known for their extraordinarily high surface areas, tunable pore size, and adjustable internal surface properties. These properties, together with the extraordinary degree of variability for both the organic and inorganic components of their structures, make MOFs of interest for potential applications in catalysis, gas storage, capture and separation. Additional applications in optics, electronics, drug delivery and sensing are increasingly gaining relevance. Regarding to sensing application, in the last years, Zeolite imidazolate frameworks (ZIFs) a particular class of MOFs have attracted mayor attention since they offer important advantages as its chemical and thermal robustness, extend surface area, hydrophobicity, and its easy and environmental friendly synthesis process. In this talk some results on synthesis and characterization of a ZIFs based gas sensor are discussed.

Key Words: MOFs, structures, ZIFs.

Towards strong light - matter coupling of WS2 monolayers in porous - silicon microcavities

Edgar A. CERDA MÉNDEZ[1*], Osvaldo DEL POZO ZAMUDIO[1], Francisco ROCHA REINA[1], Denise ESTRADA WIESE[2], Andrés DE LUNA BUGALLO[3], Angel TORRES ROSALES[1], Antonio DEL RÍO PORTILLA[2] y Raúl BALDERAS NAVARRO[1]

[1]Instituto de Investigación en Comunicación Óptica (IICO), Universidad Autónoma de San Luis Potosí (UASLP), Av. Karakorum 1470, Lomas 4a Secc. C.P. 78210, San Luis Potosí, México.
[2]Instituto de Energías Renovables UNAM, Priv. Xochicalco S/N Temixco, Morelos 62580 México
[3]CINVESTAV unidad Querétaro, Libramiento Norponiente #2000, Fracc. Real de Juriquilla. C.P. 76230, Santiago de Querétaro, Qro. México

*edgar.cerda@uaslp.mx

In this work, we present the advances made in the fabrication of a porous-silicon (PSi) based microcavity (MC) to produce strong light-matter coupling (SLMC) between the excitons of WS2 monolayer flakes and the confined photons. The SLM regime results from multiple coherent absorption/emission cycles of photons by the excitons, which creates a novel superposition state called polariton. Polaritons have been studied in the last decades, mostly in III-V semiconductor, for their interesting properties, such as Bose-Einstein condensation and strong non-linearity [1]. The advent of 2D materials with semiconductor properties such as transition metal dichalcogenides (TMDC), brought a strong interest in the fabrication of MCs for the implementation of SLMC based in them for novel opto-electronic devices[2]. In contrast to III-V semiconductors, the strong absorption coefficient of TMDC and large exciton binding energy (~50 meV) make them suitable for operation at room temperature. Additionally, the TMDC valleytronic properties are inherited and enhanced in the SLMC regime. We present experimental results on the fabrication of a novel and flexible MC architecture based on PSi to produce polaritons with excitons in WS2 monolayers. The MC reflectors are fabricated by a standard electrolysis procedure. The WS2 monolayers are synthesized by chemical vapor deposition on Si/SiO2 substrates and subsequently transferred to the reflector. We show photoluminescence and Raman spectra of WS2 monolayers on the PSi reflectors, which show that the transfer procedure is very efficient. We also demonstrate the fabrication of a MC containing TMDC monolayers by the mechanical deposition of a PSi reflector previously removed from a separate substrate on the reflector where the monolayers were deposited. This work is relevant for the implementation of valley-optoelectronic devices based on TMDC.

Key Words: 2D materials, exciton-polaritons, valley optoelectronics

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Optical properties of gold nanoparticles and silver deposited on optical fibers for sensing pH

Ivan Hernández Gutiérrez[1*], Georgina Beltrán Pérez[1], Martín Rodolfo Palomino Merino[1], Iván Edoardo Gil García[1], Juan Castillo Mixcóatl[1], Severino Muñoz Aguirre[1], Juan de la Cruz Quiroga[1], Hugo Méndez Martinez[1]

[1]Facultad de Ciencias Físico Matemáticas, Benemérita Universidad Autónoma de Puebla. Apartado Postal 1152, 72000, Puebla, Pue. México

*txuzivan17@gmail.com

In this work we measured some optical properties of gold and silver nanoparticles deposited on optical fiber such as the emission and light absorption spectra in the visible and infrared range. The fiber coating was performed using Sol-gel technique on a SiO_2 base at different molar concentrations, using as a TEOS precursor. Optical experiments were performed using a white halogen lamp for the visible range (350-900 nm) and a superluminescent laser diode (1400 - 1650 nm). The spectra were obtained in the infrared and visible range respectively by using an optical spectrum analyzer (OSA) and a spectrophotometer (visible range). In order to give the application as a method of census to indicate the degree of acidity or alkalinity of a solution, was varied the pH in a range of 1 to 13, observing changes in amplitude at each one of the variations. The main idea of this sensor is the excitation of surface plasmon resonance (SPR) due to the interaction of the evanescent field generated by optical devices with a thin metal film, in this particular case the gold and silver nanoparticles.

Key Words: sensor, pH, nanoparticles, plasmon, and fiber.

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MOF-derived nanocarbons: synthesis, properties, and applications

Boris I. Kharissov,* César M. Oliva González, Ana de Monserrat Navarro, Thelma Serrano, Yolanda Peña, Oxana V. Kharissova.

Universidad Autónoma de Nuevo León, Ave. Universidad, San Nicolás de los Garza, N.L., Mexico 66455.

*bkhariss@hotmail.com.

Metal-organic frameworks (MOFs) are multi-dimensional nanoporous structures composed of metal ions (or clusters) coordinated to rigid organic molecules (linkers). The choice of the metal ion and linker species completely determines the structure and functionality of the resulting MOF. Common organic linkers include bidentate carboxylics (e.g., HOOC–COOH), tridendate carboxylates, 1,4-benzenedicarboxyalte (BDC), and azoles. The great freedom with which the linkers and metal ions can be chosen and combined is reflected in the more than 20,000 MOF species that have been reported in the last two decades. The MOFs built from metal ions and polyfunctional organic ligands have proved to be promising self-sacrificing templates and precursors for preparing various carbon-based nanomaterials, possessing high BET surface areas, abundant metal/organic species, large pore volumes, and extraordinary tunability of structures and compositions. MOf-derived nanocarbons are obtained by carbonizing carbon precursor (*i.e.*, MOF) usually in inert atmosphere. Type of pyrolysis (in vacuum or inert gas) is an important factor. The pore structure and surface area of the MOFs can be tuned by changing the calcination temperature (600-1000^{o}C). The resultant carbon structures possess high surface areas and distinct properties.

In comparison with other carbon-based catalysts, MOF-derived carbon-based nanomaterials have great advantages in terms of tailorable morphologies, hierarchical porosity, easy functionalization with other heteroatoms and metal/metal oxides, which make them highly efficient as catalysts directly or as catalyst supports for numerous important reactions. Other uses of MOF-derived carbons include other electrochemical applications, for example for batteries. In whole, heat treatment of metal–organic frameworks, resulting MOF-derived carbons, belongs to green energy applications. Among other applications, we note CO2 capture, fabrication of pseudo-capacitance electrodes, adsorbents for removal of heavy metals and toxic species from drinking water, drug delivery carriers, electrolyte/membrane materials for fuel cells, sulfur hosts for lithium–sulfur batteries, etc. Oxygen Reduction Reactions (ORR) are also a promising field of applications of MOF-derived carbons.

This presentation is dedicated to the state of the art of the MOFs area and selected experimental results of our research group.

Biomimetic synthesis of composite polyaniline/O-doped carbon nitride as flexible supercapacitive microelectrodes

M. E. MARTÍNEZ-CARTAGENA[a,b]*, S. FERNÁNDEZ-TAVIZÓN[a,b], J. ROMERO-GARCÍA[a], R. TORRES-LUBIÁN[a], U. SIERRA[a,b], A. MERCADO[a,b], E. CUARA[a,b]

[a]*Centro de Investigación en Química Aplicada; Blvd. Enrique Reyna No. 140, Col. San José de los Cerritos, 25294 Saltillo, Coah.*
[b]*Laboratorio Nacional de Materiales Grafénicos; Blvd. Enrique Reyna No. 140, Col. San José de los Cerritos, 25294 Saltillo, Coah*

*Eduardocartaa@gmail.com

Various applications requiring the conduction of electricity make use of PANI as a convenient substrate; commonly PANI is synthesized by oxidative polymerization of aniline using a variety of protocols[1]. The enzyme-catalyzed aniline polymerization has been presented in a scant number of articles and while convenient[2], the use of enzymes have important limitations, among them its high cost and limited pH range use[3]. As PANI´s conductive properties are pH dependent, it would be advantageous to use enzyme-like catalysts that would allow to polymerize aniline at fairly low pH[4]. We present the use of hematin as an enzyme substitute that allows said polymerization in a 1-2 pH range of. We have found that hematoporphyrin can be easily deposited onto graphitic carbon structures and the resulting composite used as an aniline polymerization catalyst. The graphitic carbon nitride allows the template formation of planar PANI-gOCN composites while the carbon nitride's stability and ease of dispersion at very low pH protects the hematin deposited on their surface. Through the use of this catalyst, high-quality PANI can be obtained with yields of > 70%. XRD, FTIR and UV vis analysis substantiate the formation of the polymer while SEM and TEM observations demonstrate its laminar form. The prepared composite material can be advantageously used in the preparation of supercapacitors, as shown by its electrochemical evaluation. Moreover, this polymerization technique let *in situ* fabrication of microsupercacitors by the layer by layer method, basically we demonstrate that is possible a deposition of hematin onto g-OCN and use this substrate as catalyst of aniline polymerization in presence of hydrogen peroxide to create a stack of multilayers of polyaniline/g-OCN/hematin that it has a 200-300 nm of height. All the layers are supported in flexible substrate of PET-ITO to obtain a functional electrode that was used in electrochemical characterization.

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Study of several lubricants doped with carbon nanoparticles

Estefany TOVAR S.[1]*, Oxana Vasilievna KHARISSOVA[1], Patsy ARQUIETA[1], Demofilo MALDONADO[2], Laura PEÑA[2]

[1]Facultad de Ciencias Físico Matemáticas, UANL, Ciudad Universitaria SN, San Nicolás de los Garza, C.P. 66455, N.L., México
[2]Universidad de Monterrey, Av. Ignacio Morones Prieto 4500, Jesús M. Garza, C. P. 66238, San Pedro Garza García, N.L. Monterrey, N.L. México

*Estefany.tovars@splinter.com.mx

During the present investigation, the effect of lubricity was analyzed in various lubricants such as, Ecodraw, Sigralub, doped with carbon nanoparticles (0.5% -2%). The nanoparticles used to dope these lubricants were: multilayer carbon nanotubes, carbon nanotubes functionalized with -OH groups, -COOH groups, nanotori, among others. During the investigation, improvements in the properties of the lubricants were noted (Figure 1).

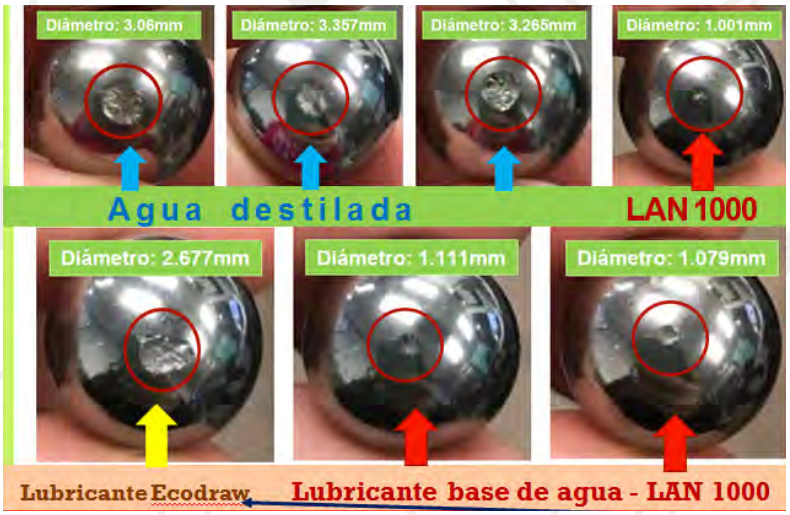

Figure 1 –Tribological test with four balls.

The best results were obtained by doping nanoparticles of nanotori with percentages >1%. The anti-wear properties were improved 80% higher compared to lubricants without the presence of nanoparticles. It was noted a higher presence of carbon on the surface, which protects the surface and improves the quality of the same.

Key Words: lubricants, nanoparticles, carbon, doped, improvement, industry.

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WEDNESDAY

Influence of different process parameters on the characteristics of liposomes prepared by a solvent emulsion-solvent evaporation technique

Daniela Ortiz Ríos[1,2]

[1]*University Medical Center Groningen, 2 TEVA Pharmachemie*

danny.qfb.ortiz@hotmail.com

Liposomes are an attractive delivery system due to their flexible physicochemical and biophysical characteristics, which allow an easy manipulation to address different drug-encapsulation considerations [1]. Some liposome characteristics may vary depending on the lipid composition and the preparation method [2]. Therefore, the objective of the present study was to investigate the influence of different process parameters on the characteristics of liposomes prepared by a solvent emulsion – solvent evaporation and technique [3].

To study the influence of different solvent systems, liposomes were prepared using either dichloromethane/methanol/water or chloroform/methanol/water. On the other hand, to study the influence of different evaporation temperatures, solvents were evaporated at a temperature either below or above the phase transition temperature of the lipids [4]. Also, we investigated the effect of different concentrations of copper gluconate/triethanolamine in the hydration solution [5].

Results indicated that the use of different process parameters has an influence in certain liposome characteristics such as encapsulation efficiency, particle size, and surface charge. Nevertheless, characteristics such as morphology and phase transition temperature were not affected. In conclusion, our results provided more insights on the influence of different process parameters on the characteristics of liposomes. This understanding might help to establish key process parameters that can serve to tailor required liposomal characteristics in further liposomal formulations and moreover, we provide a possible approach to control them.

Key Words: Liposomes, solvent emulsion, copper gluconate, triethanolamine. References

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Conjugated Linoleic acid liposomes: possible brain cancer drug delivery system

Gómez-Bustamante, D. E.[1*], Navarro-Tovar, G.[1], González, C.[1], Rocha-Uribe, A.[1]

[1]*Chemical Sciences Faculty, UASLP. Av. Manuel Nava, #6, C.P. 78210, San Luis Potosí, México.*

egomezbustamante@outlook.com

A blend of bioactive conjugated linoleic acid (CLA) isomers, with anticarcinogenic properties, was obtained by microwave-assisted alkali isomerization of cooking oil according to Silva-Ramirez [1]. Afterward, assembled into liposomes mixing different CLA and cholesterol mass ratios in aqueous solution at biological pH (~7.3), adapting Zhang's method [2]. CLA liposomes (LCLA) size, emulsion stability and drug encapsulation were evaluated using dynamic light scattering (DLS), ξ potential and UV–Vis spectroscopy. LCLA hydrodynamic diameter and surface electrostatic charge, directly related to liposome stability, is summed up in *table 1*. Best relationship between those features was registered in batches with 2:1 lipid mass ratio, so they were used in every cells viability experiment.

Table 1. LCLA batches size and surface charge with standard deviation (n=3).

CLA:cholesterol proportion	Diameter (nm ± SD)	ξ potential (mV ± SD)
1:0	34.89 ± 12.35	-36 ± 12.35
1:1	54.09 ± 15.01	-39.9 ± 5.96
2:1	57.71 ± 13.64	-46.4 ± 3.6

Cytotoxicity was evaluated via MTT colorimetric assay on *C6* glioma cells, fitting van Meerloo's protocol [3]. All LCLA batches tested, showed glioma cells growth inhibition (*Fig. 1A*) below 20 mM, while H_2O_2 and culture media acted as positive and negative damage control, respectively. Encapsulation of photoactive anticancer drug in LCLA, was monitored over time (*Fig. 1B*), via UV-Vis spectroscopy until maximum absorbance become constant.

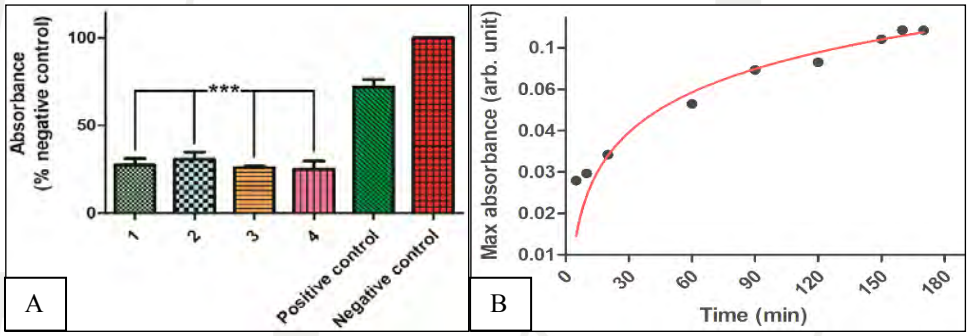

Fig. 1. A: MTT assay of different LCLA batches (1-4) and damage controls. *** Statistical significance ($p<0.001$) against controls. **B**: Plot of drug highest absorbance against sampling time.

Key Words: Liposomes, Conjugated Linoleic Acid, Brain Cancer, Fatty Acids, Drug Delivery.

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Preparation, characterization and UV crosslinking of PVA/DEXTRIN nanofibers as aplication for dressing wound healing

Ortíz Linda K [1], Estrada- Villegas G. Mayeli[2*], Betancourt Rebeca[3]

[1]CONACYT-Centro de Investigación en Química Aplicada, Alianza Sur 204, C.P. 66629, Parque de Investigación e Innovación Tecnológica, Apodaca, Nuevo León, México.
[2]Centro de Investigación en Química Aplicada, Blvd. Enrique Reyna Hermosillo No.140 C.P. 25294 Saltillo, Coahuila México

*mayeli.estrada@ciqa.edu.mx

Nanotechnology is applied with remarkable success in the development of fibrous matrices; being a need the study and development of new materials that give optimal results with high yields. Thanks to this, the electrospinning technique has been considered a novel process due to its simplicity and profitability to manufacture nanofibers polymers being of great importance for the industry and the academy [1]. Therefore, in this study, nanofibers were fabricated using a mixture of polyvinyl alcohol (PVA) with dextrin by the electrospinning technique from an aqueous solution PVA/Dextrin with a ratio of 90:10, 80:20, 70:30, 50:50. The solutions were prepared by dissolving PVA in 100 ml of deionized water by magnetic stirrer until its dissolution to subsequently Dextrin addition. All solutions were prepared at 10% of the total mixture (w/v). According to the literature for the electrospinning process the solutions were supplied at a temperature of 25 ° C with relative humidity 30% and programmed flow rate at 0.5 mL/h with a voltage of 21kV. To collect the nanofibers, aluminum was used on a cylindrical collector with a horizontal distance of 15 cm from the tip of the needle [2,3]. The nanofibers obtained were characterized by means of scanning electron microscopy (SEM), FTIR spectroscopy and thermogravimetric analysis (TGA). Additionally, PVA-Dextrin electrospun nanofibers were crosslinked using succinic acid as crosslinking agent and UV-254nm as initiator. The fibers solubility was tested in pure water and in simulated body fluid (SBF).

Key Words: Electrospinning, PVA, Dextrin, SBF.

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Gold nanoparticles synthesized by Zornia thymifolia plant extract

X. Delgado Martínez[1*], G. A. Rosas Trejo[2]

[1,2]Instituto de Investigación en Metalurgia y Materiales, edificio U., UMSNH, Avenida Francisco J. Múgica S/N Ciudad Universitaria, C.P. 58000, Morelia, Michoacán, México.

*xitla.203.dm@gmail.com

Nanoparticles have gained considerable attention in recent years due to their technological importance. Gold has shown a particularly promising behavior or when it is on a nanometer scale (1-100 nm), becoming extremely reactive [1], due to which gold nanoparticles are the most important due to their use in various biomedical, catalytic, electronic applications, optical and biological [2-3].

In this work, the synthesis of gold nanoparticles was carried out using ecological biosynthesis employing tetrachloroauric acid (HAuCl4) as a precursor salt, and Zornia thymifolia extract as a reducing and stabilizing agent. The volumetric ratio of extract and salt (1:1-1:8, 2:1-8:1), the concentration of the extract (0.01-0.1 g / ml), the concentration of the salt (6, 8, 10, 12 and 14 mM) and the influence of magnetic stirring were varied (2-10 str). The nanoparticles were characterized by UV-vis, scanning electron microscopy (SEM), X-ray diffraction (XRD) and Fourier Transform Infrared Spectrometry (FTIR).

The results accepted the formation of spherical, stable and dispersed Au NPS as the reducing and stabilizing agents of the extract. XRD confirmed the crystalline nature (fcc) of the gold nanoparticles. The influence of the concentration of the extract concerning the number of nanoparticles was noted, being higher when increasing the concentration of the extract, but obtaining a most homogenous size distribution. The high stability of the nanoparticles was observed, since the solution was analyzed in MEB after 4 and eight months after the reaction, finding the same morphologies from the first time it was examined.

Key Words: Ecological synthesis, nanoparticles gold, characterization.

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Design and Fabrication of Bio-Nanosensors featuring Hybrid Structures NEMS-MOS

M. A. García-Ramírez[1*], M. A. Bello-Jiménez[2], R. E. López-Estopier[3], J. T. Guillén-Bonilla[1], M. E. Macías-Rodríguez[1]

[1]Universidad de Guadalajara, Centro Universitario de Ciencias Exactas e Ingenierías (CUCEI), Blvd. Marcelino García Barragán 1421, C.P. 44430, Guadalajara, Jalisco, México
[2]Instituto de Investigación en Comunicación Óptica (IICO), Universidad Autónoma de San Luis Potosí, Av. Karakorum No. 1470 Lomas 4a Secc., 78210, San Luis Potosí, México
[3]Consejo Nacional de Ciencia y Tecnología (CONACYT), Av. Insurgentes Sur No. 1582, Col. Crédito Constructor, Del. Benito Juárez, México, D.F. 039040, México

*seario@gmail.com.

We present a hybrid structure for bio-sensing applications that features the co-integration of nano-electromechanical systems with the well-known metal-oxide-semiconductor technology[1-4]. The structure proposed features a MOSFET as a readout element, a doubly-clamped beam that is isolated from the substrate by a thin air-gap as well as by a tunnel oxide layer. The beam structure is functionalized by a thin layer of biomolecules that it is aiming to detect a particular set of enzymes, toxins or biogenic amines. In here, a three-dimensional finite element analysis is performed in order to study the behavior of the doubly-clamped functionalized beam. Preliminary results for the fabrication and characterization processes show good agreement between the simulated and measured characteristics.

Key Words: Hybrid Structures, NEMS, Biosensors, Electro-Optic Devices

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Non-enzymatic electrochemical sensor based on Amine funcionalizated Graphene sheets

Salvador Fernández, Alfonso Mercado, Uriel Sierra, Edgar Cuara, Alonso Cortes

National Laboratory of Graphene Materials, Reseacrh Center in Applied Chemistry Enrique Reyna Hermosillo 140, P.O. 25294, Saltillo, México.

lab_grafeno@ciqa.edu.mx

According to the world health organization, the number of adults with Diabetes has quadrupled in the past 25 years making it a major cause of death and disability. Currently it is estimated that diabetes causes over 1.6 million deaths yearly worldwide1. Therefore, monitoring blood glucose concentration is essential for the management of the disease. During the last 50 years several continuous monitoring technologies has been significantly improved in order to maintain glucose concentration on check2,3. However, there is still some challenges to overcome in order to obtain an accurate and reliable glucose monitoring device, most of them are related to the sensor materials themselves. Due to its intrinsic properties, Graphene composites surges as an attractive alternative to produce Non-enzymatic sensor material for the determination of glucose without the need of an enzymatic mediator 4,5. The aim of this work was dedicated to develop an economic alternative to produce a fast, highly sensitive non-enzymatic glucose sensor via amine functionalization of Graphene sheets under the hydrogen peroxide RedOx approach.

X-Ray Diffraction, Raman Spectroscopy, Sweep Electron Microscopy, Transmission Electron Microscopy were used to characterize physicochemically the obtained material. Electrochemical analyses were performed in a corrosion cell using a 1M Ag/AgCl and Platinum Mesh as reference and counter electrode respectably. Working electrodes were fixed using the sample in a 2:1 mixture with Poly(vinylidene fluoride) powder from Aldrich. Electrolyte was composed by a dissolution 0.1M of Phosphate Buffer Solution fixed with Potassium monobasic Phosphate and Potassium bibasic phosphate also from Sigma Aldrich. All reagents were used as arrived. All solutions were prepared with ultra-pure water (18.2 Mohms cm).

The obtained materials present sheets like appearance with apparent high porosity and active area. Physicochemical analysis suggest that the graphene material was effectively funcionalizated with the corresponding amine. Results also shows that the obtained material is not composed entirely by single graphene sheets but rather multi layered lattice, the electrochemical activity of the amine funcionalizated graphene allows the quantification of hydrogen peroxide contained in blood simulated medias. This behavior can be further exploited to generate electrode material in the determination of glucose levels in the human body.

Key Words: Graphene, amine.

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Carbon nanospheres for electrochemical detection of heavy metals in water

Svetlana Kashina[1*], Araceli Jacobo Azuara[1], Marco Balleza[2], Maria del Rosario Galindo Gonzalez[3]

[1]Department of chemistry, Natural and Exact Sciences Division, University of Guanajuato. Noria Alta S/N; C.P. 36050; Guanajuato, Gto., México
[2]Department of physics engineering, Sciences and Engineering Division, University of Guanajuato. Loma del Bosque 103, Lomas del Campestre CP 37150. León, Gto., México.
[3]CONACyT cathedra, Natural and Exact Sciences Division, University of Guanajuato. Noria Alta S/N; C.P. 36050; Guanajuato, Gto., México

*ersinia@msn.com

Carbon materials is a large area of investigation due to unique properties of these materials and it is known that nanometric size results in different properties. On the other hand, heavy metals contamination is another research challenge, so new materials for their detection should be developed. Some nanometric forms of carbon were used successfully in electrochemical systems for metal detection with low detection limits [1]. A relatively new nanometric form of carbon – nanosphere – have been investigated extensively but its use in electrochemical detection systems was not assessed. So, the main objective of this study was to synthetize carbon nanospheres and apply them in electrochemical systems. Three carbon materials (SG-1, SG-2 and SG-3) were synthetized using sol-gel process described [2] varying temperature and time of synthesis. SEM images showed that particles of these materials are spherical and have a size of 700 nm, approx. FTIR spectra did not present any peak of functional group. BET surface area was estimated as 400-480 m^2/g for three materials.

Electrochemical characterization was performed in standard three electrode electrochemical cell. Cyclic voltamperogramm obtained for all three materials did not evidenced presence nor anodic nor cathodic peaks. Simultaneous detection of heavy metals (Cu and Pb) was performed using anodic striping voltammetry [1]. Detection limits for Cu was 1.01, 0.1 and 0.02 ppm for SG-1, SG-2 and SG-3, respectively, that is lower than limits established for drinking water. Detection limits for Pb was 0.52, 0.09 and 0.02 ppm for SG-1, SG-2 and SG-3, respectively. As a conclusion, all three carbonaceous materials can be utilized as working electrode material in systems for electrochemical detection of heavy metals in water.

Key Words: Carbon nanospheres, sol-gel process, heavy metals, electrochemical detection.

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Effect of the synthesis method in the obtaining of a polymeric nanored based on chitosan and pectin for the treatment of parkinson's disease

Villavicencio-Carvajal C.G.[1], Valverde-Aguilar M.G.[1], Vergara-Aragón P[2], Quiroz-Reyes C. N.[1]

[1]Cicata-Legaria, Instituto Politécnico Nacional, Legaria 694, Col. Irrigación. Del. Miguel Hidalgo. C.P. 11500, México D.F.
[2]Physiology Department, Faculty of Medicine, Universidad Nacional Autónoma de México. CDMX, México, C.P. 04510.

*azuranano@gmail.com.

Parkinson's disease (PD) is a chronic and progressive disorder that affects the central nervous system (CNS), causing the death of dopamine-producing cells, located in substantia nigra pars compacta (SNpc). Dopamine (DA) is a neurotransmitter that participates in the control of movement and since there is a deficit of DA the signal of how and when to move will be transmitted in a wrong way [1]. Among the current therapies are pharmacological, deep brain stimulation and cell replacement therapies, but none has managed to cure the disease, prevent its progression or have any proven neuroprotective effect. An ideal treatment would be to deliver the DA directly into the striatum gradually, as well as a neuroprotective, such as Curcumin (Cur), a poly-phenolic compound isolated from the Curcuma Longa plant that has antioxidant properties and is being investigated for treat various neurodegenerative diseases, such as Alzheimer's and PD [2]. However, both the Cur and the DA not cross the blood-brain barrier (BBB) and are susceptible to light, pH and temperature. In the present project, the effect of the synthesis on the formation of a polymeric nano-network, self-destructive and regulated by electrostatic charges, capable of releasing dopamine / curcumin by diffusion, was evaluated to be administered intranasally in a rat model with hemiparkinsonism.

Key Words: Parkinson's disease; chitosan, pectin, curcumin; dopamine; nano-network.

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THURSDAY

Advances in visible light driven photocatalysis of Non-biodegradable pollutants

C. A. Huerta-Aguilar[1,2*], J. Narayanan[1], P. Thangarasu[2]

[1]*Division of Nanotechnology, Universidad Politécnica del Valle de México, Tultitlán, Estado de Mexico, C. P. 54910, México.*
[2]*Faculty of Chemistry, Universidad Nacional Autónoma de Mexico, Coyoacán, CDMX, C. P. 04510, México.*

caha_09@comunidad.unam.mx

The application of different materials as catalysts for achieving non spontaneous reactions has increased significantly. Ranging from organic synthesis to pollutant degradation, scientists are looking for inexpensive and efficient processes such as the utilization of nano-engineered semiconductors and sun irradiation as light source. However, visible light photocatalysis still have drawbacks due to exciton (e- /h+) recombination, low Reactive Oxygen Species (ROS) production and recovery processes for catalyst reutilization. With these concerns in mind, our research group has been exploring the degradation of numerous non-biodegradable pollutants by multiple photocatalysts having as main goal the development of new materials that can be activated under sunlight irradiation: core-shells ($ZnO@TiO_2$ and $Fe_3O_4@TiO_2$), composites (ZnO/TiO_2), magnetically recoverable particles (MFe_2O_4, M=Fe, Co, Zn, Ru and Ce), surface deposition of transition metals (TiO_2- M, ZnO-M and Fe_3O_4-M; M=Ni, Cu, Ag, Au) and transition metal complexes ($[M^{3+}8HQ]$, M=Fe, Co, Cr). The photocatalytic studies include UV-Vis, photocatalytic activity, removal efficiency, reaction rates and byproduct formation. Moreover, the arise of computational chemistry has open new possibilities where a reaction mechanisms is proposed based on product analysis and then its feasibility is proven via thermodynamical DFT calculations. A review on recent advances in environmental photocatalysis, its applications, limitations and new possibilities based in developing technologies and informatics.

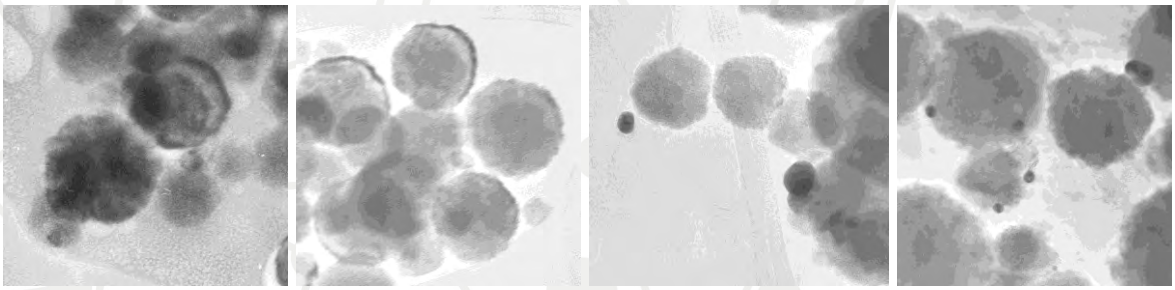

Figure 1. TEM images of doped magnetite materials a) Fe_3O_4-Ni doped nanoparticles; b) Fe_3O_4-Cu doped nanoparticles; Fe_3O_4-Ag doped nanoparticles and d) Fe_3O_4-Au doped nanoparticles.

Key Words: visible light photo catalysts, Density Functional Theory, pollutant degradation, reaction mechanisms.

Up-conversion nanomaterials for photo-induced therapies

Ramírez-García GONZALO[1]*, López-Luke TZARARA[1], De la Rosa-Cruz ELDER[1]

[1]Centro de Investigaciones en Óptica, Nanophotonics and Advanced Materials Lab., C.P. 37150, León, Guanajuato, México.

gonzalo.ramirez@cio.mx

A set of novel up-conversion nanohybrids with effective properties for simultaneous imaging and photo-induced therapies is introduced. The 975 nm laser irradiation absorbed by the up-conversion nanomaterials (UCNPs) can be converted to emissions at different wavelengths according to the dopant's nature and concentrations. That light could be specifically modulated to transfer energy towards the elements decorating their surface, activating a therapeutic mechanism. In this context, some conjugated UCNPs have been developed in our lab: i) UCNPs covalently linked to a zinc phthalocyanine for deep penetration photodynamic therapy [1], ii) UCNPs/metallic oxides core/shell nanoparticles for photodynamic therapy, and iii) gold-decorated UCNPs for photothermal therapy. The design and synthesis of these nanomaterials was described and accompanied with the corresponding systematic physicochemical and optical characterization. The selectivity of the nanohybrids was achieved by conjugation with specific monoclonal antibodies, and their specific interactions with breast cancer cell structures was verified by confocal microscopy. The pharmaceutical activity and mechanisms (free radicals production and heat generation) were then evaluated by standard and complementary methods, and finally their effects on culture cells evaluated. The tracking and therapeutic doses were determined, finding practically inert nanoconjugate concentrations in absence of infrared light exposure, but activating cell death by irradiation with 975 nm light for short periods of time. These novel nanohybrids have a great potential as individual or complementary agents for breast cancer diagnosis and treatment.

Key Words: Up-conversion nanoparticles, photodynamic therapy, photothermal therapy, breast cancer.

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Green Synthesis of bimetallic nanoparticles silver-gold, using the extract of the hamelia patents plant

K. Chávez[1], G.Rosas[1].

[1]*Instituto de investigaciones en metalurgia y materiales. Universidad Michoacana de San Nicolás de Hidalgo, Avenida Francisco J. Múgica s/n, Ciudad Universitaria, C. P. 58030. Morelia, México*

ingquimica269@hotmail.com

The nanoparticles (Nps) of noble metals present great interest due to their properties and as a consequence of their wide variety of applications in which they are actively used. In the nanometric scale, the properties of nanoparticles improve with respect to their micrometric counterparts, which is why they have become essential for their study in biosensors, electrocatalysis, and optical applications. The nanostructures can be configured in different ways, highlighting those of the core-shell type.

The conventional methods of synthesis for the obtaining of nanoparticles, use chemical reagents that cause harmful residues to the environment, for that reason the biosynthesis is used, which uses reagents of natural origin, like the extracts of the plants to reduce and stabilize the Nps. Consequently, the byproducts are friendly to the environment.

In this work we present the study on the biosynthesis and characterization of bimetallic Nps of Ag core-Au shell, using the extract of the Hamelia Patens plant. To achieve this objective, the strategy consisted of synthesizing Ag seeds and later growing the gold Nps taking advantage of a heterogeneous nucleation. NPs were structurally characterized by UV–vis spectrometry, X-Ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The infrared spectroscopy (FTIR) technique was also used to determine the chemical groups of the plant extract involves in the bioreduction. SEM analysis showed spherical particles with aggregation but studies as a function of reaction time indicate that the Hamelia Patens plant has inadequate quantities of stabilization agents. TEM observations show that the sizes of the bimetallic nanoparticles varied in 15 to 50 nm with an average size of 32 nm. FTIR spectroscopy confirmed the presence of phenolic compounds as the reductant agent of the NPs.

Key Words: Green synthesis; Gold- Silver; Nanoparticles.

Single photon emitters in hexagonal boron nitride at room temperature

Osvaldo DEL POZO-ZAMUDIO[1]*, Francisco J. ROCHA-CARDENAS[1], David ARIZA-FLORES[1], Raúl E. BALDERAS-NAVARRO[1], Edgar A. CERDA-MENDEZ[1]

[1]*Instituto de Investigación en Comunicación Óptica, Universidad Autónoma de San Luis Potosí, Av. Karakorum 1470 Lomas 4a. 78210 San Luis Potosí, S.L.P., México*

*odelpozo@cactus.iico.uaslp.mx

Single-photon emitters (SPEs) have gained attention due to their application in quantum technologies, such as quantum computation and communication. Solid-state SPEs are promising due to their high stability and scalability in addition to the excellent optical properties. Recently, the layered semiconductors WSe_2 and WS_2 have been shown to host SPEs [1,2,3] at low temperature. Hexagonal boron nitride (hBN), a layered van der Waals material, exhibits bright and narrowband single-photon emission at room temperature in a range from 570 to 700 nm [4]. These emitters emerge from defects or vacancies in the hexagonal lattice (fig. 1a) similar to color centers in diamond. Typical photoluminiscence (PL) spectra show a narrow zero phonon line (ZPL) and a phonon side band well separated from each other (fig. 1b). Further investigation of SPEs in hBN is currently focusing on the implementation to photonic devices like optical microcavities to study light-matter interaction by coupling the emitter to the photonic mode. These experiments open interesting possibilities for cavity-enhanced SPEs in a layered material for a wide range of applications in nanophotonics and quantum information technologies.

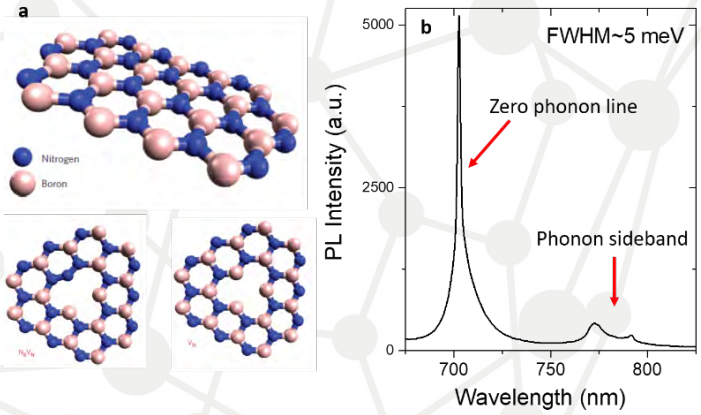

Figure (a) Crystal structure of hBN and two different types of defects on the lattice (Taken from ref. [4]). (b) Typical photoluminescence spectrum of a single-photon emitter in hBN.

Key Words: 2D materials, nanophotonics, quantum optics

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Polymers and small molecules for large area electronics

J.A. Ávila-Niño

[1]*CONACYT – Centro de Investigación y Desarrollo en Electroquímica, Parque Tecnológico Querétaro s/n, Pedro Escobedo, Querétaro, México.*

javila@cideteq.mx

Recent progress in large area electronics has been made in order to economize the manufacturing process of the electronic components. The use of organic small molecules and polymers has led to the fabrication of flexible and very low cost electronic devices with the advantage of a facile and low temperature manufacturing processes [1]. The flexibility of the organic films has led to fabricate electronic circuits onto flexible substrates like PET, paper and clothes, so those devices can be used as wearable circuits. One of the most important devise in order to fabricate more complex logic circuits is the transistors. In this work, results of all-evaporated organic thin film transistors (OFETs) [2] are discussed and also their advantages and disadvantaged in comparison with the inkjet-printed OFETs. Furthermore, organic electrochemical transistors (OECTs) [3] are also discussed. The OECTs has been used as chemical and biological sensors with perspectives to be used as “Point Of Care” applications due to their flexibility and their low cost of manufacture.

Key Words: Polymers, small molecules, flexible electronics

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Matter-wave packets diffracted by stationary electromagnetic waves, a numerical treatment

Alejandro Castellanos-Jaramillo[1*], A. Castellanos[1] , Ramirez-Rodriguez L.P.[1]

[1]*Universidad de Sonora, Blvd. Luis Encinas J. & Calle Av. Rosales, Centro, C.P. 83000, Hermosillo, Sonora, México*

*alejandrocastellanosjaramillo@gmail.com

It is well known that X rays are diffracted by periodic arrays of atoms, but few people know that massive particles can be diffracted by light, provided that a periodic behavior of the electromagnetic fields are available. This phenomena was proposed theoretically by P. Kapitza and P. Dirac in 1933, but it was observed for electrons until 2001. The aim of this work is to deal with this effect by using a numerical method that simplifies its study and makes it available for students taking a course in quantum mechanics. The system under consideration is a spinless particle with mass m that crosses a laser of nanometric width. The theoretical description is based in a wave packet that evolves according to the time-dependent Schrödinger equation and crosses a region of standing waves represented by a ponderomotive potential. The solution is found using the finite differences time domain method (FDTD) working in a rectangular box of large enough dimensions that the phenomenon of interest is not impacted by the physical boundaries. The diffraction can be observed as it happens and the interference patterns produced in the configuration and momentum spaces can be registered. A movie can be obtained if the student wants.

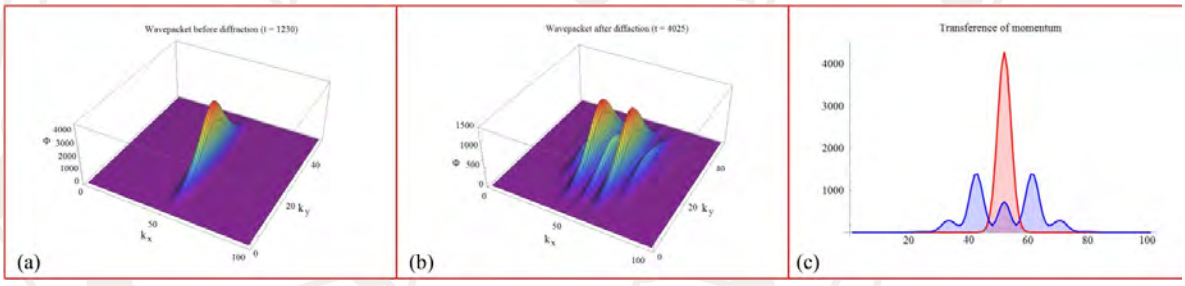

Figure - Description in the momentum space. The absolute value of the Fourier transform is presented for two times: before and after the diffraction. (a) Momentum in Kx is a sharp peak. (b) The diffracted wave packet has a momentum shift in Kx with several peaks.

Key Words: Matter-wave diffraction, Momentum shift, Time domain simulation, computer simulation.

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POSTERS SESSION

MONDAY

Synthesis and characterization of gold and palladium nanoparticles loaded on Lithium disilicate nanostructures

Jáuregui-Gómez Daniel[1*], Bárcena-Soto Maximiliano[1], Gutiérrez-Becerra Alberto[2]

[1]*Chemistry Department, University of Guadalajara.*
[2]*Engineering Department, University of Guadalajara. Av. Nuevo Periférico Oriente 555, C.P. 45425, Tonalá, Jalisco, México.*

ing.danieljauregui25@gmail.com

Nowadays there is an increasing number of studies focused on the application of metallic nanoparticles in different scientific fields e.g. biotechnology, catalysis, energy storage, advanced materials, etc. In the catalysis field, many attempts have been made to achieve the "perfect" catalyst that combines metallic nanoparticles with very low size and irregular shapes and a support that serves as vehicle for the nanoparticles. Nanoparticles of gold, platinum, palladium and rhodium have been used the most for this propose, due to their high catalytic properties in hydrogenation reactions and carbon monoxide conversion. On the other hand, the most employed supports are SiO_2, Al_2O_3, ZrO_2 and Fe_2O_3, however, there are many supports that have not been studied like lithium disilicate ($Li_2Si_2O_5$). Lithium disilicate is a glass-ceramic material that contains polycrystalline lithium disilicates immersed in a glass matrix [1]. The main advantage of using $Li_2Si_2O_5$ is that it grows up as nano-sized polycrystals which can be crushed by means of a planetary ball mill until reaching 100 nm nanorods. Different studies have shown that the method in which the nanoparticles are dispersed through the support determines the final catalytic effectiveness. Hence, in this work, we propose two methods to add the nanoparticles to the $Li_2Si_2O_5$ nanorods. First, we proposed a methodology using "gold ruby glass" method to add the nanoparticles directly inside the glassy matrix by thermal decomposition at 1300°C achieving gold and palladium nanoparticles and with low size and narrow size distribution [2]. On the other hand, the second methodology consists in the impregnation of chloride auric and palladium salts on the Li2Si2O5 nanorods followed by a colloidal borohydride/ citrate reduction [3]. The nano-catalyst was characterized by means of X-ray diffraction and transmission/scanning electron microscopy. Furthermore, the catalytic activity was measured indirectly by the hydrogenation of 4-nitrophenol with sodium borohydride by means of UV-vis spectroscopy.

Key Words: Gold nanoparticles; Palladium nanoparticles; Glass; Catalysis.

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Self-assembled supramolecular nanostructures of TDAP-TCPP on Au(111)

E. Sánchez-Muñoz, R. Aguilar-Sánchez, J.L. Gárate-Morales, J. M. Hernández-Pérez

Facultad de Ciencias Químicas, Benemérita Universidad Autónoma de Puebla. 22 Suy y Av San Claudio, C.U. San Manuel. 72570. Puebla, México

ras747698@gmail.com

Facile electron transfer and photon connectivity are crucial factors to increase efficiency in molecular devices and new materials that mimic photosynthesis. Self-aggregation of porphyrinic systems plays a key role to mediate light harvesting and charge transfer processes. The high degree of order within supramolecular nanostructures may provide a basis to relate structural characteristics to electron and energy transport and to photon capture. Supramolecular nanostructures of porphyrins can be constructed from different chemical environments that allow a better control of their chemical and physical properties. Non-covalent interactions (hydrogen bond, ligand-metal interactions, and electrostatic interactions [1]) permit a wide variety of structures of a host-guest type system through self-recognizing that can be performed in solution. In this work we use molecular self-assembly processes to form supramolecular nanostructures based on tetra (4-carboxyphenyl) meso porphyrin (TCPP) and tetra (4-dimethyl amino phenyl) meso porphyrin (TDAP) building blocks. The formation of the supramolecular nanostructure was followed by UV-vis spectroscopy and electrochemical techniques and the structure was explored by scanning probe microscopies. It was demonstrated that porphyrin has a strong interaction with the substrate and can form ordered adlayers parallel to the Au (111) surface in electrochemical environment.

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Synthesis of $CoAl_2O_4$ nanoparticles by an ultrasound-assisted colloidal method and their structural and morphological characterization

Víctor Emmanuel Muñoz Moreno, Juan Pedro Mariscal Martinez, Erwin Said Guillen López, Marciano Sanchez Tizapa, Miriam Marcela Tostado Plascencia, Celia de la Mora Orozco, Juan Pablo Morán Lázaro*

[1] *CUValles, Universidad de Guadalajara, Carretera Guadalajara-Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México.*

juan.moran@profesores.valles.udg.mx

Cobalt aluminate ($CoAl_2O_4$) is a material commonly known as Thenard´s blue. Cobalt aluminate is an interesting material that due to its good physical and chemical properties has been used as a catalyst, sensor and as electrode for photo-electrochemical cells. In this work, $CoAl_2O_4$ nanoparticles were synthesized by a simple and efficient ultrasound-assisted colloidal method, using ethanol and dodecylamine as solvent and surfactant, respectively. Studies by X-ray diffraction showed that single-phase $CoAl_2O_4$ was obtained when a calcination temperature at 900 °C was used. The surface morphology of the $CoAl_2O_4$ powder was analyzed by scanning electron microscopy (SEM), and a porosity with pores of irregular shape was observed. A particle size distribution of 30-90 nm was measured from SEM images. Vibrational modes and absorption bands characteristic to $CoAl_2O_4$ were registered by Raman and UV-vis spectroscopy. These last characterizations verified the formation of the $CoAl_2O_4$ phase at a calcination temperature of 900 °C.

Key Words: Cobalt aluminate, nanoparticles, ultrasound

Structural conversion of gas-phase $Cu_{4-x}Pt_x$ (x = 0 - 4) clusters induced by the adsorption of CO_2

Luis E. GÁLVEZ-GONZÁLEZ[1]*, J. Octavio JUÁREZ-SÁNCHEZ[2], Rafael PACHECO-CONTRERAS[2], Ignacio L. GARZÓN[3], Lauro Oliver PAZ-BORBÓN[3], Alvaro POSADA-AMARILLAS[2]*

[1]Programa de Doctorado en Ciencias (Física), División de Ciencias Exactas y Naturales, Universidad de Sonora, Blvd. Luis Encinas & Rosales, 83000, Hermosillo, México
[2]Departamento de Investigación en Física, Universidad de Sonora, Blvd. Luis Encinas & Rosales, 83000 Hermosillo, Sonora, México
[3]Instituto de Física, Universidad Nacional Autónoma de México, Apdo. Postal 20-364, 01000 Cd. de México, México

*luis.galvez@correo.fisica.uson.mx

Transition and noble metal clusters have proven to be critical novel materials, potentially offering major advantages over conventional catalysts in a range of value-added catalytic processes such as carbon dioxide transformation to methanol. Motivated by this, we studied the adsorption of CO_2 on $Cu_{4-x}Pt_x$ (x = 0 - 4) metal tetramers using a Density Functional Theory scheme. We first performed a first-principles Basin-Hopping global optimization to find the ground-state and some low-lying isomers of the clusters. Then, we analyzed the adsorption process of the CO_2 molecules on the ground-state configurations of each cluster. For the Cu_3Pt_1 and Pt_4 clusters, we observed a structural conversion between the ground-state geometry and the corresponding first isomers upon adsorption of the CO_2 molecule. To explain this behavior, we calculated the energy difference and the transition state energy barrier between the ground-state and the respective first isomer structures, for all clusters. Compared to the clusters that did not exhibit conversion, both the energy barrier and the energy difference were rather small in the cases that underwent structural conversion.

Key Words: Nanocatalysis, CO_2 adsorption, Fluxionality, DFT

Magnetic interaction on multilayer nanowires

María Fernanda Ruiz Villegas*, Juan Manuel Martínez Huerta, Armando Encinas

División de Materiales Avanzados, Instituto Potosino de Investigación Científica y Tecnología, Camino a La Presa de San José 2055, 78216 San Luis Potosí, S.L.P, México.

*maria.ruiz@ipicyt.edu.mx

In the past years the interest in understanding the behavior of magnetic nanoparticle assemblies has been increasing. Among these systems, magnetic multilayer nanowires have received considerable attention due to their possible applications in information storage, as electrical and biological sensors, as well as for spintronic devices. These type of systems are complex since their magnetic properties depend on the competition between the shape anisotropy of the magnetic segments and the intra and inter wire dipolar interactions (figure 1a). That's why most of the studies that exist on the subject have focused only on studying the intra-wire interaction while neglecting the dipolar interaction between nanowires [1]. There are a few studies that consider the both interactions [2,3] but these calculations are restricted to particular cases or require large computational resources. In the present work we propose a simple analytical model for multilayer nanowires, which incorporates the combined effects of the shape anisotropy and both intra and inter wire dipolar interactions. A systematic study has been done considering the geometric parameters of the system only such as the height of the wires, the thickness of the magnetic layer and the non-magnetic layer, the center-to-center distance of the wires, as well as the diameter of the wires (figure 1b). The results obtained show a overall agreement with a large number of published experimental studies and with the predictions of previously reported models under the same limiting conditions.

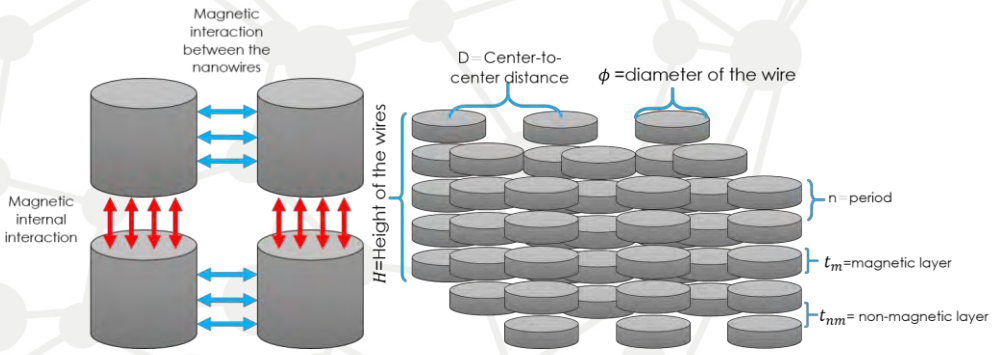

Figure 1a Present interactions on the systems **1b** Geometrical parameters used for the model.

Key Words: Multilayer nanowires, intrawire dipolar interactions, inter dipolar interactions.

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Determination of the interaction field distribution and the intrinsic switching field distribution in nanowire networks using minor loops and forces

K. Hintze-Maldonado[1*], J. M. Martínez-Huerta[1], L. Piraux[2] and A. Encinas[1]

[1]División de Materiales Avanzados, Instituto Potosino de Investigación Científica y Tecnología, Camino a La Presa de San José 2055, 78216 San Luis Potosí, S.L.P, México.
[2]Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Place Croix du Sud 1, B-1348, Louvain-la-Neuve, Belgium

*kevin.hintze@ipicyt.edu.mx

In this work we propose and validate a method to determine the interaction field and the intrinsic switching field distribution in assemblies of particles between which there is a magnetic dipolar interaction using minor magnetization loops or first order reversal curves (FORCs). Experimentally, NiFe magnetic nanowire networks with diameters of 18.29 nm in diameter, average heights of 18 micrometers and with volume fractions of 4.5, 5 and 11.4% were used to vary the intensity of the interaction field. The magnetometry measurements were made using an alternating gradient magnetometer with the field applied parallel to the axis of the nanowires and all measurements were made at room temperature. The method allows to measure the interaction field and intrinsic switching field distribution for minor loops and FORCs, from the differences between the remanences of the demagnetization loop and magnetization loops of the minor loops or FORCs. So that measuring a greater number of minor loops or FORCs allows obtaining the interaction field and the intrinsic switching field distribution for the same number of points on the hysteresis cycle. The results obtained by this method are consistent with the average value of the interaction field obtained from the remanence curves IRM and DCD and with the value obtained from the mean field model for nanowire networks.

Key Words: Minor loops, switching field distribution, dipolar interactions.

Demagnetizing effects in non-continuos magnetic media

Elia Oliva Moreno*, A. Encinas

División de Materiales Avanzados, Instituto Potosino de Investigación Científica y Tecnológica, Camino a la Presa San José 2055, Lomas 4ta sección,78216 San Luis Potosí SLP, México

*elia.oliva@ipicyt.edu.mx

In this work a study of the demagnetizing field and the magnetic anisotropy in non-continuous magnetic materials is presented. The aim of the study is to understand the effect of discontinuities, pores and non-magnetic inclusions in the bulk of a soft magnetic material, both in the demagnetizing field as well as in its magnetic anisotropy. Nickel, cobalt and iron materials with interconnected pores have been considered whose characteristic dimensions vary significantly in scale. In particular, commercial sponges with pores of average diameter of hundreds of micrometers, thin films deposited by electrochemistry in commercial membranes with pores of characteristic diameter of hundreds of nanometers as well as packed spheres have been magnetically characterized. The results are analyzed from a medium field model that considers the distribution of magnetic charges generated inside the bulk of the material at the pore boundary. The model allows to make a correlation between the perpendicular susceptibility to the plane and the effective magnetic anisotropy with the porosity of the material and the average geometry of the pores.

Fabrication and magneto-structural characterization of magnetic wood composites

Carlos Eduardo Niño González[1*], Armando Encinas[2]

[1]Facultad de Ciencias, Universidad Autónoma de San Luis Potosí, Zona Universitaria, Av Manuel Nava, 78290 San Luis, S.L.P., México
[2]Instituto Potosino de Investigación Científica y Tecnológica A.C., Camino a La Presa de San José 2055, Lomas 4 sección, 78216 San Luis, S.L.P., México

*peyroxvsreaper@hotmail.com

Wood is a natural renewable and highly abundant natural resource. Moreover, it possesses a highly anisotropic hierarchical structure which is part is responsible for its outstanding mechanical properties and it posses no environmental threats. Its structure consists in long, well oriented parallel cavities. In this work we have performed the infiltration of these cavities with ferric and ferrous chloride in order to co-precipitate magnetic nanoparticles and thus obtain magnetic responsive wood. The experiments were successfully performed in wood sticks, tooth picks, slabs and sawdust. In all cases, scanning electron microscopy, X-ray diffraction and Infrared spectroscopy confirm the presence of magnetic nanoparticles embedded in the wooden support. Magnetic hysteresis loops performed at room temperature further confirm the superparamagnetic nature of the magnetic wood.

Key Words: Wood, magnetic nanoparticles, superparamagnetic composite.

Hydrogen Storage on Volleyballene

Alfredo Tlahuice-Flores*

Universidad Autónoma de Nuevo León, CICFIM-Facultad de Ciencias Físico-Matemáticas, San Nicolás de los Garza, NL 66455, México.

*tlahuicef@gmail.com

This study is devoted to the hydrogenation of the volleyballene ($Sc_{20}C_{60}$) compound [1]. It is determined that up to 70 H atoms can be adsorbed on the volleyballene structure, and its hydrogenated structure ($Sc_{20}C_{60}H_{70}$) holds a 1.1 eV HOMO-LUMO gap value. The new structure is comprised by scandium atoms forming part of the framework, which avoid their clustering and enhance the H2 uptake. Worthy of note is a calculated H_2 uptake capacity of 4.20 wt %, with a calculated -0.11 eV/H2 adsorption energy value. Moreover, calculated thermodynamic properties as enthalpy (negative sign) and entropy (positive sign) assure that the hydrogenation reaction of volleyballene can be obtained at ambient temperature. The calculated IR and Raman spectra do not feature imaginary frequencies attesting the experimental convenience of the predicted $Sc_{20}C_{60}H_{70}$ cluster

Key Words: Hydrogen storage, DFT, Volleyballene, Raman.

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Photoluminescence and Raman study of GaN and $Al_xGa_{1-x}N$ films

L.A. Martínez Ara[1*], P. Maldonado Altamirano[2], J. R. Aguilar Hernández[1], M. A. Hernández Pérez[3], G. S. Contreras Puente[1]

[1]ESFM-IPN Edificio No. 9 U. P. A. L. M. Lindavista C. P. 07738, Ciudad de México.
[2]Doctorado en Nanociencias y Nanotecnología, CINVESTAV-IPN, San Pedro Zacatenco, C. P. 07360, Ciudad de México.
[3]ESIQIE-IPN Edificio No. 7 U. P. A. L. M. Lindavista C. P. 07738, Ciudad de México.

*mtzara1984@gmail.com

Gallium Nitride (GaN) and AlxGa$_{1-x}$N films were deposited on three diferent susbtartes, silicon (111), sapphire (0001) and quartz, using Laser Ablation technique with a Nd:YAG pulsed laser. Photoluminescence (FL) signal was obtained at room temperature, the yellow band is observed at 2.3 eV, also another band around 3.0 eV associated with donor-acceptor pair transitions. As well a signal due to aluminum vacancies at 2.63 eV on $Al_xGa_{1-x}N$ films is presented. The FL spectra obtained at 10 K present emissions in the Ultra-violet region and there are presence of phonon coupling with vibrational frequency associated to the E_1 (TO) mode of gallium nitride. The Raman spectra show the A_1 (LO) mode of the GaN, the ternary films also have a peak at 773 cm^{-1}, these signal is associated to aluminium incorporation.

Key Words: Gallium Nitride, Photoluminescence, Raman

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Biological and nonlinear optical applications of silver nanoparticles fabricated by laser ablation protocols

Reynoso Héctor[1], Álvarez Jonathan[1], Ruvalcaba Juan M.[1], Martínez-Borquez Alejandro[1] Gutiérrez-Juárez Gerardo[1], Ramos-Ortiz Gabriel[2] and Castro-Beltrán Rigoberto[1]*

[1]División de Ciencias e Ingenierías, Universidad de Guanajuato Lomas del Bosque 103 Lomas del Campestre, León Guanajuato, México.
[2]Centro de Investigaciones en Óptica Lomas del Bosque 113 Lomas del Campestre, Leon Guanajuato, México.

*cbrigoberto@fisica.ugto.mx

Nowadays metallic nanoparticles (MNPs) has been synthesized and optically characterized by using several methods which determinate their shape, size and main optical properties. From all the standard methods to fabricate MNPs, laser ablation (LA) procedure permits direct fabrication, highly stable and homogeneously dispersed MNPs on different solvents. Three different laser exposure times were considering as protocol for comparison purposes through which, three concentrations allowed to obtain spherical particles from 5 nm to 20 nm of diameters. Silver NPs were optically characterized using UV-Vis, SEM, AFM, COMSOL Multiphysics simulation, digital image processing and Z-scan measurements. Z-scan open aperture configuration showed that at different peak intensities Silver MNPs switch from saturable absorption (SA) to reverse saturable absorption (RSA) presenting potential opportunities to optical limiting applications. In addition, MNPs were deposited on a silica surface to Surface Enhanced Raman Spectroscopy (SERS) applications. We were able to achieve SERS effect on rhodamineG6 (RG6) at 3 different concentrations: 10^{-3}, 10^{-4} and 10^{-6} M. From all these results we demonstrated that MNPs fabricated by LA protocols presented strong third-order nonlinear optical behavior and can be used in hybrid substrates to boost Raman signals of organic molecules.

Figures (Left) Results of SERS at different molar concentrations (center) 3D Topography of the hybrid substrate and (right) Z-scan open aperture configuration results.

Key Words: Laser Ablation, Nanoparticles, Z-Scan, SERS, COMSOL simulation.

Use of microwaves for the synthesis of nano and microparticles of silver with different morphologies

[1]Susana Elizabeth Rocha González*, [1]Esmeralda Dhamar Rayas Urdiano, [1]Erika Fabiola Hernández Elizarrarás, [2]Hugo Getzael Rodríguez Acosta, [2]Jose Maria Tapia Rivera, [4]Adalberto Zamudio Ojeda, [3]Ernesto David García Bustos

[1]Licenciatura en Ciencias de los Materiales, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México.
[2]Ingeniería de Nanotecnología, Centro Universitario de Tonalá, Tonalá, Jalisco, México.
[3]Cátedras Conacyt, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México. 4Departamento de Física, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México.

susana.E.R.G.20@hotmail.com

In the actuality the nanoscience is taking great relevance both for research in basic science and for the development of new technologies. In particular, the properties of silver nanoparticles, which are dependent on the size and shape of these, may have different technological applications [2]. So it is of great importance develop simple and economical methodologies for the synthesis of nano and microstructures with controlled morphologies. The method developed on this work consists of solutions of silver nitrate and sodium citrate, the latter being the reducing and stabilizing agent [1]. Usually the control of the morphologies is done by using templates, or by making the synthesis in prescence of presintetized particles. The novelty of this process is that it makes use of a conventional microwave and that depending on the power or reaction time, different morphologies (spherical, cubic, elongated) or sizes of nano and microparticles can be obtained. The nano and microparticles obtained were characterized by the following characterization techniques: UV-vis spectroscopy, Scanning electron microscopy (SEM) and Transmission Electron Microscopy (TEM).

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Influence of pH on silver nanoparticles synthesis using dextrose as a reducing agent

Daniel Araujo Avila[1], Natale Quetzali Martínez Gutérrez[1], Iyoy Sarahí Molina Rodríguez[1], Alexis Misael López Lara[1]

[1]Universidad de Guadalajara, Centro Universitario de Ciencias Exactas e Ingenierías, Departamento de Química
[2]Universidad de Guadalajara, Centro Universitario de Ciencias Exactas e Ingenierías, Departamento de Madera celulosa y papel
[3]Universidad de Guadalajara, Centro Universitario de Ciencias Exactas e Ingenierías, Departamento de Física. Blvd. Marcelino García Barragán No. 1421, Guadalajara, Jalisco, C.P.44430, México

Daniiiel_9508@hotmail.com

Nanoparticles have revolutionized the world, the ability to manipulate matter at a nanometric level allows us to generate nanoparticles with great potential for innovations and applications in different areas such as chemistry, medicine, textiles, food and energy to mention just a few. Therefore, the great importance of looking for cheap and simple methodologies to synthesize particles of different sizes or morphologies since the properties of these depend on the shape and size, the chemical synthesis methods in aqueous media allow to synthesize silver nanoparticles (AgNPs) in a simple and economical way. In this work the influence of pH on silver nanoparticles is studied, the reducing sugars present a free carbon in their structure and can reduce under certain conditions to metal salts, the synthesis method will be carried out by the "bottom-up" method. The physicochemical properties of silver nanoparticles will be characterized from visible ultraviolet spectrophotometry (UV-vis), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and dynamic light scattering (DLS).

Fabrication of flexible MOS devices using ZrO_2

S G Chávez-Veloz[1*], A G Rodríguez[2] and A Encinas[1]

[1]Instituto Potosino de Investigación Científica y Tecnológica (IPICYT) A.C., Camino a la Presa San José 2055, Lomas 4 sección, 78216 San Luis Potosí, S.L.P., México.
[2]Coordinación para la Innovación y la Aplicación de la Ciencia y la Tecnología (CIACyT) Universidad Autónoma de San Luis Potosí, Álvaro Obregón 64, 78000 San Luis Potosí, S.L.P., México.

*sara.chavez@ipicyt.edu.mx

The development of electronic devices, which are important due to their multiple applications, has been advancing over the years; the current objectives are to reduce their size and cost. Actually, a new need appears, which is to develop devices with the particularity that they are flexible and, therefore, functional for some applications that demand it, reducing their cost and increasing their performance. In this work, the fabrication and characterization of flexible MOS (metal-oxide-semiconductor) capacitors were carried out. ZrO_2 was used as oxide. Thin layers of this material were deposited by spin coating, by the sol-gel chemical route, on flexible metallic tapes of Ni-Mo-Cr alloy (Hastelloy C-276), which were used as substrates. A 0.1 M solution was prepared dissolving Cl_4Zr (Zirconium tetrachloride) in C_3H_8O (isopropanol) with stirring and bathed in iced water (10 °C) for 2 h and aged at 18 °C for 24 h. The semiconductor used was type p silicon and was grown by sputtering. The structural characterization for both samples (ZrO_2/hastelloy and Si-p/ZrO_2/hastelloy) was performed by x-ray diffraction and Raman spectroscopy. The capacitive behavior was verified by electrical measurements to determine the complex impedance of the devices as a function of frequency.

Key Words: Flexible MOS, ZrO_2, spin coating, sputtering.

The effect of water incorporated in the electrolyte solution on dye-sensitized solar cells

[1]Alfredo Romero Contreras*, [2]Julio Villanueva-Cab

[1,2]Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apdo. Postal J-48, Puebla, Pue. 72570, México.

*aromero@ifuap.buap.mx

A new cheap and easy way to get energy from the sun is through a photovoltaic cell, called Dye Sensitized Solar Cell (DSSC). These cells are made with an electrode (a semiconductor oxide thin layer sensitized to visible light with a monolayer of dye supported by an FTO-Glass), an electrolyte and a counter-electrode (a platinum deposition over FTO-Glass). Researches have been focused on the improvement of efficiency, trying to apply new and environmentally-friendly materials. One example is the substitution of organic solvents, present in the electrolyte, by water. The first study about water in DSSCs was made by S. Lindquist et. al [1]., they noticed efficiency decreased when the water concentration in the electrolyte increased. Brian O'Reagan et. al. [2] performed a similar experiment employing a hydrophobic dye and water vol. from 0 to 100% related to the electrolyte amount (3-methoxypropionitrile used as solvent) showing slightly change on cell efficiencies. By another side, Frank et. al. [3] performed experiments with 0 and 10 % of water and a Z907 dye using acetonitrile and valeronitrile as solvents, they noticed that the DSSCs efficiency was improved from 7% to 7.5 % when water was added. Now, there is not a quantitatively study elucidating the electrodynamic contribution in DSSCs when water is introduced on the electrolyte. In this work, we quantitatively study the effect of water on the performance of DSSCs through conventional optical and electronical characterization techniques for DSSCs with a hydrophobic dye (Z907) and an electrolyte (iodine/triiodide with acetonitrile and valeronitrile as solvents) with 0, 1, 2, 5, 10, 20 and 40 % of water content. This work highlights how the solvent plays an important role on the kinetics of device.

Key Words: Aqueous-DSSCs, electrodynamic, electrolyte, solvent.

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Green synthesis of silver nanoparticles using solar radiation and loeselia mexicana leaf extract

R. Herrero-Calvillo[1*], G. Rosas[1]

[1]*Instituto de Investigación en Metalurgia y Materiales, UMSNH, Av. Francisco J. Mújica S/N, C.P. 58030, Morelia Michoacán, Mexico.*

*roy619@gmail.com

This paper shows that is possible the bio-reduction of $AgNO_3$ using *Loeselia Mexicana* extract by sunlight activation. Photocatalytic action due to solar radiation was necessary for the silver nanoparticles production and stabilization, due to the low-efficiency antioxidant activity in the absence of sunlight. *Loeselia mexicana* leaf extract showed a low antioxidant capacity in the absence of sunlight. However, the reduction capacity considerably increased when exposed to solar radiation, obtaining silver nanoparticles in just 0.75 min. Some samples were obtained varying the time under a reported irradiance of 694 W/m^2 and analyzed by UV-Vis, scanning electron microscopy (SEM), transmission electron microscopy (TEM) and x-ray diffraction (DRX). The results obtained from the previous techniques show the formation of crystalline nanoparticles using an economic and sustainable synthesis technique. Silver nanoparticles with spheroidal morphology and another shape almost spherical are appreciated. It is also shown that the nanoparticles have a narrow size distribution with sizes from 13 to 23 nm. It is important to highlight the stabilizing capacity of the leaves extract, due to that the aggregates amount was minimal and no precipitation occurred after the synthesis. Solar exposure time has utmost importance because solar irradiation excess leads to the formation of tiny nanoparticles with bimodal distribution and submicron particles, outside the nanometric range.

Key Words: nanotechnology, silver nanoparticles, green synthesis, solar radiation.

Ab-initio calculations of structural and electronic properties of graphene quantum dots

A. Nascir Pérez M., I. G. Avendaño-García, Ma. Luisa Ojeda M., Celso Velásquez O. and Miguel Ojeda M.

[1]Universidad de Guadalajara, Centro de Investigación en Nanociencia y Nanotecnologías, CUVALLES Carretera Guadalajara-Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México

miguelojedama@gmail.com

Nowadays, the nanomaterials based on graphite as graphene, nanotubes, fullerenes or quantum dots have been attracted much attention due to the possible applications on medicine, electronics or sensors [1]. Graphene quantum dots, which are nanometer-sized fragments of graphene where the electronic transport are confined in the three spatial dimensions, are very attractive for the tunable modification of the band gap by the quantum confinement effect [2]. In this wok, we performed a theoretical study of structural and band gap modification on graphene quantum dots with the diameter dependence.

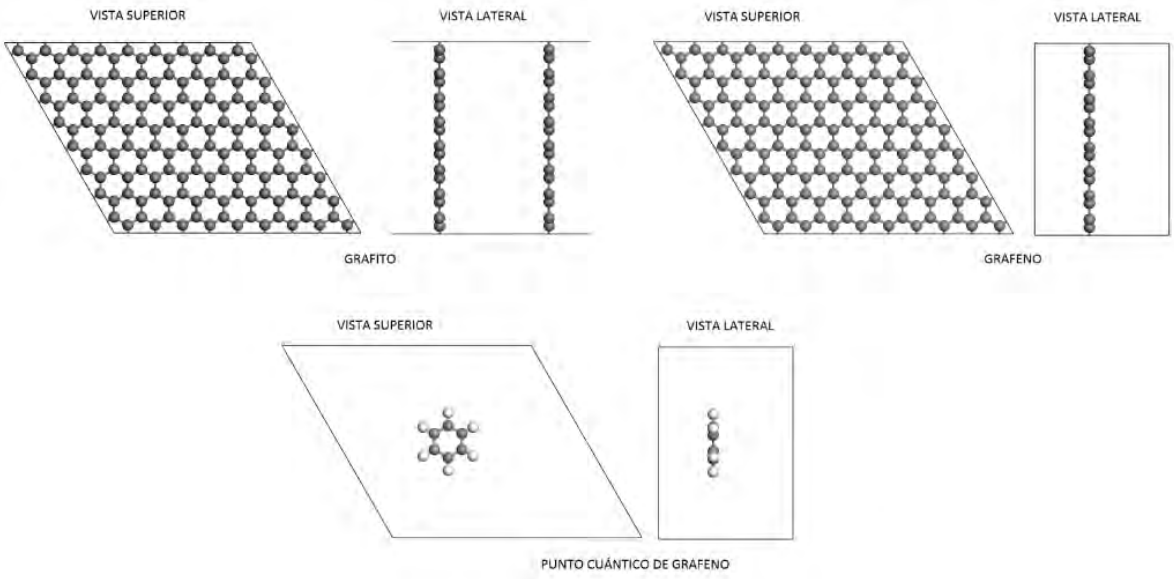

Figure 1 Schematic representation of graphite, graphene and graphene quantum dot.

Key Words: quantum dots, graphene, graphite, band gap.

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Cu-Ag nanoalloys using green synthesis

M. Cortez-Valadez[1], O. Rocha-Rocha[2], H. Arizpe-Chávez[2] and M. Flores-Acosta[2]

[1]CONACYT - Departamento de Investigación en Física, Universidad de Sonora. Apdo. Postal 5-88, 83190, Hermosillo, Son. México
[2]Departamento de Investigación en Física, Universidad de Sonora. Apdo. Postal 5-88, 83190, Hermosillo, Son. México
[3]Departamento de Física, Universidad de Sonora. Apdo. Postal 5-88, 83190, Hermosillo, Son. México

manuelcortez@live.com

Employing the Opuntia ficus-indica wild plant extract were obtained bimetallic Nanoparticles of Ag/Cu. Core-shell and Janus morphologies were found. Transmission Electronic Microscopy (TEM) showed a sample size of 15 and 25 nm for Core-shell and Janus nanoparticles, respectively. Uv/Vis spectroscopy shows two absorption bands located in 440 and 500 nm for Core-shell and Janus nanoparticles, respectively. These absorption bands are attributed to surface plasmon resonance in bimetallic nanoparticles of Ag/Cu. A Raman band centered approximately at 220 cm-1 after the formation of bimetallic nanoparticles was experimentally detected. Additionally, was used the density functional theory (DFT) to predict the vibrational modes in small low-energy clusters of (AgCu)n. The vibrational modes predicted in small clusters were correlated with the experimental Raman band detected in bimetallic nanoparticles.

Key Words: Bimetallic nanoparticles, Surface Plasmon Resonance, Vibrational properties.

ChargenQ, an easy toolkit to visualize charge density

M. de la Rosa-Escareño[1 *] and P. G Nieto-Delgado[2]

[1]Universidad Politécnica de San Luis Potosí (UPSLP), Urbano Villalón num.500, Col. La Ladrillera, 78363 San Luis Potosí, SLP, México.
[2]Departamento de Físico-Matemáticas, Universidad Autónoma de San Luis Potosí (UASLP), Niño Artillero s/n, Zona Universitaria Poniente, 78290 San Luis Potosí, SLP, México.

guillermo.nieto@uaslp.mx

In the current literature, it is useful to report changes in charge density associated with biomolecules. However, in order to get such information from output files generated from software like Quantum Espresso could be repetitive and long time-consuming. With this in mind, we present ChargenQ, which is a set of scripts developed in “python”, thus, from the typically files from charge density of Quantum Espresso, ChargenQ delivery a new file, that It could be visualized with a very popular software of biomolecular visualization: Pymol. Thus, with ChargenQ, in a simple way, we convert the charge density data in a visualize file, with several options to display.

Key Words: Charge density, pyMol, Quantum espresso.

Processing and characterization of micro-nanostructured CdS thin films

R. Navarro Jiménez[1], P. G. Gutierrez Z-B[2], K. Gutierrez Z-B[2], J. Sastré-Hernández[3], and G. Contreras-Puente[2]

1Instituto Tecnológico y de Estudios Superiores de Monterrey, ITESM, Carretera Lago de Guadalupe Km. 3.5, Colonia Margarita Maza; Atizapán de Zaragoza, Estado de México.
2Instituto Politécnico Nacional, Escuela Superior de Física y Matemáticas, Departamento de Física, U.P.A.L.M., San Pedro Zacatenco, Ciudad de México, 07738, México.
3Tecnológico de Monterrey, Escuela de Ingeniería y Ciencias, Av. Carlos Lazo No. 100, Col. Santa Fe, Álvaro Obregón, 01389, México D. F., México

A01746885@itesm.mx

Nowadays we can find different types of solar cells that have any amount of compounds that cause many possibilities for processing the optimized final device. That's why in this work we are focusing on nano-structured layers of cadmium sulfide (CdS). To achieve the highest efficiency in the ability of getting the growth of nanowires at different flows and different boiling temperatures, a mixture of alcohol with nanoparticles of Bismuth are used as the catalyst , which once placed in the sample an evaporation on a grill at 80 ° C to leave the bismuth nanoparticles in the substrate [1]. Several tests were performed in which we varied only the deposition time and temperature of growth. The parameter of growth that are being handled are: nitrogen (N2) flow of 0.1 and 0.2 standard liter / min, high (around 300 ° C) and low temperatures (around 200 ° C). In the case of high temperature we have the growth of nanotubes with a diameter of the micron range, in the case of low temperatures a nucleus surrounded by very thin nanotubes; these results are expected according to the Vapor-Liquid-Solid model (VLS). After that, we will make the change of flow to analyze if the results remains constant as before. We observed two types of results: 1) a type of coarse threads with the absence of thin nanowires on the catalyst drops. 2) Several amount of thin nanowires in contact with a small amount of coarse threads or simply implanted in the drop of the catalyst. The different processes that were followed to achieve growth and repeatability events are presented and the SEM images and Raman Spectroscopy of the processing CdS nanowires are also analyzed [2].

Key Words: Cadmium Sulfide, VLS, Nanowires.

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Synthesis of CaO nanoparticles by citric acid-assist SOL-GEL method

H.Y. LOPEZ[1,2*], E. M. MUZQUIZ[1], C. M. LOPEZ[1], M. HERNANDEZ[2], F. HERNANDEZ[2]

[1]Universidad Autónoma de Coahuila, Blvd. V. Carranza s/n Col. Republica Oriente, C.P. 25280, Saltillo, Coahuila, México.
[2]Universidad Autónoma Agraria Antonio Narro, Calzada Antonio Narro 1923 Buenavista, C.P. 25315, Saltillo, Coahuila, México.

*yajaira.lp@gmail.com

Calcium oxide (CaO) is an important inorganic material [1], nanoparticles exhibit various advantages in applications, can be used as bactericide, adsorbent, and catalyst [2]. This type of nanoparticles can be synthesized by various methods, such as sol - gel and thermal decomposition [3]. In this work the CaO nanoparticles were synthesized by a citric acid-assist sol-gel method [4]. The particles were characterized by TGA-DSC, XDR, FT-IR analysis. The thermal decomposition behaviour was investigated to determine the calcination temperature, the TGA-DSC analysis shows that the temperature of 700°C was chosen as the calcination temperature to ensure fully calcined products are obtained. XDR confirms that the final products are pure, single phase and of cubic shape. The crystallite size calculated using Scherrer's formula was about 40 nm. It can be concluded that it was possible to synthesize CaO nanoparticles by this method.

Key Words: Calcium oxide, sol-gel method, citric acid, calcination.

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Reduced graphene oxide as a hole transport layer in OPVs and the influence of number of layers in the efficiency

P. G. Olvera-Otal[1,2]*, J. L. Maldonado[2] and R. Castro-Beltrán[1]

[1]*División de Ciencias e Ingenierías, Universidad de Guanajuato Loma del Bosque #103, Lomas del Campestre, C.P. 37150. León Gto., México.*
[2]*Research Group of Optical Properties of Materials (GPOM), Centro de Investigaciones en Óptica, A.C. Loma del Bosque #115, Lomas del Campestre, C.P. 37150. León Gto., México.*

*pg.olveraotal@ugto.mx

In this work is reported the analysis of contribution of the number of deposited layers of reduced Graphene Oxide (rGO) functionalized with phenylhidrazine (PHrGO), as a hole transport layer [1] (HTL), in organic photovoltaic (OPV) power conversion efficiency (PCE). OPVs cells were fabricated under the bulk heterojunction architecture with the configuration glass/ITO/PHrGO/P3HT:PC61BM/FM. Field's metal (FM) is a eutectic alloy, composed by 32.5% Bi, 51% In and 16.5% Sn, that melt at 65°C and is easily deposited on top of the electron transport layer (ETL) at low temperature (~ 90 °C) [2]. PEDOT:PSS film as a HTL is used as a control device. An improved PCE was observed, from 1% to 1.4%, by depositing a second PHrGO film and consequently the short-circuit current density (Jsc) increases from 4.8 mA/cm^2 to 6.2 mA/cm^2 because of the increase in charge carrier collection. In comparison with the values of the control device, where a PCE of 1.7% and Jsc of 7.3 mA/cm^2 were obtained, this PV performance achieved with this alternative HTL is promising and could be a replacement option of PEDOT:PSS that degrade the OPVs devices.

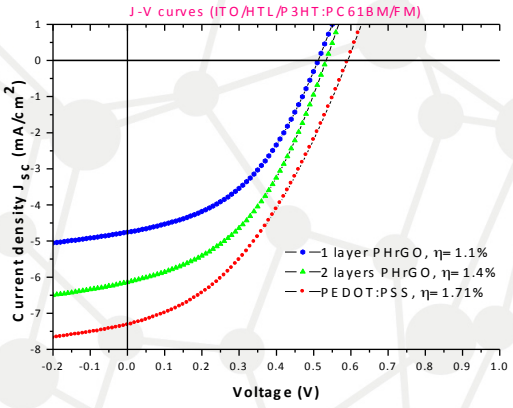

Figure 1 J-V curves for OPVs devices.

Key Words: OPVs, reduced graphene oxide, HTL, PHrGO.

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Fluorescent carbon nanoparticles from sodas

Jesús Antonio Orozco Frías[1], Juan José Martínez Fuentes[1], Juan Luis Mares Alvarado[1], Alberto Gutiérrez Becerra[1], Armando Pérez Centeno[2], Juan Pablo Morán Lázaro[3], Adalberto Zamudio Ojeda[2]

[1]Ingeniería en nanotecnología Universidad de Guadalajara, Centro Universitario de Tonalá, Tonalá, Jalisco, México.
[2]Departamento de Física, Universidad de Guadalajara, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México.
[3]Departamento de ciencias computacionales e ingeniería, Universidad de Guadalajara, Centro Universitario de los Valles, Ameca, Jalisco, México.

orozcofrias58@gmail.com

Fluorescent nanoparticles have a wide variety of promising applications, especially in the area of biology and medicine. However, many of the materials which these particles are made of, are toxic or can generate an environmental risk, presenting limitations for their application, such is the case of cadmium sulfide, so it is necessary to use materials such as carbon which are biocompatible, for both in vitro and in vivo uses. For this reason, carbon-based fluorescent nanoparticles present advantage for having this characteristics such as: low cytotoxicity, good photostability [1] and therefore can enter in the cells, which makes them suitable candidates to be used as biomarkers [2]. Based on this, carbon particles have been synthesized, obtained from the sugars of orange juice and candle smoke, some of them received a hydrothermal treatment and, in some cases, a reflux post treatment in different acids [1,3]. In this case the photoluminescent carbon nanoparticles were prepared by a simple microwave treatment, using polyethylene glycol and the sugar of the sodas as a source of carbon particles [3]. The photoluminescent properties of carbon nanoparticles are analyzed with respect of exposure time, number of cycles and microwave power. The samples were characterized with fluorescence spectroscopy, scanning electron microscopy, transmission electron microscopy and UV-Vis spectroscopy.

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Optical and morphological characterization of CdSe nanoparticles processed by LASER ablation in liquid

Patricia MALDONADO-ALTAMIRANO[1*], Jaime SANTOYO-SALAZAR[2], Luis Arturo MARTÍNEZ-ARA[3], Ma. de los Ángeles HERNÁNDEZ-PÉREZ[4], Fernanda GARCÍA-MEJÍA[3], Jorge R. AGUILAR-HERNÁNDEZ[3]

[1]Programa de Nanociencias y Nanotecnología, CINVESTAV- Instituto Politécnico Nacional, Av. Instituto Politécnico Nacional 2508, Gustavo A. Madero, San Pedro Zacatenco, 07360 Ciudad de México, CDMX.
[2]Depertamento de Física, CINVESTAV- Instituto Politécnico Nacional, Av. Instituto Politécnico Nacional 2508, Gustavo A. Madero, San Pedro Zacatenco, 07360 Ciudad de México, CDMX.
[3]ESFM- Instituto Politécnico Nacional, Edif. 9, IPN, U.P.A.L.M., Col. Lindavista. C.P. 07738, CDMX.
[4]ESIQIE-Instituto Politécnico Nacional, Edif. 8, IPN, U.P.A.L.M., Col. Lindavista. C.P. 07738, CDMX

*pma8410@gmail.com

In this work we present some results and analysis concerning the processing of semiconducting CdSe nanoparticles obtained by laser ablation of diluted CdSe powder in acetone. A Nd-YAG pulsed laser was used for ablation, tuned at the first harmonic, λ=1064 nm, 50 Hz frequency repetition during 60 minutes. The experiment was performed at different power intensities. UV-Vis, PL and Raman spectroscopies were used to characterize the CdSe nanoparticles, whereas atomic force microscopy and transmission electron microscopy were used to determine the morphology and size of the particles finally, TEM and XRD were used to describe the CdSe nanoparticles morphology. According to the UV-Vis results it was confirmed a shift of the band edge towards high energy (blue shift) until 2.2 eV. Raman spectroscopy show the LO phonon at 207 cm-1 with two phonon replicas. The samples shown room temperature emission which depends of power intensity. The size, approximately 20 nm, was estimated through AFM and TEM pictures. A deep analysis of the results is presented and discussed.

Key Words: Liquid laser ablation, nanoparticles, PL, Raman.

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Optical, structural and electrical properties from ZnO:Ta doped films obtained by HFCVD approach

V. Herrera[1*], T. Díaz-Becerril[1], G. García-Salgado[1], R. Galeazzi[1], C. Morales[1], E. Rosendo[1], A. Coyopol[1], R. Romano[1], F. G. Nieto-Caballero[1]

[1]Centro de Investigación en Dispositivos Semiconductores, Universidad Autónoma de Puebla, 14 sur y Av. San Claudio, C. U., C.P. 72570, Puebla, México.

pds_vherrera@hotmail.com

ZnO:Ta doped films were obtained by hot filament chemical vapor deposition (HFCVD) approach. A pill source fabricated with a mixture of ZnO and Ta_2O_5 powders were used as a solid source to grow this films. Hydrogen flow was used as reactant gas at temperature of 800°C, all experiments were carried out at atmospheric pressure, and were obtained on a silicon substrate (100) n-type. Films obtained shows a green luminescence visible at the naked eye when these are excited under an ultraviolet lamp. From X-ray diffractograms we could confirm the presence of zinc oxide in wurtzite phase, and metallic zinc with hexagonal structure, in case of tantalum atoms, these seem not to have effect on the structure of the films, but in morphology of each one, because roughness of the films increases as the amount of tantalum is increased in source pill. The reason of this effect could be attributed to the difference of atomic radii between Zn and Ta atoms because we are observing a substitutional effect between this two atoms, and tantalum is slightly smaller than zinc atoms, causing a compressive stress in structure. Regarding to electrical behavior of the films, we can observe an increment of carrier concentration as tantalum is increased in the films, therefore we can conclude that Ta atoms are contributing with free electrons in the film, and also, these free electrons are benefiting to decrease resistivity value in the films. Luminescence observed is attributed mainly to oxygen vacancies, according to several reports, and range of emission in the films.

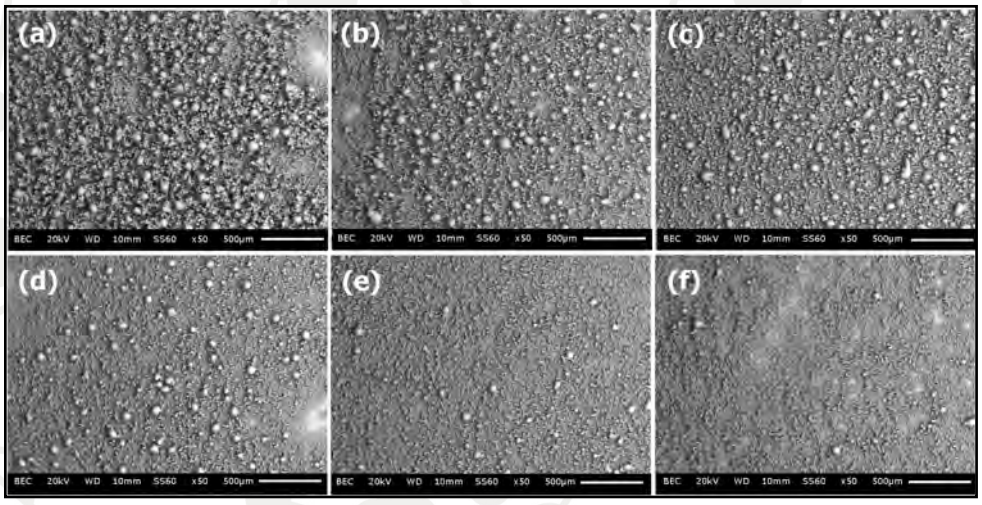

Figure 1 – Results SEM-50x of films ZnO:Ta doped growned on silicon substrates with (a) 0% Ta2O5, (b) 10% Ta2O5, (c) 20% Ta2O5, (d) 40% Ta2O5, (e) 50% Ta2O5, (f) 60% Ta2O5 on pill source.

Key Words: Zinc oxide, tantalum oxide, ZnO:Ta doped films, substitutional alloy.

Study of effect of pH, temperature and the surfactant on the size of ZrO_2 nanoparticles by central composite design synthesis

M. M. Luna[1], R. A. Estrada[1], J. Narayanan1, C. A. Huerta[1]

[1]Universidad Politécnica del Valle de México, Av. Mexiquense s/n, Col. Villa Esmeralda, C.P. 54910, Tultitlán, Estado de México, México.

mayra.luna@live.com.mx

Surfactants are useful to control the particle size [1-2]. The present work evaluate the effect of surfactant, temperature and pH of the reaction in the size-controlled synthesis of ZrO_2 nanoparticles by response surface method. Ultraviolet–visible spectroscopy is used to determine the most relevant factors for the size distribution of the ZrO_2. XRD, TEM, AFM, and DLS techniques were used to determine the nanoparticles size and the diameters were between 35-150 nm.

Key Words: ZrO_2, Nanoparticles, Effect, pH, Temperature, Surfactant.

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Morphological Characterization with STM and SEM of CdSe Nanostructures in function of pH

Sánchez Legorreta GABRIELA[1], Rosendo Francisco PORFIRIO DOMINGO[1], Olea Mejía OSCAR[2]

[1]Facultad de Ciencias, UAEM, Campus "El Cerrillo, Pierdas Blancas". Carretera Toluca – Ixtlahuaca, Km. 15.5, CP. 50200 Toluca de Lerdo, México.
[2]Centro Conjunto de Investigación en Química Sustentable UAEM-UNAM. Carretera Km. 14.5, Unidad San Cayetano, Toluca - Atlacomulco, C. P. 50200 Toluca de Lerdo, México.

*g.sanchez.legorreta@gmail.com.

The cadmium selenide (CdSe) semiconductor nanostructured is a material very interesting due their optical and physical property that depend of their morphology and size [1-5]. For this reason, we synthetized nanoparticles of CdSe using the colloidal method and we varied, as mean parameter in the growing, the pH value: 8 to 12 to know the effect of pH on the physical properties of the samples. The nanoparticles were characterized using the SEM to know the morphology of the samples and the STM to obtain imagen of the electronic cloud on the surface of nanoparticles. In each case, was found different sizes (from 6 to 11.5 nm) and shapes as filaments (fibbers), bars and spheres of CdSe nanoparticles and the 3D-FFT was obtained too. The results are analyzed and discussed.

Key Words: Cadmium Selenide, pH value, colloidal synthesis, SEM, STM.

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Optical and microestructural study of HfO_2-Nd/Si-NCs thin films

Baños Sánchez Saúl[1*], Tetyana V. Torchynska[2], Díaz Cano Aarón Israel[1] and Leonardo G. Vega Macotela[3]

[1]UPIITA, Instituto Politécnico Nacional, Ciudad de México, 07340, México.
[2]ESFM, Instituto Politécnico Nacional, Ciudad de México, 07340, México.
[3]ESIME, Instituto Politécnico Nacional, Ciudad de México, 07340, México.

kgvd6@icloud.com

In recent years, the development of metal-oxide semiconductor devices has evidenced the SiO_2 limitations in semiconductor technology. The study of high dielectric constant K materials has proposed new alternatives to substitute SiO_2 and overcome its limitations HfO_2 oxide being one of the main candidates [1]. Meanwhile optical properties of rare earth (RE) ions suggest they can be used as efficient optical centers while embedded in HfO_2/Si matrix [2].

In present work the thin films of HfO_2-Nd / Si- nanocrystals (NCs) have been investigated in dependence on the temperatures of thermal annealing. A post-deposition treatment leads the re-crystallization of films and to creation of Si NCs. The films were characterized using SEM, EDS, XRD and PL methods, which show a homogeneity of deposited films, the presence of neodymium atoms, as well as a significant increase of emission in the visible to infrared range (400-900 nm) related to the presence of rare earth atoms coupled to the HfO_2 matrix enriched with Si NCs.

Key Words: Rare earths, optical properties, high dielectric constant, re-crystallization.

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Tailoring Physicochemical Properties of 1D Nanostructures

H. A. Borbon-Nuñez[1*], D. Domínguez[2,3], J. López[1], M. Herrera-Zaldiar[2], J. M. Romo-Herrera[2], F. Muñoz-Muñoz[4], M. Landeros[4], G. Soto[2], H. Tiznado[2]

[1]CONACyT- Centro de Nanociencias y Nanotecnología. Universidad Nacional Autónoma de México, Km 107 Carretera Tijuana-Ensenada s/n, Ensenada, B.C., C.P. 22800, México
[2]Centro de Nanociencias y Nanotecnología. Universidad Nacional Autónoma de México, Km 107 Carretera Tijuana-Ensenada s/n, Ensenada, B.C., C.P. 22800, México
[3]Posgrado en Ciencias de la Ingeniería, Instituto Tecnológico de Tijuana, Calzada Del Tecnológico S/N, Fraccionamiento Tomas Aquino, Tijuana, Baja California, México.
[4]Universidad Autónoma de Baja California, Facultad de Ingeniería, Arquitectura y Diseño. Km 107 Carretera Transpeninsular Ensenada-Tijuana 3917, Ensenada, B.C. C.P 22860, México

*hborbon@cnyn.unam.mx

The applications of nanostructured materials are driven by their properties and shape. Since the discovery of carbon nanotubes (CNTs), has increased intensive research to characterize the structure and properties toward the nanoscale phenomena and technology. Recently, the one-dimensional (1D) nanostructure, such as wires, belts, rods and tubes have also become the focus of research owing to their unique applications on fabrication of nanoscale devices. In special, the 1D semiconductor nanostructures have attracted considerable research activities because of their great potential for fundamental studies of the role of dimensionality and size in the physical and chemical properties as well as for applications in electronic and optoelectronic nanodevices. A comprehensive understanding of properties and its modification while controlling its size, shape, topology, etc., is of key importance. This manner, a nanostructure can become a building block to create the upcoming nano-technological stages, where the final characteristics of devices are controlled at will. At the present work, we present the development of 1D nanostructures with desirable composition and properties, by engineering surface approach. From dielectric to metal nanostructures, using atomic layer deposition, and carbon nanotubes as templates, were grown, and structural and morphologically characterized.

Key Words: Nanostructures, Atomic layer deposition, unidimensional, Nanotubes

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Influence of the control temperature in the graphene oxide synthesis

Bravo González Edith[1], León Nataret Yosemik Arjuna[1*], Díaz Cano Aarón Israel[1], Rubio Rosas Efraín[2]

[1]SEPI-UPIITA, Instituto Politécnico Nacional, Ciudad de México, 07340, México.
[2]CUVyTT, Benemérita Universidad Autónoma de Puebla, Puebla, 72570, México.

aidiaz@ipn.mx

Synthesis and characterization of graphene oxide (GO) have allowed developing different mechanisms of control to improve its mechanical, optical and structural properties [1-2]. The temperature control in the synthesis process is an important factor that defines the quality of the microstructure, chemical exfoliation, the functionalization with different organic groups and some relevant changes in the crystal structure [3]. A study was conducted by controlling temperature rise which originates from exothermic process reaction with H_2O & H_2SO_4. Which allowed observing the influence of the released heat in the material reaction. The GO was characterized using techniques XRD, SEM, AFM, EDX, FTIR, which noted the shift of the plane (001) in 7° to 12° (2 theta), a high level of degradation on the material surface, it witch to leave it exposed to the exothermic process reaction (85°C) and how it was corrected with the temperature control at 15°C, was analyzed the influence of surface degradation through images of topology and phase to identify the change affecting the microstructure of the material, a qualitative analysis was applied to meet the stoichiometry of the material and the level absorption of the organic groups present during the process of functionalization.

Key Words: temperature control, microstructure, surface degradation, functionalization.

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Growth of ultra-thin films of ZnO on Magneto-Controllabe core-shell nanoparticles encapsulated with a removable SiO_2 template

A. Ortiz[1] - Atondo, J. López[2*], F. Muñoz – Muñoz[1], J. M. Romo[3], H. Tiznado[3]

[1]Facultad de Ingeniería, Arquitectura y Diseño, UABC, Universidad Autónoma de Baja California, Km. 106 Carr. Tij-Ens, Ensenada, C. P. 22800, México
[2]CONACYT - Centro de Nanociencia y Nanotecnología, UNAM, Ensenada, B.C. México, Km 107 Carretera Tijuana-Ensenada s/n, Ensenada, B.C., C.P. 22800, México
[3]Centro de Nanociencia y Nanotecnología, UNAM, Ensenada, B.C. México. Km 107 Carretera Tijuana-Ensenada s/n, Ensenada, B.C., C.P. 22800, México

javierlo21@cnyn.unam.mx

Nowdays, a research area of great interest in nanotechnology is the development of nanoparticles for different applications. This work focus in core-shell nanostructures synthesis based on $Co_{0.25}Zn_{0.75}Fe_2O_4$ ferrite nanoparticles with superparamagnetic behavior via chemical co-precipitation method from aqueous salt solutions in alkaline medium and coated with a silica shell (SiO_2), through the sol-gel method as removable template. ZnO ultrathin layer was growth over SiO2 template via atomic layer deposition technique (ALD). After coating the template with ZnO, it was removed via chemical method in order to obtain a functional material with interesting properties that can be applied in photocatalysis, magnetic separation and drug transport. Nanostructures were characterized by XRD, VSM and TEM in order to study the structural, magnetic behavior, removable template morphology, particles size and ZnO coat thickness. TEM measures for zinc-cobalt ferrites coated with silicon oxide allows to observe nanoparticles with a diameter size distribution between 7 and 11 nm and ZnO layer thickness with approximately 30 nm. Magnetic measures from M vs H loops, indicate a tendency superparamagnetic behavior which is a good indicator of the high magnetization capacity. X-rays diffraction pattern allowed confirm spinel structure formation, features this kind of ferrite. This results opens the possibility to use this functional materials in different nanotechnology fields.

Key Words:

Acknowledgment
This work was partially supported by Dirección General de Asuntos del Personal Académico DGAPAUNAM, through research projects: PAPIIT IN105114, IN112117, IN107715, PAPIME 2017 project PE101317 and FORDECYT - CONACYT 272894 project.

Development of Sb_2S_3 nanoparticles for its application in sensitized solar cells

Andrea CERDÁN-PASARÁN[1,2*], Nini MATHEWS[1]

[1]*Instituto de Energías Renovables-Universidad Nacional Autónoma de México, Priv. Xochicalco s/n, C.P. 62580, Temixco, Morelos, México.*
[2]*Universidad Autónoma de Nuevo León, Av. Universidad s/n, C.P. 66455, San Nicolás de Los Garza, Nuevo León, México.*

andreaqcp@gmail.com

In the study of photovoltaic devices, it is important the development of solar cells based on non-toxic, stable and environmental friendly materials. The Sb_2S_3 is a semiconductor that present convenient properties for photovoltaic applications, such as band gap of 1.6-1.8 eV and high absorption coefficient (105 cm-1) [1]. The highest power conversion efficiency reported for solar cells based on Sb_2S_3 is 7.5 % [2]. Therefore, there is still wide potential for its development. In this work, we study the synthesis of Sb_2S_3 nanoparticles for its application as sensitizer in TiO_2 sensitized solar cells. We synthetized Sb_2S_3 nanoparticles by hot-injection method using toluene as solvent. Colloidal nanoparticles of spherical shape with ~40 nm diameter were obtained. After annealing in nitrogen atmosphere at 300°C for 30 min, they became crystalline with stibnite phase according to the results from XRD characterization. Furthermore, the shape of particle change to rods and size increased to 4 µm in length and 850 nm in diameter, see Figure 1. The thermal treatment was studied in a temperature range from 275 °C to 400°C and photoresponse were analyzed. The highest photosensitivity was obtained at 300°C.

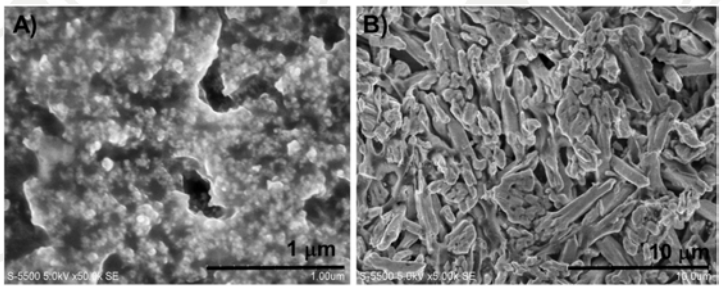

Figure 1 SEM image of the Sb_2S_3 nanoparticles A) before and B) after of the annealing at 300°C for 30 min.

Key Words: colloidal Sb_2S_3, sensitized solar cells, hot-injection, TiO_2.

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ZnO and ZnS photo-luminescents quantum dots as a possible new method to improve solar cell efficiency

A. Zazueta-Raynaud[1, 2], J. E. Pelayo[1,3], R. Lopez-Delgado[1, 2], E. Alvarez[2] and A. Ayon[1]

[1]University of Texas at San Antonio, Dept. of Physics and Astronomy, MEMS Research Lab, One UTSA Circle, San Antonio, TX 78249, USA.
[2]Universidad de Sonora, Departamento de Física, Blvd. Luis Encinas y Rosales, Col. Centro, Hermosillo, Sonora, México. CP 83000.
[3]Universidad de Guadalajara, Centro de Ciencias Exactas e Ingenierias, Blvd. Gral. Marcelino García Barragán 1421, Olímpica, 44430 Guadalajara, Jalisco, México.

aldo.zazuetaa@gmail.com

Silicon solar cells have captured more than eighty percent of the current photovoltaic market due to their relatively high efficiency, and, in spite of their relatively high manufacturing cost, still are the preferred market choice. On the other hand, the relatively poor UV absorption of crystalline silicon (c-Si) limits the aforementioned efficiency precluding their proliferation in a larger number of settings. Higher efficiency is, therefore, the greatest challenge for their expanded utilization. Solar cell technology still needs to be developed and improved further to obtain optimal efficiency and cost. In this work, Zinc Oxide (ZnO) and Zinc Sulfide (ZnS) quantum dots were synthesized to study the electric influence in the devices. The excitation wavelength of these quantum dots is between 340 to 350 nm with different emission wavelength over 500 nm. These nanoparticles allow us to convert high energy photons to lower energy photons that can be absorbed by the poly-Si solar cell.

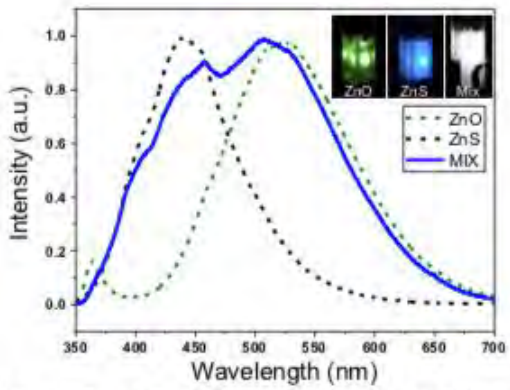

Figure 1. Photoluminescence spectra of synthesized ZnO & ZnS QDs and mix with visible light emission images.

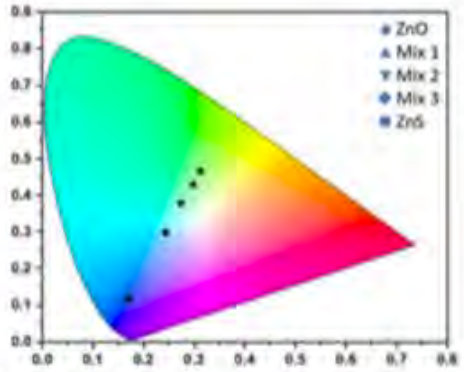

Figure 2. CIE Chromaticity diagram of different mix samples.

Key Words: quantum dot, solar cell, down shifting, zinc oxide, zinc sulfide, photo voltaic.

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Synthesis and characterization of materials used to build a dye sensitized solar cell using the colorant protoporphyrin IX

P. I. Lopez-Picazo[*a], M.Sanchez-Tizapa[a], M. Tostado-Plascencia[a], J.P. Morán-Lázaro[b], M. Flores-Martínez[c]

[a]Departamento de ciencias Naturales y Exactas, CUValles, Universidad de Guadalajara, C.P. 46600 Ameca.
[b]Departamento de Ciencias Computacionales e Ingeniería, CUValles, Universidad de Guadalajara, Ameca, Jalisco 46600, México.
[c]Centro Universitario de Ciencias Exactas e Ingeniería, Universidad de Guadalajara, Jalisco, 44430, México.

picazo_0708@hotmail.com

The conversion of solar radiation into electricity has been done using photovoltaic devices in order to avoid environmental issues as the global warming. A cheaper variant of the solid state solar cells are the dye sensitized solar cells, specifically using organic colorants. Organic dyes have a broad absorption band, and when are coupled with nanocrystalline oxide films it is possible to collect a wider fraction of the sunlight [1]. In this work we describe the use of the protoporphyrin IX in a dye sensitized solar cell. Titanium oxide synthesized by Sol-Gel was used as the working electrode, and reduced graphene oxide was the counterelectrode. The synthesis of graphene oxide was carried out by the modified Hummer method and the reduction was done by sonication. The materials were characterized by X-ray diffraction, Raman, ultraviolet-visible, and infrared spectroscopies. X-ray diffraction and Raman showed the presence of anatase phase of the titanium dioxide. Raman spectroscopy showed the characteristic signals of graphene oxide and reduced graphene oxide, i.e. the bands D and G, as well as important changes in these bands as the change from graphene oxide to reduced graphene oxide was carried out. The band gap calculation of titanium dioxide by ultraviolet-visible spectroscopy resulted in 3.2 eV. Infrared spectroscopy of protoporphyrin IX resulted in strong signals of hydroxyl groups, double bond C=O, and C-N bonds, all of these signals are characteristic of porphyrin-like compounds.

Key Words: graphene, titanium dioxide, dye sensitized solar cells, charge transport, porphyrin

Solar cells efficiency improvement employing multilayered films of quantum dots

A Cordova-Rubio[1,2], R Lopez-Delgado[1,2], A Zazueta-Raynaud[1,2], M E Alzarez-Ramos[2], and A Ayon[1]

[1]*University of Texas at San Antonio, One UTSA Circle, San Antonio, TX 78249, USA*
[2]*Universidad de Sonora, Blvd. Luis Encinas y Rosales, C.P. 83000, México.*

ale.cordovar@gmail.com

The Quantum dots (QD) are semiconductor structures that confine charge carriers to a nanoscale region that are described by quantum mechanics, exhibit different behavior compared to bulk materials because the surface/volume ratio affects their physical and chemical properties, their electronic properties are strongly related to its size [1] and by varying their size it is possible to obtain emission in different wavelengths [2]. Thus, judiciously employed, the ability of quantum dots (QDs) to absorb high energy photons and emit photons with lower energy could be exploited to increase the efficiency of solar cells.

We report the synthesis and characterization of silicon (Si) and zinc oxide (ZnO) quantum dots (QDs), that exhibit down-shifting photoluminescent characteristics, and their deployment on photovoltaic devices. The ZnO QDs were synthesized in an ethanol-based colloidal solution, while the Si QDs were synthesized in a water-based colloidal solution. The deployment of the aforementioned films as photon down shifting layers on solar cells enabled improvements in the efficiency of the photovoltaic devices from 14.42% to 15.41%. These observations indicate an improvement of ~6.8% in the power conversion efficiency.

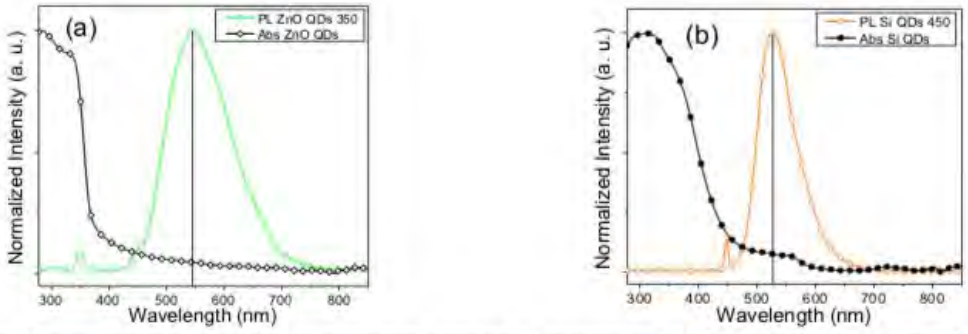

Figure 1 Absorption and photoluminescence spectra characterization for (a) ZnO QDs and (b) Si QDs.

Key Words: Quantum Dots, Solar cell, Power Conversion Efficiency, photovoltaic devices.

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Emission and HR-XRD study of GaAs/AlGaAs heterostructures with quantum dots covered by strain reducing capping layer

Georgiy POLUPAN[1*], Tetyana TORCHYNSKA[2], Leonardo G. VEGA MACOTELA[1], Ricardo CISNEROS TAMAYO[1] and Arturo ESCOBOSA ECHAVARRÍA[3]

[1]ESIME, Instituto Politécnico Nacional, Av. IPN, México D.F, 07738, México
[2]ESFM, Instituto Politécnico Nacional, Av. IPN, México D.F. 07738, México
[3]Solid State Electronics Section, CINVESTAV-IPN, Av. IPN, México D.F. 07320, México

*gpolupan85@yahoo.com.mx

InAs quantum dots (QDs) embedded in MBE grown GaAs/Al0.30$Ga_{0.70}$As/AlGaInAs/$Al_{0.30}Ga_{0.70}$As/GaAs quantum wells (QWs) have been investigated in as grown state and after thermal annealing at 710℃ for two hours. Three types of QD structures with the different compositions of AlGaInAs capping layers and the same composition of buffer layers are compared and studied by means of photoluminescence (PL), X-ray diffraction (XRD) and high resolution HR-XRD methods. The next types of QD capping layers have been used: GaAs (#1), $Al_{0.30}Ga_{0.70}As$ (#2) and $Al_{0.10}Ga_{0.75}In_{0.15}As$ (#3). XRD and HR-XRD techniques are applied with the aim to control the quality of crystal structures, as well as varying the material compositions and elastic strains in QW layers at thermal annealing.

The highest PL intensity, smaller PL band half width and lower energy of ground state (GS) emission are detected in the structure with the $Al_{0.10}Ga_{0.75}In_{0.15}As$ capping layer. Thermal annealing leads to the shift of PL spectra into higher energy range and the value of this shift is more essential in the structure with the $Al_{0.10}Ga_{0.75}In_{0.15}As$ capping layer as well. The variation of GS emission peak versus temperature has been monitored within the range of 10-450 K for as grown and annealed states and it compared with temperature shrinkage of band gap in the InAs and GaAs bulk crystals. It permits to reveal that the QD composition in #3 is closer to InAs and the efficiency of Ga/In intermixing at annealing in #2 is less than in #1 and #3.

Finally the reasons of PL spectrum transformation at annealing, the mechanism of PL thermal decay, and the advantages of the QD structure with strain reduced $Al_{0.10}Ga_{0.75}In_{0.15}As$ capping layer have been analyzed and discussed. The composition variation of QDs and QWs at annealing has been modeled using the simulation of HR-XRD results with Xpert Expitaxy software.

Síntesis de oligoiminas conjugadas para el desarrollo de celdas solares orgánicas

L. E. Castaños Padilla[1], B. D. Gerardo Iribe[2], C. L. Moraila Martínez[1,2]

[1]Universidad Autónoma de Sinaloa, Facultad de Ciencias Físico Matemáticas Av. de las Américas y Blvd. Universitarios 80010 Culiacán, Sinaloa, México.
[2]Universidad Autónoma de Sinaloa, Parque de Innovación Tecnológica cl. Josefa Ortiz de Domínguez, Ciudad Universitaria 80013 Culiacán, Sinaloa, México.

*ing.denicegerardo@gmail.com

Nowadays scientific community is working in a worlds common problem: How to obtain clean energy?. Photovoltaic devices development is a good alternative to obtain clean energy reducing in this manner the ambiental impact caused the natural resources as the fossil resources to obtain energy. Solar cells silica based used currently are expensive to produce therefore the acquisition of solar panels are expensive and they are not suitable for most population in our country.

Organic nanostructurated materials are presented as a good alternative to create solar cells (and many other optoelectronic devices). In this work conjugated oligoimines were synthesized by means of conventional and mechanochemical synthesis, and they were characterized by spectroscopic methods. Furthermore, the optical, electronic and chemical properties were analyzed. Besides, thin films of the materials synthesized were deposited using the spin coating technique. Finally, solar cells were performed successfully.

(a) (b)

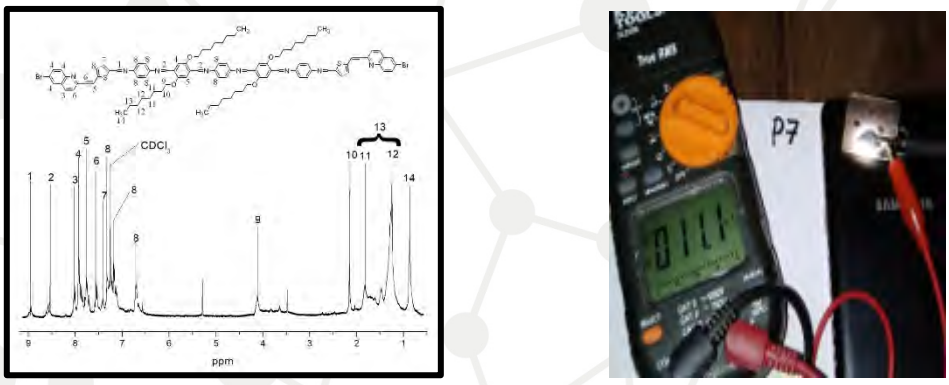

Figura 1- (a) Proton Nuclear Magnetic Resonance Spectrum (RMN-1H) of the compound OICF7,(b) Activity test in fabricated solar cell Cell of OICF7 (P7).

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Novel Co_xS_{x+1} Quantum Dots from Cobalt Sulfide (CoS_2.Bulk): Synthesis, characterization and application in solar cells

M. A. Honorato-Colin[1], C. Gomez-Solis[2], Tzarara Lopez-Luke[1] & E. de la Rosa[1*]

[1]Nano photonics and Advanced Materials Group (NAMG), Centro de Investigaciones en Óptica, A.C., Loma del Bosque 115, Lomas del Campestre León, Guanajuato, México. Zip Code 37150.
[2]Universidad de Guanajuato, Campus León, División de Ciencias e Ingenierías, 37150 León, Guanajuato, México.

elder@cio.mx

Cobalt Sulfide (Co_xS_{x+1}) Quantum Dots (CoSQDs) were prepared from bulk CoS_2 directly by a thermal-chemical etching process with some modification [1] and is obtained the same chemical composition, but in 0-dimensions (Quantum confinement) in different solvents. This is shown in Energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD) and Scanning Electron Microscope (SEM). The UV-Vis spectra show that there are many peaks of absorption, one peak is around 680nm to UV, this is good for application in the solar cell. The CoSQDs show strong blue emission as well as down conversion behavior under UV excitation, which can be used as universal energy-transfer components in visible-light-driven metal-free photocatalytic [2], bioimaging, biolabeling and solar cells systems [3]. In addition, it shows Photoluminescence (PL) spectra, when the excitation is varied, PL lifetime and the PL Quantum Yield is 10-27% depending on the solvent. finally it is demonstrated that there is a small increase in the efficiency of the solar cell by the electrophoresis method.

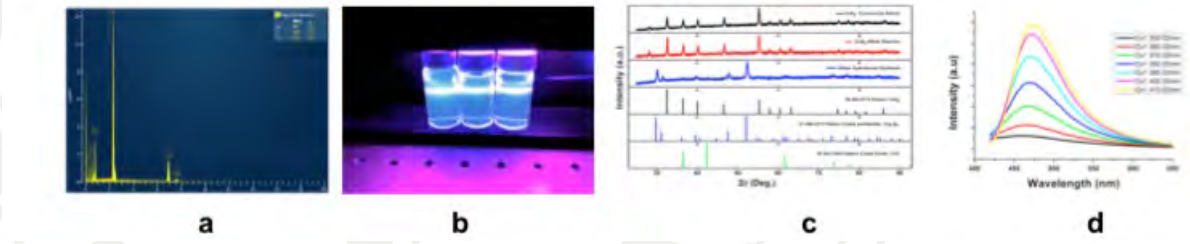

Fig 1. a) EDS spectra, b) Blue emission under UV excitation, c) XRD and c) PL.

Key Words: Quantum dots, down conversion, thermal-chemical etching.

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Effect of potential on the synthesis of porous Alumina templates for metalic nanowires electrodeposition

D. Levi QUIROZ-AGUILERA[1]*, J. Ernesto NERI CRUZ[2], Héctor A. CALDERON BENAVIDES[3], Luz A. GARCÍA SERRANO[4], Mayela GARCIA DE ALVA MAGOS[5]

[1,2]Instituto Politécnico Nacional – Escuela Nacional de Ciencias Biológicas, Prolongación de Carpio y Plan de Ayala s/n, Col. Sto. Tomás, C.P. 11340, Del. Miguel Hidalgo, CDMX, México.
[3]Instituto Politécnico Nacional – Escuela Superior de Física y Matemáticas, Av. Instituto Politécnico Nacional s/n, Ed. 9, Col. San Pedro Zacatenco, C.P. 07738, Del. Gustavo A. Madero, CDMX, México.
[4]Instituto Politécnico Nacional – Centro Interdisciplinario de Investigaciones y Estudios sobre Medio Ambiente y Desarrollo, Calle 30 de Junio de 1520 s/n, Barrio la Laguna Ticomán, C.P. 07340, Del. Gustavo A. Madero, CDMX, México.
[5]Instituto Politécnico Nacional – Centro de Desarrollo de Productos Bióticos, Carretera Yautepec – Jojutla, Km. 6, Calle CEPROBI No. 8, Col. San Isidro, C.P. 62731, Yautepec, Morelos, México.

iqpquiroz@gmail.com

In this work, we observe the growing of Anodic Porous Alumina Templates witch different electrical potentials are applied with different profiles, under a specific amperage pulse, witch influence structure characteristics of Anodic Alumna Templates (AAT), on which it is intended to synthesize metallic nanowires usable in artificial photosynthesis processes, will be studied in main characteristics such as interpore distance (D_c), pore diameter (D_p), Wall thickness (W), barrier layer thickness (B) and porosity (α) to secure an adequate penetration of the catalytic nanoparticles over the nanowires' surface. Also, is important to know the pore density (η) over the template, to calculate the proximal number of nanowires that could be synthetized. So, we made a theorical calculation of all the interest parameters based on literature about synthetic process of Anodic Alumina Templates (AAT)[1]–[8] to compare the theorical results with the experimental ones.

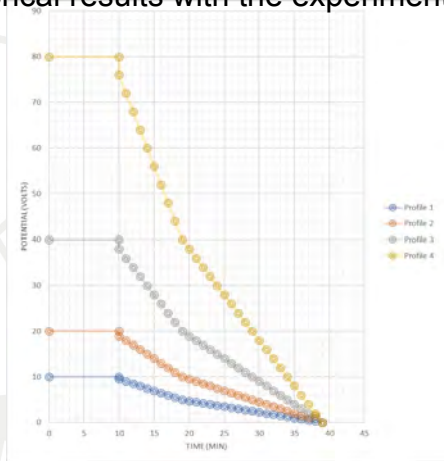

Figure 3 – Experimental Potential Profiles.

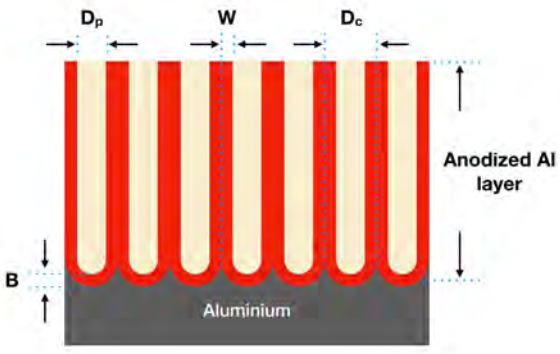

Figure 2 – Cross-sectional view of anodized layer with the main parameters marks.

Therefore, we use a modified two steps synthesis process of the reported one by O'Sullivan et al [1], where we use 10, 20, 40 and 80 V, shown at Fig.1 as electrical potential for 10 minutes and then a diminution gradient profile just 0 V, that represent 39 minutes of synthesis, with a amperage pulse of 6 milliseconds of a positive mA, following for a 4 milliseconds of a negative mA, and finally a neutral amperage of 0 V for 90 milliseconds, into a solution of $H_2C_2O_4$ at 0.5 M. Then, the characterization was made with XRD and BET analysis, and SEM imaging to obtain the experimental parameters of D_c, D_p, W, B, α, and η, to compare with the theoretical data, calculate a standard deviation (σ_{st}), and determinate the range of voltage with the lowest D_p, and largest D_c.

Key Words: Porous, Alumina, Templates, Synthesis, Nanowires, Electrodeposition.

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Investigating the synthesis of delafossite CuFeO2 using as precursors single Cu and Fe oxide layers prepared by AACVD

P. Pizá-Ruiz[1,4], A. Román-Loya[2], A. Sáenz-Trevizo[4], Y. Verde-Gómez[3] and M. Miki-Yoshida[4]

[1]Centro de Investigación en Materiales Avanzados, S.C., NANOTECH, Miguel de Cervantes 120, Complejo Industrial Chihuahua Chihuahua, Chih. México. C.P. 31136.
[2]Universidad Tecnológica de Chihuahua Sur, Km. 3 Carretera Chihuahua a Aldama S/N, Chihuahua, Chih Mexico.
[3]Instituto Tecnológico de Cancún, Div. de Estudios de Posgrado, Av. Kabah, Km. 3 Cancún Quintana Roo México C.P. 77515, Col. Centro Mexico.
[4]Centro de Investigación en Materiales Avanzados, S.C., Departamento de Física de Materiales, Miguel de Cervantes 120, Complejo Industrial Chihuahua Chihuahua, Chih. México. C.P. 31136.

pedro.piza@cimav.edu.mx

In recent years, the synthesis of efficient and low-cost materials for energy generation has been the focus of a vast amount of research. From available compositions, delafossite materials have shown to be appropriate candidates, in particular, for the generation of H2 by direct water splitting. Because of its chemical stability and the capability for absorption light in the visible region, delafossite $CuFeO_2$ is of interest [1]. Many synthesis methods have been employed for the growth of $CuFeO_2$ in the form of powders, particles and thin films. However, by using thin films supported onto substrates, it is possible to evaluate the ability of such structures to generate H_2 when exposed in direct contact with water. In this work we investigated the possible synthesis of $CuFeO_2$ via aerosol assisted CVD (AACVD) technique. This was achieved by growing consecutive layers of Cu and Fe oxides onto Au coated silicon wafers and borosilicate glass substrates. Single Cu and Fe organometallic salts were used as precursors for the growth of the respective layers of the oxide materials. The growth temperature was set at 723 K. Different characterization techniques, including scanning electron microscopy, x-ray diffraction, Raman spectroscopy and energy dispersive x-ray spectroscopy were used. Outcomes revealed the feasible formation of $CuFeO_2$ during the sequential synthesis of the layers. It was assumed that the evolution from Cu and Fe oxides layers to $CuFeO_2$ was to be promoted by the reaction of the Cu oxide layer as the Fe precursor arrived at the surface of the substrate. The prepared $CuFeO_2$ films were uniform in composition, presence Fe of Cu oxides were identified. The efficiency and stability of the synthesized samples during the generation of H_2 has to be evaluated in order to stablish its functionality.

Key Words: Delafossite $CuFeO_2$, AACVD technique, H_2 generation

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Banded iron formation for efficient nitrogen-doped carbon nanotubes production

Luis E. Jiménez-Ramírez[1*], Juan. L. Fajardo-Díaz[1], Sanjeet. J. Verma[2], Florentino López-Urías[1], and Emilio Muñoz-Sandoval[1]

[1]División de Materiales Avanzados, IPICYT, Camino a la Presa San José 2055, Col Lomas 4a sección, San Luis Potosí S.L.P., 78216, México
[2]División de Geociencias Aplicadas, IPICYT, Camino a la Presa San José 2055, Col Lomas 4a sección, San Luis Potosí S.L.P., 78216, México

luis.jimenez@ipicyt.edu.mx

Banded iron formation (BIF) powders are sedimentary rocks formed mainly by iron-oxide and silica-rich. We have used BIF powders from the Bundelkhand craton located in the north of India as catalyst for the high production of nitrogen-doped multiwalled carbon nanotubes (N-MWCNTs) in an aerosol assisted chemical vapor deposition (AACVD) experiment. The N-MWCNTS were grown on BIF powders located inside the reactor at a temperature of 850 °C and under the presence of benzylamine ($C7H_9N$) vapor as carbon and nitrogen source which was dragged by Ar/H2 flow during 40 min. It was considered pristine BIF powder and those ball milled during 1, 2, and 3 h under an ethanol atmosphere. The BIF powders and N-MWCNTs sample morphology and composition profiles were analyzed by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS) Raman spectroscopy, and thermogravimetric analysis (TGA). BIF powder XRD characterizations revealed that this is formed by mainly formed by quartz and hematite as also confirmed by Raman spectroscopy. TGA measurements revealed that BIF powder subjected to a ball milling increases their weights as the temperature increases, suggesting a surface modification of hematite and quartz grains. It was found that the yield production and morphology of N-MWCNTs depend strongly of the BIF powder (pristine and those ball milled). Efficiency of 340 % wt./wt. in the yield production of N-MWCNTs was obtained for BIF powder ball milled during 1 h. The specific surface area of N-MWCNTs estimated by Brunauer–Emmett–Teller (BET) for the N-MWCNTs reached up to 275 m2/g. The type of nitrogen doping (pyrrolic, pyridinic, quaternary), different nitrogen and oxygen functional groups (carbonyls, carboxylics, and nitrogen-oxide), Si species (SiO_2, SiO, Si^{4+}) and carbon species (sp2 and sp3) hosted at the surface of N-MWCNTs were quantified by the XPS characterizations. We have also investigated the electrochemical response of electrodes made of N-MWCNTs by cyclic voltammetry in order to assess the applications of our synthesized materials as energy storage and sensor systems.

Key Words: Carbon nanotube sponges, doping, nitrogen, hematite, nanoparticles, BIF, CVD

Obtention of Hydroxyapatite coatings by calcium carbonate precursor transformation

G. Amor[1], A. Vázquez[2], B. Kharissov[1*]

[1]*Universidad Autónoma de Nuevo León, Facultad de Ciencias Químicas. Av. Pedro de Alba S/N, Cd. Universitaria, San Nicolás de los Garza, C.P. 66450, Nuevo León, México.*
[2]*Centro de Investigación en Biotecnología y Nanotecnología, Facultad de Ciencias Químicas, Universidad Autónoma de Nuevo León, Parque de Investigación e Innovación Tecnológica, Km. 10 Autopista al Aeropuerto Internacional Mariano Escobedo, Apodaca, C.P. 66629, Nuevo León, México.*

*bkhariss@hotmail.com

Hydroxyapatite (HA) has proven to be an important material for environmental and biomedical applications due to its excellent biocompatibility, non-toxicity, human bone-like chemical structure, good capacity of drug/dye adsorption and high chemical stability. HA coatings could be used for enhancing biocompatibility of metallic implants, immobilization of different pollutants or drugs, among other applications. However, the control of the HA coating morphology has been difficult by direct synthesis/deposition methods, but recently a novel type of strategy called precursor transformation has been used, allowing the advantage that the morphological control can be performed in the precursor and in a final step this precursor is just transformed into HA. In this project $CaCO_3$ was obtained by microwave irradiation method starting from $Ca(NO_3)_2$, $NaHCO_3$ and sodium citrate as a stabilizer. $CaCO_3$ precursor was deposited on aluminum substrates using an electrophoretic process for 6 h and variations of the applied voltage. Electrophoretic deposition method is used in this work due to its benefits like ease of operation, low cost and the possibility to be scaled to an industrial level. Finally, the precursor deposits were transformed into HA by an immersion method in a reflux system of the substrates in a Na2HPO4 solution. The materials were characterized by FTIR, XRD, AFM and SEM. The obtained coatings presented brain-like morphology and the transformation of the precursor into HA was successful. Applications like metallic implants or drug/dye adsorption are promising due the roughness of these type of nanostructures.

Key Words: hydroxyapatite, calcium carbonate, precursor transformation, electrophoretic deposition.

Development of nanoemulsions with stability for insect repellents

Andrea LÓPEZ MARTÍNEZ[1,2], Janneth BERNARDO LINO[1,2], Abril FONSECA GARCIA[2], Reyna Araceli MAURICIO SÁNCHEZ[2], Luz Ma. Reina AVILÉS ARELLANO[2], Gabriel LUNA BERCENAS[2]

[1]Universidad Tecnológica Fidel Velázquez, Emiliano Zapata s/n, col. El tráfico, 54435 Villas Nicolás Romero, Estado de México, e-Mail: janny509@hotmail.com.
[2]Centro de Investigación y de Estudios Avanzados del I.P.N, Unidad Querétaro, Querétaro, 76230, México.

*gabriel.luna@cinvestav.mx

In this research, nanoemulsions of citronella were prepared by high energy. Citronella is an essential oil with great medical applications such as in the absorption of drugs through the skin [1]. Also, this essential oil have a huge bactericidal potential and the smell is unpleasant to the insects, so citronella can be used as repellent [2]. For this reason, the objective of this research was to develop nanoemulsions that can be stables during a suitable period, for its application as repellent without damage to humans. Silver nanoparticles (Npa Ag) in non-cytotoxic concentration to humans (lower than 10 µg/L) were added to the nanoemulsions. The Npa Ag help to potentiate the bactericidal effect from the essential oil. The Citronella was stabilized in two kinds of emulsions, by oil-in-water (O/W) emulsion and by water-in-oil (W/O) emulsion. Tween 80 is the surfactant employed to the preparation of these emulsions. We found that the O/W emulsion was not stable after 24 hours. However, white W/O emulsion were stable during 4 weeks. However, white W/O emulsions were stable during 4 weeks. FTIR spectroscopy was required to characterization of the essential oil and the surfactant

Key Words: Nanoemulsiom, Citronella, oil-in-water, water-in-oil.

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Characterization and bioactive effect in vivo of nopal nanoparticles

Jocelyn Madrigal-Acevedo[1], José Jorge Chanona-Pérez[1], Leticia Manuel-Apolinar[2], Martha Quetzalli Marín-Bustamante[1], Liliana Edith Rojas Candelas[1]

[1]Instituto Politécnico Nacional, Escuela Nacional de Ciencias Biológicas, Departamento de Micro y Nanobiotecnología. Unidad Profesional Adolfo López Mateos, Av. Wilfrido Massieu s/n C.P. 07738. Gustavo A. Madero, México.
[2]Unidad de Investigación Médica en Enfermedades Endócrinas, Hospital de Especialidades, Centro Médico Nacional Siglo XXI, Instituto Mexicano del Seguro Social. Avenida Cuauhtémoc 330, Doctores, C.P. 06720. Cuauhtémoc, México.

jocelynmadrigal580@yahoo.com.mx

Nanoparticulation increases the availability and reactivity of its bioactive components, which allow a greater speed of diffusion and assimilation in target organs to perform their function and / or nutraceutical activity [1]. On the other hand, obesity is a public health problem, that cause chronic diseases [2]. Objective: Obtain nanoparticles of nopal powder (Opuntia ficus indica) less than 100 nm, from high impact milling, and evaluate its physical, chemical, structural and bioactive properties. Material and methods: Particle size (Zetasizer nano s90). High impact milling (Premium line pulverisette 7, Fritsch, Alemania). Morphology and composition of powder (Sonics vibracell VCX130, SEM Joel Field Emission 6701F, TEM JEM-2100 Jeol USA. Obese rats Sprague Dawley, males and females, group 1 control, group 2 hypercaloric diet, group 3 hypercaloric diet with nanoparticulate powder. Results: Figure 1:

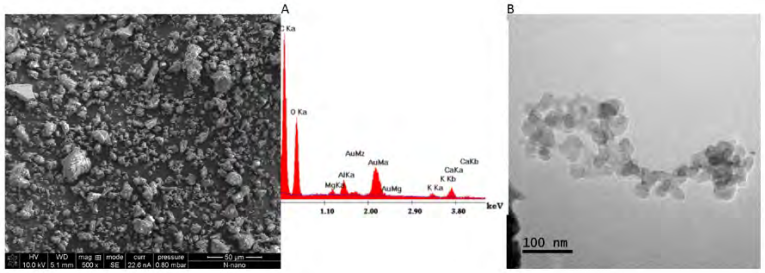

Figure 1. A) SEM image of nopal nanoparticles and EDS spectrum, B) TEM image of nanoparticles and diffraction pattern.

It is observed that trace elements are Al, Ca, Mg and K, Ca, salts (K) and contaminants (Al). And the particle size is 92 ± 26.39nm. The effect in female rats its better in low triglycerides, atherogenic index and glucose, as well as an increase in HDL-cholesterol than in male rats. Conclusion: The high impact milling allowed obtaining nopal nanoparticles to perform EDS, SEM and TEM that showed size and the chemical elements of nanoparticles and in vivo studies, suggest that the powder it is good for health.

Key Words: Nopal nanoparticles, High impact milling, effect of nopal, obesity.

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Crystallization synthesis modification for elaboration of inorganic perovskite quantum dots $CsPbX_3$, X = Cl, Br, I

J. P. Guerrero[1*], V. H. Romero[1], T. Lopez-Luke[2], E. De la Rosa[2]. B. C. Sulbarán-Rangel[1]

[1]Centro universitario de Tonalá de la Universidad de Guadalajara, División de Ciencias, Tonalá Jal. Nuevo Periférico #555, 48525, México.
[2]Centro de Investigaciones en Óptica, A. P. 1-948, León Gto. 37160, México.

*pablinguerrero@hotmail.com

Inorganic Cesium Lead Halide Perovskite Quantum Dots PQD's $CsPbX_3$, X=Cl, Br, I, have shown great opticals and electronic properties, there are attractive for the manufacture of electroluminescent devices. In the present work, PQD's $CsPbX_3$, X = Cl, Br, I, were prepared by 3 different synthesis techniques, Hot-Injection synthesis, crystallization synthesis, and a modification to the crystallization synthesis; in which the crystallization synthesis route was changed, combining it with the hot-injection technique for the elaboration of QPD's $CsPbX_3$, X = Cl, Br, I. The absorption and emission spectra of PQD's $CsPbX_3$, X = Cl, Br, I, were adjusted to the entire visible spectral region by a variation of their composition and particle size (quantum confinement effects). The photoluminescence of all the quantum dots of perovskite was remarkably bright with high quantum efficiencies. The absorption threshold of PQD's $CsPbX_3$, X = Cl, Br, I were found at 434 nm, 515 nm, and 690 nm, respectively; and the emission peaks were 440 nm, 520 nm, and 700 nm, and are characterized by having a narrow emission spectrum. The analysis of the results has allowed us to find the advantages and disadvantages of each of the synthesis method, and their use in optoelectronic devices.

UV-Vis, SEM and photoluminescence in Nanoprisms of Ag

Iván Edoardo Gil García[1*], Georgina Beltrán Pérez[1], Martín Rodolfo Palomino Merino[1], Hugo Méndez Martínez[1], Juan Castillo Mixcóatl[1], Juan de la Cruz Quiroga[1], Severino Muñoz Aguirre[1], Ivan Hernández Gutiérrez[1]

[1]Facultad de Ciencias Físico Matemáticas, Benemérita Universidad Autónoma de Puebla. Apartado Postal 1152, 72000, Puebla, Pue. México

*edoardogil@hotmail.com

This work was born with the need to have a major control in the size and shape of Ag's nanoparticles. With this in mind the absorption spectra were studied for Ag's nanoprisms that were obtained by oxide reduction process, which were applied the technique of photoluminescence with a maximum electric power of 13 watts through an exposure period of 24 Hours, due to that nanoparticles of Ag are sensitive to radiation. The nanoparticles were exposed to RGB light with the colors blue, green, red, yellow and white, obtaining as a result different visible tonalities of the nanoparticles as changes in their UV-Vis spectra. All the changes of Ag's nanoparticles were submitted to a cleanliness by centrifugation, the RPM were calculated according to the expected size of the nanoparticles. To be able to obtain their morphology SEM was applied obtaining finally nanoprisms of 8nm in diameter with potential bio-medical applications.

Key Words: photoluminescence, nanoprisms, nanoparticle, SEM.

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Tunable laser source based on a fiber optic tapered coated with Au and Ag nanoparticles

Hugo Méndez Martínez[1*], Georgina Beltrán Pérez[1], Martín Rodolfo Palomino Merino[1], Ivan Hernández Gutiérrez[1], Juan Castillo Mixcóatl[1], Juan de la Cruz Quiroga[1], Joaquín Munive Parra[1], Severino Muñoz Aguirre[1], Iván Edoardo Gil García[1]

[1]Facultad de Ciencias Físico Matemáticas, Benemérita Universidad Autónoma de Puebla. Apartado Postal 1152, 72000, Puebla, Pue. México

*hugosan67@gmail.com

Lasers based on erbium-doped fibers play an important role in many applications. This work presents the characterization and implementation of an annular cavity laser, in which we used as an active element 30 cm of erbium-doped fiber (ER 30). As a tuner element, a taper was performed by means of an electric arc generated by a splicer on a standard fiber which was coated with SiO_2 doped with gold and silver nanoparticles at different molar concentrations. The coating is performed using technique sol-gel, using as a precursor TEOS. The main idea is to excite SPR due to the interaction of the evanescent wave generated by optical devices with a thin film of Au and Ag nanoparticles to apply as a filter, which generates an offset spectral making temperature variations with a Peltier plate of 20 to 80°C, with a 40nm tuning range.

Key Words: cavity, laser, nanomaterials, nanoparticles, plasmon.

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Comparing the chemistry of Al_{13} cluster and At

Bertha Molina Brito[a], Jorge Ramón Soto Mercado[a], Jorge Javier Castro Hernández[b]

[a]Facultad de Ciencias, Universidad Nacional Autónoma de México, Apdo. Post. 04510 Cd. de México, México.
[b]Departamento de Física, CINVESTAV del IPN, Apdo. Post. 14-740, 07000 Cd. de México D.F., México.

mlnbrt@ciencias.unam.mx

The alpha emitter Astatine-211, a not naturally occurring isotope, is considered one of the most promising radionuclides for targeted alpha therapy (TAT) in cancer treatment. However, due to the scarcity and short half-life of all At isotopes, its use has been hindered by its not well understood chemistry and the in vivo deastatination. Hence, any attempt to understanding it better is imperative. Adding efforts in this direction, in a previous theoretical study we showed that the halogen and alkali bonding with Al_{13} and At, presented a strong similarity on their charge transfer processes, provides a promising proof of concept that the Al_{13} cluster mimics the behaviour of At. In this work we extend our study on the possible chemical similarities between Al_{13} and At, and perform scalar relativistic ZORA-DFT calculations on the compounds corresponding to the astatination of aryliodonium salts, which have been considered as possible precursors for the synthesis of 211At labeled tracers. Next, we predict stable configurations when interchange At by Al_{13} and compare the corresponding molecular graphs of these compounds obtained from atoms in molecule (AIM) calculations.

The authors acknowledge to the Direción General de Cómputo y de Tecnologías de la Información (DGTIC-UNAM) for providing Supercomputing resources on "Miztli" through the project LANCAD-UNAM-DGTIC-298.

Key Words: Astatine, Al_{13}, aryliodonium salts, Atoms in Molecule analysis

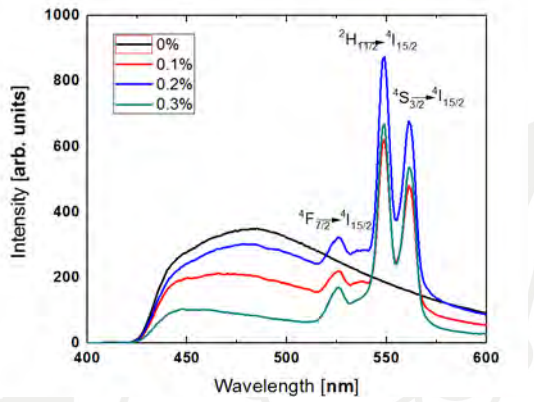
Photoluminescence spectra of ZrO_2 nanoparticles doped with Er^{3+} at different concentrations

Miguel Ojeda M.[1], Víctor M. Rentería T.[1], Ma. Luisa Ojeda M.[1] and Celso Velásquez O.[1]

[1]Universidad de Guadalajara, Centro de Investigación en Nanociencia y Nanotecnologías, CUVALLES Carretera Guadalajara-Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México

miguel.ojeda@valles.udg.mx; miguelojedama@gmail.com

Nowadays, the design of materials that could improve the electronic, optic, vibrational and luminescent properties have gained much attraction due to the possibility to generate a new variety of optoelectronic devices [1, 2]. Specially, zirconium oxide (ZrO_2) is a good candidate for optical applications, due to its high optical transparency from the visible to the near infrared region and its optical band gap, which are ranging between 5.1 to 7.8 eV [3]. By this way, ZrO_2 commonly could be doped with a luminescent rare earth ion to take advantage of the good transparency and improve the luminescent intensity emission. In this work, a study of luminescent properties of zirconium oxide (ZrO_2) doped with different Er^{3+} concentrations was performed. Four samples of ZrO_2:Er (Er^{3+}=0, 0.1, 0.2 y 0.3%) were synthesized by the sol-gel method. The measurements were performed using an excitation of 380 nm, the results show three emission bands attributed to electronic transitions $^4F_{7/2}\rightarrow{}^4I_{15/2}$, $^2H_{11/2}\rightarrow{}^4I_{15/2}$ and $^2S_{3/2}\rightarrow{}^4I_{15/2}$, all of them related to erbium. Based on the luminescent spectra we could see that the sample with an Er^{3+} concentration of 0.2% present the higher luminescent intensity



Key Words: nanoparticles, zirconium oxide, photoluminescent, rare earth.

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TUESDAY

Low-temperature ozone treatment for carbon nanotube template removal; The production of ZnO nanotubes by ALD for photocatalytic applications

D. Domínguez[1,2*], J. M. Romo-Herrera[2], F. Solorio[3], H. A. Borbón-Núñez[4], M. Landeros[3], Y. Martínez[3], J. N. Díaz de León[2], E. A. Reynoso-Soto[5], H. Tiznado[2], G. Soto[2]

[1]Posgrado en Ciencias de la Ingeniería, Instituto Tecnológico de Tijuana.
[2]Centro de Nanociencias y Nanotecnología, UNAM, Km 107 Carretera Tijuana-Ensenada Ensenada, B.C. C.P. 22800, México.
[3]Universidad Autónoma de Baja California, Facultad de Ingeniería, Arquitectura y Diseño.
[4]CONACYT-Centro de Nanociencias y Nanotecnología, UNAM, Km 107 Carretera Tijuana-Ensenada s/n, Ensenada, B.C.
[5]Centro de Graduados e Investigación. Instituto Tecnológico de Tijuana.

david@cnyn.unam.mx

This work addresses the production of stand-alone ceramic nanotubes by the template-based ALD method at low temperature. Nitrogen-doped multiwalled carbon nanotubes (CNTs) were coated with ZnO. Afterward, the template removal approach was evaluated. Two different approaches were compared: using oxidation in dry air or in an ozone-rich atmosphere. The main point is to evaluate both procedures. The samples treated by the two different methods were analyzed by XRD, TEM, SAED and Raman spectroscopy. The dry air atmosphere requires high temperatures (~700 °C) for a complete CNT removal; at that temperature the ZnO tubular shape is completely collapsed due to recrystallization. Under ozone atmosphere, the template can be removed at temperatures as low as 85 °C; this temperature is lower than the ALD preparation temperature (120 °C). The ozone treatment maintains the tubular shape of the ZnO nanostructures. The use of ozone for the template removal approach, reinforces the template-based ALD method to produce inorganic nanotubes. Finally, The ZnO nanotubes were evaluated as photocatalytic material in the degradation of the alimentary azo dye amaranth.

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Effect of plasma power modulation on CdTe thin films growth at room temperature by RF magnetron sputtering

E. Rosendo, R. Romano-Trujillo, L. Treviño-Yarce, C. Morales, T. Díaz, G. Gacía, R Galeazzi and A. Coyopol

Posgrado en Dispositivos Semiconductores, BUAP, Av. San Claudio y 14 Sur, Edificio IC5, Ciudad Universitaria, C.P. 72570, Puebla, Pue. Mexico
A. I. Oliva
Centro de Investigación y de Estudios Avanzados del IPN Unidad Mérida. Departamento de Física Aplicada. Km. 6 Antigua Carretera a Progreso, A.P. 73-Cordemex CP 97310, Mérida, Yucatán, México.
J. M. Lugo
Instituto Tecnológico Superior Progreso, ITSP, Boulevard Víctor Cervera Pacheco, S/N x 62, C. P. 97320, Progreso, Yucatán, México

enrique171204@gmail.com

We have investigated the structural, morphological and optical properties of CdTe thin films deposited on glass substrates at room temperature in order to study the effect of the RF plasma power ramps by sputtering technique. Sputtering pressure was maintained at 10 mTorr and deposition time was fixed at 120 minutes, during this time the RF plasma power varied between 40 to 30 W like a “V". The analysis of low angle X-ray diffraction (XRD) showed that CdTe films were polycrystalline with cubic structure and preferred orientation along (111) direction. The calculated average crystallite size increases from 16.6 to 29.2 nm as the RF plasma power ramps quantity increases. Raman scattering spectra showed that the peaks intensity at 123, 140 and 164 cm-1 are higher as the RF plasma power ramps quantity increases. The AFM studies showed that the rms-roughness and grain size values increase from 0.8 to 1.6 nm and 62.8 to 92.1 nm as the RF plasma power ramps quantity increases. The absorbance spectra in the UV-Visible region showed that the energy bandgap value is higher (from 1.47 to 1.54 eV) when the RF plasma power ramps quantity employed during deposition of the CdTe films increase. Obtained results show that films deposited with this technique can be used as absorber material in photovoltaic applications like the ZnO/CdTe and CdS/CdTe solar cells.

Key Words: RF magnetron sputtering, plasma power modulation, CdTe.

Morphologic analysis of functionalized Carbon Nanotubes (CNTs) by Silicon decorated process

J.S. Sanchez Nieto1, J. Martínez Reyes[1], G. Urriolagoitia Sosa[1], B. Romero Ángeles[1], G.M. Urriolagoitia Calderón[1]

[1]Escuela Superior de Ingeniería Mecánica y Eléctrica (ESIME), Instituto Politécnico Nacional (IPN), Sección de Estudios de Posgrado e Investigación, edificio 5, 2° Piso, Unidad Profesional Adolfo López Mateos, Zacatenco, C.P. 07738, Ciudad de México; México.

jsebastiansn@hotmail.com

Carbon Nanotubes has been an interesting research topic because of their mechanical, electrical and optical properties. This makes nanotubes qualified candidates for nanocomposites fabrication for different applications. However one of the most remarkable difficulties in this area is the accomplishment of nanotubes dispersion in the used matrices. Carbon nanotubes functionalization makes possible to diminish this limitation providing them functional groups that led nanotubes to adhere uniformly in the matrix. Silicon decorated is a functionalization process used for its simplicity and the low affectation of nanotubes structure. In this work is presented the morphologic analysis and chemical composition of silicon decorated multi-walled carbon nanotubes (MWCNTs) by scanning electronic microscope (SEM) and Energy-dispersive X-ray spectroscopy (EDS) respectively. The SEM analysis gives characteristics such as nanotubes diameters, length and other particles presence. Studies proved the successful silicon inclusion in nanotubes clusters and the right integrity of the nanostructures after treatment.

Key Words: Morphology, CNT, functionalization, silicon, microscopy.

Theoretical considerations in the production of silver nanoparticles by laser ablation confined in distilled water

[1]D. O. Oseguera Galindo, [2]M. T. Valenzuela López, [3]A. M. Carrillo Flores, [1]E. Oceguera Contreras and [4]S. Negrete Aragón

[1]Centro Universitario de los Valles, UdeG, Km 45.5, Carretera Guadalajara-Ameca, Ameca, 46600, Jalisco, México.
[2]Centro de Nanociencias y Nanotecnología, UNAM, Km 107 carretera Tijuana-Ensenada, Ensenada Baja California, México.
[3]Ingeniería en Nanotecnología, ITESO, Tlaquepaque, 45604, Jalisco, México.
[4]Facultad de Ciencias, UNAM, Cd. Universitaria, Ciudad de México, 04510, México

david.oseguera@academicos.udg.mx

Laser ablation is a physical method useful to obtain metallic nanoparticles, it is consist in the interaction of a high power laser on a target immersed in a liquid medium generating plasma during this interaction that is confined for the high density of the medium, while electronic recombination is attribute to the rapid cooling, causing the ions to pass to their neutral state, favoring the nanoparticles formation [1]. However to have knowledge of the silver nanoparticles amount by this method commonly is employed instruments to measurement the silver concentration in the colloidal solution. In consequence, in this research is suggesting another mechanics, taking advantage of theoretical considerations which depend of laser parameters and intrinsic properties of a silver target during the synthesis. From the calculus, this resulted a mass ablation per laser pulse ≈ 0.03 mg/ml. Additionally of the micrographs obtained with the TEM was considered the center ≈ 12 nm of the Gaussian curve in the size distribution to calculated its corresponding nanoparticle mass ≈7x10-18grs . By making a relation between the silver mass with the nanoparticle mass was calculated a concentration around 4x1012 nanoparticles/ml, being comparable with the commercial silver nanoparticles reported.

Key Words: Theoretical considerations, laser ablation, nanoparticles production.

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Surface modification of magnetite nanoparticles for the production of electrocatalizers

Cervantes-Arreola O.[1*], Rosales-de los Santos S.[1], Pérez B. V.[1], Casillas N.[1]

[1]*Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421, C.P. 44430, Guadalajara, Jalisco, México.*

*ocervantesa@gmail.com

Surface modification of magnetite nanoparticles (MNP) allows incorporating electroactive functional groups, such as carbonyl, nitro and hydroxyl or catechol and quinones molecules in alkaline media [1]. It produces magnetic core nanoparticles capable of being modified subsequently for producing electrocatalysts [2]. In this work, MNP´s are synthesized by a coprecipitation method using ammonium hydroxide as precipitating agent. Surface modification of the magnetite is carried out by sonication and vigorous stirring using tetrahydroquinone (THQ) and 1,2-dihydroxybenzene molecules. The size of the nanoparticles is controlled by varying the reaction temperature and the agitation of the medium. The results include a crystallographic characterization by XRD of the modified and unmodified magnetite nanoparticles that revels a reverse spinel type structure, a FTIR study that demonstrates the functionalization of the magnetite surface and the uses of vibrating sample magnetometer (VSM) probes a superparamagnetic response. The electrochemical characterization of the surface modified magnetite is performed by means of cyclic voltammetry (CV) in a Pt working electrode attached with a neodymium magnet in the back, in an arrangement called Magnetic Modified Electrode (MME). It is reported the irreversible oxidation of the remaining hydroxyl groups of the THQ molecule, bound to the magnetite surface via two hydroxyl groups via surface modification.

Key Words: Magnetite, THQ, Nanoparticle, Magnetic and MNP.

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Nano cobalt-ferrite as a selective catalyst for the oxidation of aromatic sulfur in aqueous medium

Mayorga Beltrán Edgar, Santiago Cuevas Alan Javier, Palacios Cabrera Cristian B, Carlos Alberto Huerta Aguilar, Jayanthi Narayanan, Cisneros Tamayo Ricardo, José Antonio Juanico Loran

Ingeniería en Nanotecnología, Universidad Politécnica del Valle de México, Av. Mexiquense s/n esquina Av. Universidad Politécnica, Col. Villa Esmeralda, Tultitlan Estado de México, México

jnarayanan@upvm.edu.mx

Cobalt-ferrite nanoparticles $CoFe_2O_4$ was synthesized by co-precipitation method and characterized by FT-IR, UV-vis, and X-ray diffractometry. Morphological analysis by TEM and AFM of synthesized nanoparticles showed the particles size of 19-100 nm with homogeneous distribution. The catalytic activity of $CoFe_2O_4$ NPs was analyzed with different sulphur compounds (thiourea, anisole and 2-mercaptobenzimidazol) by varying the reaction conditions (pH, temperature, and photo effect). The analysis of kinetic parameters and sulphur degradation percentage showed that cobalt-ferrite is a selective catalyst for the oxidation of aromatic sulphur compounds in the presence of peroxide as oxidation agent.

Key Words: cobalt-ferrite, catalytic oxidation, 2-mercaptobenzimidazole, anisole

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Nanoconcave arrays using low-purity Aluminum for plasmonics in the UV-VIS spectral range

R. González-Campuzano[1*], M. E. Mata-Zamora[2], S. López-Romero[1] and D. Mendoza[1]

[1]*Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, A. P. 70-360, Ciudad de México 04510, México.*
[2]*Instituto de Ciencias Aplicadas y Tecnología, Universidad Nacional Autónoma de México, A. P. 70-186, Ciudad de México 04510, México.*

*naedra_9999@hotmail.com

The size-controllable aluminum nanoconcave arrays were synthesized by electrochemical anodization of high and low-purity aluminum foils using oxalic, phosphoric and citric acids. The plasmonic properties of nanoconcave arrays in the two types of Al were investigated based on specular reflectance in the 190-1400 nm wavelength range. We found that their optical reflectance was dramatically reduced as compared with unstructured Al. At the same time pronounced reflectivity dips were detectable in the 280–1250 nm wavelength range for the case of high-purity aluminum while for low-purity aluminum were within 260–580 nm, which were ascribed to plasmonic resonances of first and second orders. As a proof of principle of an application, we placed graphene on top of the nanoconcave arrays and observed a Surface Enhanced Raman Scattering (SERS) effect that result in an intensity increase of the characteristic G and 2D bands of graphene induced by the plasmonic properties of Al nanoconcave arrays. The maximum increase was achieved when the plasmonic resonance almost matched with the wavelength of the excitation laser probe of the Raman system. This study is important since we used low purity aluminum at low cost to design and fabricate SERS substrates which can be used in practical applications.

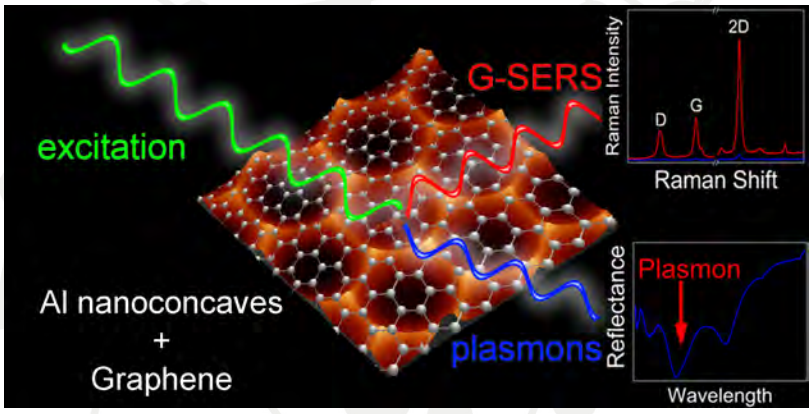

Figure 1. Plasmonic system of aluminum nanoconcave arrays to be used in Surface-Enhanced Raman Scattering (SERS) and proposed as Graphene-Surface Enhanced Raman Scattering (G-SERS) substrate.

Key Words: plasmonic aluminum, graphene, SERS, GERS

Synthesis and characterization of TiO_2 nanospheres

Kevin Manuel Esparza Ramírez[1], Virginia Francisca Marañón Ruiz[1], Corinna Janeth Enríquez Sánchez[1], Héctor Pérez Ladrón de Guevara[1], Jesús Castañeda Contreras[1], Rubén Arturo Rodríguez Rojas[1], Rita Judit Patakfalvi[1] and Roger Chiu Zarate[1]

[1]*Universidad de Guadalajara, Av. Enrique Díaz de León No. 1144, Colonia Paseos de la Montaña, C.P. 47460, Lagos de Moreno, Jalisco, México.*

vmaranon@culagos.udg.mx

In the fabrication of dye-sensitized solar cells (DSSC), titanium dioxide is one of the best photoanode materials due to its excellent photo-catalytic properties, low cost and absorption in a small range of the ultra-violet spectrum. Conventionally, nanoparticles of 15-20 nm are used as photoanode material [1]. However, there has been study on other TiO_2 morphologies for applications in DSSC's, such as nanotubes and nanospheres [2,3]. In the case of nanospheres, it has been shown that these structures duplicate conversion efficiencies when compared to traditional practice with nanoparticle materials [4]. This study encompasses both the synthesis and the characterization of hollow TiO_2 nanosphere shells by method of self-assembly in solution, using Poly (Methyl Methacrylate) [PMMA] as a hard core which is later removed by calcination at 500 oC as reported by Imhof [5]. With this method, we have obtained 3-dimensional sphere structures in the range of 30-40 nm in diameter size, as characterized by AFM and in accordance with results by Imhof [5]. We also obtained bandgap values and phase characterization by UV-VIS and XRD respectively. Bandgap values were registered between 2.89-2.98 eV. The crystallites presented Anatase phase of ~20-30%, while Rutile phase had a predominant presence of ~70-80%. These results will be useful for further application of the hollow nanosphere material in DSSC, where reports state that Anatase phase presents 30% higher short circuit current when compared to Rutile phase, however the same reports also state that this may be mostly due to pure Anatase and pure Rutile particle size differences, causing different superficial area and dye adherence [6], and with this further study, we may determine if it is necessary to obtain pure Anatase TiO_2 hollow nanospheres.

Key Words: TiO_2, Nanocomposite, Semiconductors.

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Synthesis and characterization of TiO_2 nano "bacillus"

Kevin Manuel Esparza Ramírez[1], Virginia Francisca Marañón Ruiz[1], Corinna Janeth Enríquez Sánchez[1], Héctor Pérez Ladrón de Guevara[1], Jesús Castañeda Contreras[1], Rubén Arturo Rodríguez Rojas[1], Rita Judit Patakfalvi[1] and Roger Chiu Zarate[1]

[1]Universidad de Guadalajara, Av. Enrique Díaz de León No. 1144, Colonia Paseos de la Montaña, C.P. 47460, Lagos de Moreno, Jalisco, México.

vmaranon@culagos.udg.mx

In the fabrication of dye-sensitized solar cells (DSSC), titanium dioxide is one of the best photoanode materials due to its excellent photo-catalytic properties, low cost and absorption in a small range of the ultra-violet spectrum. Conventionally, nanoparticles of 15-20 nm are used as photoanode material [1]. However, there has been study on other TiO_2 morphologies for applications in DSSC's, such as nanotubes and nanospheres [2,3]. In the case of nanotubes, it has been shown that these structures offer an increase in electron diffusion lengths, longer electron lifetimes and excellent antireflection coatings, however if grown on the transparent electrode they present deterioration of the transparent conducting oxide (TCO) layer [2,4]. This study replicates the synthesis TiO2 nanotubes by solvothermal method as reported by Suzukia [5], using 70 nm size particles and 10 M NaOH solution as precursors. With this method, we have obtained 3-dimensional tube/bacillus structures in the range of 100-200 nm in diameter size and 0.3-0.5 µm in length, as characterized by AFM. We also obtained bandgap values by UV-VIS registered around 3.19 eV. These results present slight differences from those reported by Suzukia [5], however this may be due to the difference between using a glass pressure tube (us) and a stainless steel autoclave (Suzukia) for the synthesis, meaning that pressure is a defining constant in the formation of the nanotubes. However, diameter is in accordance with particle size, since our experiment used particles 7 times larger in diameter than those reported by Suzukia [5]. This study will be useful for further application of the material in DSSC, however it has been contemplated to assure our results by replicating the experiment once more with the exact equipment used by Suzukia.

Key Words: TiO_2, Nanocomposite, Semiconductors.

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Synthesis and characterization of TiO_2 nanoparticles functionalized with an AZO-triphenilmethane dye for DSSC applications

Corinna Janeth Enriquez Sánchez[1], Kevin Manuel Esparza Ramirez[1], Samuel Mardoqueo Afanador Delgado[1], Roger Chiu Zarate[1], Jesús Castañeda Contreras[1], Miguel Mora González[1], Virginia Francisca Marañón Ruiz[1]

[1]Universidad de Guadalajara, Av. Enrique Díaz de León No. 1144, Colonia Paseos de la Montaña, C.P. 47460, Lagos de Moreno, Jalisco, México.

vmaranon@culagos.udg.mx

In the last 30 years, dye-sensitized solar cells (DSSC) have been based on porous semiconductor oxide electrodes such as TiO_2 and have been systematically studied and have become promising for the generation of solar electricity. However, the security requirements of DSSC are stricter: a photographic dye is subjected to an excitation and the subsequent redox reaction only once. On the contrary, for a photovoltaic cell, continuous photoexcitation-reaction-regeneration cycles are required [1]. In order to increase power conversion efficiency, most research has focused on the development of new metal-free organic dye sensitizers [2]. The azo-triphenylmethane dyes have both characteristics for their application in this type of cells. The z-scan technique offers us the value of the non-linear absorption coefficient, which allows knowing the color in a good prospect. Hence, the synthesis of nanoparticles of TiO_2 with a dye of this family is proposed for its application in solar cells and improve the efficiency of them. For the preparation of the nanoparticles, we used titanium isopropoxide dissolved in ethanol that was kept in a solution of dye-ethanol-water and kept in agitation for 24 hours. Subsequently, the nanoparticles were centrifuged and washed obtaining a yield of 93%, as well as a λ_{max} = 560 nm, corresponding to the dye. Finally, the z-scan technique was applied, from which values of n_2 = 3.37x10-3 and β = 1.28*105 were obtained. These results allow us to conclude that the incorporation of the dye to the nano particles is a good option to improve the efficiency of solar cells sensitized by dye.

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Design and fabrication of crossed nanowire arrays for supercapacitor applications

Wei Ge[1], Shaoxian Song[2], Armando Encinas[1]

[1]*División de Materiales Avanzados, Instituto Potosino de investigación Científica y Tecnológia, A. C., Camino a La Presa de San José 2055, C.P. 78216 San Luis Potosí, S.L.P, Mexico.*
[2]*School of Resources and Environmental Engineering, Wuhan University of Technology, Luoshi Road 122, Wuhan, Hubei, 430070, China*

wei.ge@ipicyt.edu.mx

Currently, the researches on supercapacitors mainly focus on the combination of carbon based materials (graphene, carbon nanotube) and transitional metal oxides/hydroxides [1-3]. Transitional metal oxides/hydroxides have high energy density, but their disadvantages are poor conductivity, low power density and short cycling life. In order to improve their drawbacks for supercapacitor applications, they are combined with carbon based material with high power density, long cycling and good conductivity [4, 5]. Carbon based material is used as a substrate for the growth of transitional metal oxides/hydroxides and a current collector to improve the conductivity, rate capability of the composite.

Here, a crossed nanowire arrays with porous surface structure is developed and used as supercapacitor electrode material. The crossed nanowire array is fabricated by electrodeposition of transitional metal into porous polymeric template. After removal of the template, the nanowire array is obtained and then treated by surface oxidation to produce metal hydroxide with porous structure. The obtained nanowire arrays with porous surface structure can offer large specific capacitance and collect current at the same time. This work open a new way for supercapacitor research.

Key Words: nanowire array, supercapacitor, electrodeposition, polymeric template.

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Flexible circuits for applications in wearable electronics

G. Alvarez, N. González, D. Cardona, E. Araujo*

Instituto Tecnológico y de Estudios Superiores de Occidente, Periférico Sur Manuel Gómez Morín # 8585 C.P. 45604 Tlaquepaque, Jalisco, México.

elsie@iteso.mx

The purpose of this research is to create flexible-polymer-based substrate as a Printed Circuit Board (PCB) to stand a wearable electric circuit. Since it is pretended to be used at big and small scales, on different fields, it has to be easily built and low cost; therefore, two methods were used, the first is based on film deposition with physical vapor deposition (PVD) and the second uses prefab conduct films that are added to the commercial, low-cost polymer. Because polymer-based substrates were used [1], the pollutant that is produced when manufacturing and the ones that the rigid PCB's contain are avoided. A goal is fabricated circuits using a latex-base substrate that all together with graphene and electric tracks (metallic depositions) could be used as biodegradable circuits on emerging markets as the internet of things (IoT's) and wearable electronics. Another goal was to find a deformation vs resistivity curve to material that allows adding the film and at the same time let it conduct when is flexed. For this reason, the concentration of the monomer and the catalyzer were modulated to variate the mechanical proprieties. Superficial modifications like the removal of oligomers were implemented to create a hydrophilic surface, bending and stretching test was performed at different angles measuring the changes in resistivity with an SMU Keithley 2400.

Key Words: wearable electronics, stretchable, low cost, easy to build

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Study and fabrication of a microporous foam for water-oil separation from a non expensive and commercial silicone rubber

N. González, E. Araujo*

Instituto Tecnológico y de Estudios Superiores de Occidente, Periférico Sur Manuel Gómez Morín # 8585 C.P. 45604 Tlaquepaque, Jalisco, México

*elsie@iteso.mx

Saving water to save the planet is what we need to do now. Hydrocarbon is the wide contaminants of water in the world [1]. In this work, we proposed the study and fabrication of a low-cost alternative material to separate oil from water. Specific we create a non-expensive an oleophilic porous material from a commercial silicon rubber OOMOO 30® which is commonly used to create molds copying surfaces. For the present work, sugar and salt crystals were used as sacrificial templates to "copy" for inducing porous within rubber volume to increase the surface area. Different proportions of monomer and catalyzer were used to tailoring mechanicals properties and hydrophobicity. The oil mass sorption capacity (M_{abs}) and volume absorption (V_{abs}) capacity were evaluated by using the following equation: $M_{abs} = (m - m_0)/m_0$ $V_{abs} = (m - m_0)\ \rho_0/\rho m_0$ where m is the weight of the sample after sorption, m_0 is the initial weight of the sample, ρ_0 and ρ are density values of the absorbent material and absorbed oil, respectively [2]. Different kinds of oils were used. Repeated absorption-desorption cycles of oils were performed to evaluate sponge reusability.

Key Words: Micro-porous foam, silicone rubber, oil separation, hydrophobicity.

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Magneto-mechanical piezoresistive caltilevers as magnetic field sensors

R. S. Osorio Velázquez*, J. A. Montenegro Ríos, A. Encinas

División de Materiales Avanzados, Instituto Potosino de Investigación Científica y Tecnológica A.C. (IPICYT), Camino a la Presa San José # 2055., Col. Lomas 4 sección, CP. 78216. San Luis Potosí, S.L.P., México

*r.selene.osorio@gmail.com

This work describes the fabrication process of a piezoelectric cantilever based on paper, employing Rochelle salt and magnetic nanoparticles. All the elements used in the fabrication of this sensor are eco-friendly, low-cost and highly available. The working principle is based in that Rochelle salt presents piezoelectric properties in response to applied mechanical stress. Coupling the salt with superparamagnetic nanoparticles incorporates magnetic functionalities. In particular, the magnetic nanoparticles allow generating deflections of the cantilever in response to an applied magnetic field. The fabrication of the paper-based cantilevers is done by infiltrating the porous structure of paper with a saturated solution of Rochelle Salt in which the magnetic nanoparticles are dispersed. In this work we present the results of the cantilever output voltage as a function of the magnitude of the applied magnetic field for several magnetic nanoparticle concentrations as well as for different cantilever configurations. Preliminary results suggest that these cantilevers can be used as magnetic field sensors. We propose that the cantilever can be used to monitor the energy usage in electrical networks. When the cantilever is located close to an electrical wire, the current that circulates through it, produces a magnetic field and the cantilever is deflected proportionally. This deflection produces a voltage that is sensed with an Arduino board and correlated with energy consumption in the electrical network by means of a calibration procedure.

Key Words: Piezoresistive, Rochelle Salt, Magneto-mechanical, magnetic field sensors.

Photodegradation of rhodamine 6G by AG_2O and AG/AG_2O under visible-light irradiation

Ma. De L. Ruiz Peralta[1*], M. Padilla Villavicencio[1], J. H. Camacho García[1], L. Rojas Blanco[2]

[1]Benemérita Universidad Autónoma de Puebla, Facultad de Ingeniería Química, Avenida San Claudio y 18 Sur, C.P. 72570 Puebla, Puebla, México.
[2]Universidad Juárez Autónoma de Tabasco, Avenida Universidad S/N, Zona de la Cultura, Col. Magisterial, Centro, Villahermosa, Tabasco 86040, México.

*lourdes.ruiz@correo.buap.mx

In recent years, different photocatalytic materials and nanocomposites have been fabricated, to date, TiO_2 has proven high efficiency in the oxidative decomposition of dyes, pesticides, and anti-inflammatory drugs. However, its band gap (3.2 eV), and rapid recombination rate of electron-hole pairs lowers the quantum efficiency [1,2], as an alternative metal/ semiconductor nanocomposite have been fabricated, due to metal nanoparticles act as electron scavengers. Nevertheless, TiO_2, and, ZnO can be only excited in the UV region of the electromagnetic spectrum, which is 4% of the solar radiation energy [3], as a result the use of different semiconductors as Ag_2O have been received attention as a promising photocatalyst with narrow band gap of 1.3 eV. In this work, Ag_2O and Ag/Ag_2O nanocomposites were fabricated via two-step approach. The crystal structures, morphology and optical properties were characterized by X-ray diffraction (XRD), SEM, and Diffuse Reflectance Spectroscopy (DRS). The obtained materials were evaluated as a photocatalyst in the degradation of Rhodamine 6G under visible light irradiation, the results show a quantum efficiency of 85% in presence of Ag_2O, however no significant degradation was achieved when the Ag/Ag_2O nanocomposite was evaluated. A photocatalytic mechanism is proposed.

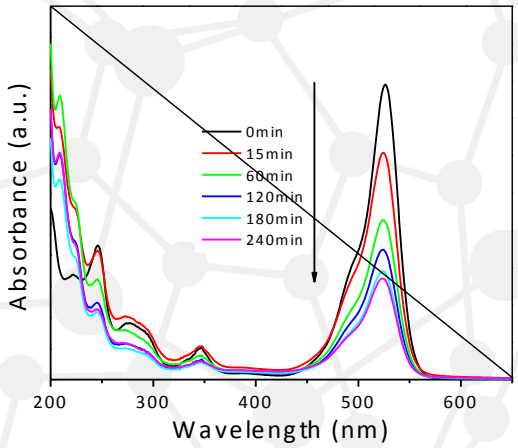

Figure 1. UV-Vis absorption spectra of Rhodamine 6G aqueous solution in presence of Ag_2O.

Key Words: Ag_2O, Rhodamine 6G, photocatalysis.

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Fabrication and characterization of monodisperse calcium ferrite nanoparticles via precursor route

Carlos Alberto Huerta Aguilar[2], Harpreet Kaur[*1], B. S. Randhawa[3] and Jashanpreet Singh[*1]

[1]*School of Chemical Engineering and Physical Sciences, Lovely Professional University, Phagwara, India-144411,*
[2]*Division of Nanotechnology, Polytechnic University of the Valley of Mexico, Tultitlán, Mexico-54910*
[3]*Department of Chemistry, Guru Nanak Dev University, Amritsar, Punjab-143005, India*

*jashanpreet.21529@lpu.co.in; harpreet.21520@lpu.co.in

Monodisperse calcium ferrite nanoparticles have been prepared by the thermal decomposition of propionato and butyrato-ferrate(III) precursors in flowing air atmosphere at a heating rate of 10 °C min^{1}. The reaction mechanism has been obtained from the thermolysis of ferricarboxylate precursors leading to calcium ferrite nanoparticles using Simultaneous thermogravimtery-differential thermogravimtery-differential thermal analysis (TG-DTG-DTA). Direct decomposition of ferricarboxylate intermediates into oxide phase facilitates the formation of ferrite nanoparticles at lower temperature as compared to conventional ceramic methods. The intermediates formed during the reactions have been investigated by Fourier Transform Infra-red (FTIR) and Mössbauer spectroscopy. Further, the final ferrite nanoparticles were characterized by powder X-ray diffraction, Transmission electron microscopy (TEM) and Mössbauer spectroscopy. X-ray diffraction analysis shows the formation of cubic phase spinel calcium ferrites. TEM showed the monodisperse spherical ferrite nanoparticles (~25 ± 0.5 nm) from both precursors. Room temperature magnetic measurements reveals the superparamagnetic nature of all the ferrite nanoparticles. These analysis makes them the potential candidate to be applicable in nanoelectronic devices.

The effect of annealing treatments in the electrical properties of Ti-Cu thin films

Susana Martínez[1], Valeria García[1], José Quiñonez[2], Elsie Araujo[1], Carlos Hernández[3], Rubén Montelongo[1], Dagoberto Cardona[1*]

[1]ITESO, Anillo Perif. Sur Manuel Gómez Morín 8585, Santa María Tequepexpan, C.P. 45604 San Pedro Tlaquepaque, Jalisco, México
[2]Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421, Olímpica, C.P. 44430 Guadalajara, Jalisco, México
[3]Doctorado en Nanotecnología, Cinvestav-IPN, México, DF 07360, México.

dagobe@iteso.mx

The purpose of this work is to improve the electrical properties of titanium thin films through the incorporation of copper as an alloying element and study its performance as an electrical contact in applications for the design and manufacturing of different silicon-based semiconductor devices. In these applications titanium is widely used as an electrical contact because of its Fermi level which varies between 3.6 and 4.3 eV, on the other hand, copper has a high conductivity (1.759x10-6 Ω·cm) but with a high oxidation degree.

The Magnetron Sputtering technique was used to synthesize titanium-copper thin films. The relation Ti/Cu was changed by means the control over the experimental parameters such as deposition rates of titanium and copper and sputtering power applied simultaneously in two different targets (one titanium and other copper), achieving copper incorporation in the range of 5 to 95 at%. P- and N-type Silicon (100) were used as substrates. To evaluate the electrical properties of the samples the four-probe technique was used, and the preliminary results showed a resistivity value of 423 μΩ·cm.

To decrease the substrate influence in the electric measurements the films were deposited with thicknesses greater than 500 nm to reduce the electric resistance values of the samples. The samples were annealed up to 800 °C in Ultra-High Vacuum and the evolution of their electrical properties were evaluated.

Key Words: Electrical properties, thin films, Titanium-Copper, magnetron sputtering, annealing.

Green synthesis of silver nanoparticles using wood industry residual bark

Jose Luis SALAZAR-PEREZ[1*], Diana BARRAZA-JIMENEZ[1], Manuel FLORES-HIDALGO[1], Ma. Del Socorro VAZQUEZ-MENDIETA[1], Abel HURTADO-MACÍAS[2]

[1]Universidad Juárez del Estado de Durango, Av. Veterinaria S/N, Circuito Universitario C.P. 34120, Durango, Dgo. México.
[2]Miguel de Cervantes 120, Complejo Industrial Chihuahua. C.P. 31136, Chihuahua, Chih. México.

*pepszr@gmail.com

Aqueous extracts of wood industry residual bark were used to synthesize stable Ag nanoparticles (AgNPs) from a 0.01 M $AgNO_3$ solution without the aid of any other reductant or stabilizer. Extracts were prepared with different bark weight to solvent volume ratios (1/10, 1/20, 1/50). Extracts were characterized by chemical methods: antioxidant activity was tested by Fe ion reduction and tannin content was evaluated in reaction with lead acetate. AgNPs colloidal solutions were characterized by FTIR. Quinone evaluation was performed to both extracts and colloidal solutions via HCl oxidation. Catechins seem to be present in extracts; and catechinones (quinone form), in resultant colloidal solution. Transmission electron micrography was performed to obtain AgNPs size and morphology. Semi-spherical ~7nm AgNPs aggregates are formed in the surface of a stabilizing molecule. This process confirms the use of residual bark of sawmills in Durango, Mexico as a source of reducing and stabilizing biomolecules for AgNPs green synthesis.

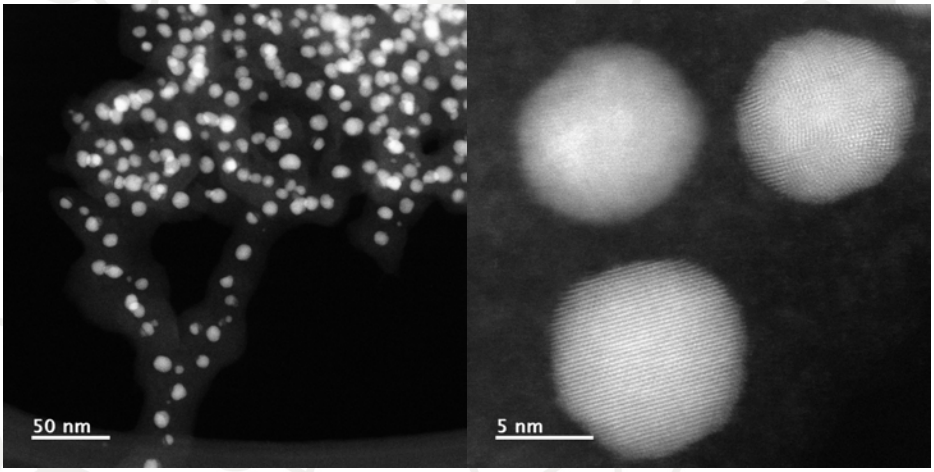

Figure 1 – AgNPs synthesized with 1/50 extract transmission electron micrography.

Key Words: green synthesis, silver nanoparticles, residual bark of sawmills

Synthesis and characterization of Core-Shell Ag0@Fe3O4 nanostructures

Luis F. Vázquez G.[1], Miguel Ojeda M.[1], Karely Chamé F.[1], Victor M. Rentería T.[1] and Celso Velásquez O.[1]

[1]*Centro de investigación en Nanociencia y Nanotecnologías, Centro Universitario de los Valles, Universidad de Guadalajara.*

fergc3939@outlook.com

The synthesis of Ag@Fe_3O_4 was obtained by the hydrothermal method. The XRD spectrum for the obtained sample of Ag@Fe_3O_4 reveal that the magnetite with a single phase. In Figure 1, some intense peaks are observed around 2θ = 30°, 35°, 43°, 53°, 57°and 62°that peaks represent a crystalline phase, cubic spinel structure and free of impurities. In addition, there are some peaks corresponding to Ag (●) at 2θ = 38, 44° and 64°with centered cubic phase. The FT-IR spectrum shown that the sample Ag@Fe_3O_4 exhibits an intense peak at 573 cm^{-1} due to the vibration stretch associated with the absorption band of metal-oxygen (Fe-O in the crystal lattice of Fe_3O_4), peaks between 1000 and 1700 cm^{-1} show bending vibration due to the OH of the water molecule, a peak in 873 cm^{-1} also belonging to the OH bond. The Raman spectrum obtained for the sample of Ag@Fe_3O_4 is shown, in the spectrum we can observe a strong signal around 670 cm^{-1} assigned to the vibration mode A 1g (symmetric stretching of oxygen atoms along the Fe-O bond) and a peak at 218 cm^{-1} assigned to the T_2G mode associated with the translation movement of the whole Fe_3O_4 unit [1-3]. The NPs of Fe^{3+} and Ag^{+} are dispersed among themselves, but with the addition of ethylene-glycol the NPs are reduced to Fe_3O_4 and Ag_0, respectively.

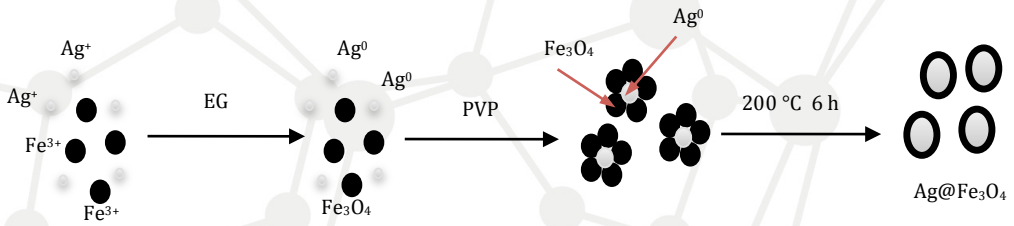

Figure 1 Schematic representation of the formation process of Ag@Fe_3O_4

Key Words: core shell, magnetite, Ag silver, nanoparticles.

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Mechanical and electronic properties of tin carbide structures in three, two and one dimensions

Alma L. Marcos-Viquez*, Alvaro Miranda Durán, Miguel Cruz-Irisson, Luis A. Pérez López

Instituto Politécnico Nacional, ESIME Culhuacán, Av. Santa Ana 1000, 04430 Ciudad de México, México
Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20- 364, 01000 Ciudad de México, México.

*almalorenamarcos@gmail.com

We have theoretically studied the mechanical and electronic properties of tin carbide in bulk phase (zincblende structure), in the form of two-dimensional graphene-like sheets and also in the form of nanowires with a diameter of 1.5 nm and grown along the [100] and [111] crystallographic directions. To obtain these properties, we performed density- functional calculations within the generalized gradient approximation by using the SIESTA code. In particular, we studied how the electronic band structures, the electronic densities of states and the semiconducting gaps are modified by changing the structure dimensionality. Likewise, we calculated the energetic stability and the Young moduli of the different structures studied.

Key Words: tin carbide, electronic properties, DFT.

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CTAB and sodium oxalate for two-steps synthesis of ultrasmall Cu-Pt bimetallic nanoparticles as promising electrocatalyst for the oxygen reduction reaction

I. E. Pech-Pech[1,2*], Y. Verde Gómez[1], R.H. Valencia-Ruiz[1], A.M. Valenzuela-Muñiz[3]

[1]TecNM/Instituto Tecnológico de Cancún, Departamento de estudios de posgrado e investigación (DEPI), Av. Kabah, Km. 3, Cancún, Quintana Roo, México C.P. 77515.
[2]Centro de investigación en corrosión, Universidad Autónoma de Campeche, San Francisco de Campeche, Campeche, C.P. 22860, México
[3]CONACyT-TecNM/Instituto Tecnológico de Cancún, Departamento de estudios de posgrado e investigación (DEPI), Av. Kabah, Km. 3, Cancún, Quintana Roo, México C.P. 77515.

*ildepech@uacam.mx

Metal nanostructures have shown a substantial impact in catalysis field. The replacement of platinum with no-noble metals is a current trend in the proton exchange membrane fuel cell (PEMFC) technology. In this sense, copper nanoparticles have received considerable attention due to its high conductivity and low cost. This work reports the influence of hexadecyltrimethylammonium bromide (CTAB) and sodium oxalate (SO) on the synthesis of CuNPs by a chemical reduction method in aqueous medium under normal atmospheric conditions. In addition, the electrochemical behavior of these particles alloyed with platinum for the oxygen reduction reaction (ORR) in acid medium is presented. The surface plasmon (SP) obtained by UV-Vis spectroscopy was used to identify the formation of CuNPs in aqueous solution. The SP has only been observed when the Cu^{+2} ions are reduced with sodium borohydride (BH) in presence of CTAB. The incorporation OS has demonstrated increasing the intensity of SP signal. The Cu^{+2}:BH:CTAB:SO ratio, which allows to qualitatively know the metallic copper yield, has been optimized as a function of SP signal intensity. A complete disappearance of SP signal is observed when the Pt^{+4} ions are reduced on Cu NPs surface. XRD analysis of these catalysts supported on a carbon surface revealed the formation of metallic copper and copper oxides during the first step of the synthesis, and the formation of Pt-Cu bimetallic nanoparticles (possibly as core-shell structures) in the second step. TEM analysis shows that these nanostructures mainly grow in form of clusters of ultrasmall bimetallic nanoparticles (<5nm). The electrochemical characterization has demonstrated that these nanostructures supported on a carbon surface are stable and active to catalyze the ORR in acid electrolyte. These results could have a significant contribution on the design of new nanostructured catalysts with low percentages of platinum for the ORR in a PEMFC.

Key Words: Sodium Oxalate, Copper nanoparticles, Catalysts.

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Composite films formed by a mixture of silicon oxide and tantalum oxide obtained by HFCVD approach

T. Díaz-Becerril[1,*], V. Herrera[1], G. García-Salgado[1], R. Galeazzi[1], C. Morales[1], E. Rosendo[1], A. Coyopol[1], R. Romano[1], F. G. Nieto-Caballero[1]

[1]*Centro de Investigación en Dispositivos Semiconductores, Universidad Autónoma de Puebla, 14 sur y Av. San Claudio, C. U., C.P. 72570, Puebla, México.*

*tomas.diaz.be@gmail.com

In this work, we report some properties of composites constituted of nanostructures of tantalum oxide and silicon immersed in silicon oxide obtained by hot filament chemical vapor deposition approach (HFCVD). A mixture of Ta_2O_5 and silicon powders compressed to form a pill were used as solid source to grow the films. Percentage of tantalum oxide and silicon were varied in weight in an amount 20mg (Table 1). Molecular hydrogen flow was used as gas reactant and all experiments were carried out at atmospheric pressure. The films were deposited on silicon substrates (100) n-type at temperature processing of 800°C and 1000°C for 10 minutes. The synthesized films were characterized structurally, chemically and optically. By XPS technique it is possible to observe a composite conformed by all the expected elements: silicon, oxygen and tantalum, these results show that samples fabricated at higher temperature present a more stoichiometric relation of SiO_2, while at lower temperature films contain silicon excess forming a silicon rich oxide film. HRTEM pictures displayed an amorphous structure (silicon oxide) and a several conglomerates of silicon nanoparticles and TaO_x in different zones of the film. Photoluminescence results shows an emission band running from 490nm to 880nm, attributed to an overlap of two main bands, one corresponding to (490nm-650nm) due to the presence of the tantalum oxide nanoparticles, and the second one corresponding to silicon nanoparticles (650nm-880nm). Less stoichiometric relation enhances the intensity band in range of TaO_x, reason could be owing to a more creation of oxygen vacancies under this experimental condition.

Table 1 – Experimental details of the power mixture used as source reactants in HFCVD sistem.

Sample reference name	Amount of silicon (mg)	Amount of Ta_2O_5 (mg)
Si-Ta_1	100	0
Si-Ta_2	80	20
Si-Ta_3	60	40
Si-Ta_4	40	60
Si-Ta_5	20	80
Si-Ta_6	0	100

Key Words: Composite, tantalum oxide, silicon oxide, silicon nanocrystals.

Environmental impact of Cu nanoparticles

Martínez BEATRIZ[1], Martínez LUIS[1], Bautista EDUARDO[1], Santiago JESÚS[1]

[1]*Universidad Politécnica del Valle de México, Av. Mexiquense s/n, C.P. 54910, Tultitlán, Estado de México, México*

betymp21@yahoo.com.mx

Copper Nanoparticles (NPs-Cu) have been focus of attention in recent decades because of its electric properties. The synthesis methods of NPs-Cu Involve processes of Oxide-Reduction [1,2] and the environmental impact of this type of synthesis has not been evaluated. In this work, Life Cycle Assessment was developed, based on ISO standards 14040:2006, to analyze the environmental impact of this chemical synthesis of NPs-Cu. As a result of the work it was observed that there are CO_2 emissions in the synthesis of copper nanoparticles towards the environment, we attribute the emissions to the process and propose to improve it or make a subsequent treatment.

Key Words: Environmental, Impact, Cupper, Nanoparticles, CO2.

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Ring-like colloidal deposits formed at uniformly-driven contact lines in saturated atmosphere, effect of the particle electric charge

Gerardo Guerrero-Félix[1], Diego Noguera-Marín[2], Miguel Cabrerizo-Vílchez[2], Miguel Á. Rodríguez-Valverde[2], Carmen Lucía Moraila-Martínez[1]

[1]Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Sinaloa, México.
[2]Biocolloid and Fluid Physics Group, Department of Applied Physics, University of Granada, E-18071 Spain

grardo.g.f@gmail.com

In order to produce well-ordered structures via evaporation of colloidal suspensions (1), it is essential to control the evaporation flux, solute concentration, etc. Several authors have reported that the pH of the solution modifies the final deposit pattern (2-4). Bhardwaj et al. (2) explained the transition between different patterns by considering how the electrostatic and van der Waals forces (known as DLVO forces) alter the particle deposition process. Moraila-Martínez et al. (3) concluded that the morphology of the nanoparticle deposits is modulated to a different extent by the strength of the particle–particle repulsion, the substrate–particle wettability and the substrate receding contact angle. Droplet drying has been widely investigated in many fundamental studies and has been used for several applications like, printing, bioassay manufacturing, colloidal assembly/templating, micro and nanowires fabrication, etc. In this work we used the low rate dynamic contact angle technique using a methodology called Quadratic Flow Rate (QFR) where the liquid flux was varied to obtain a constant contact line velocity during the entire experiment (3). We utilized a microinjector for the drop injection/suction and we analyzed the contact line dynamics during the experiment. As substrate we used PMMA and nanoparticles of SiO_2 of 90 nm. We varied the nanoparticle electric charge and the relative humidity (RH). We obtained that the morphology of the nanoparticle depositions can be controlled by varying and controlling the ambient RH. Furthermore, particle depositions can be even suppressed under certain pH and RH conditions.

Key Words: Drop Coffee Effect, Relative Humidity, Nanoparticles.

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Facile Synthesis of Cu_2O particles with different morphologies

M.S. Aguilar*, G. Rosas

[1]*Instituto de Investigación en Metalurgia y Materiales, UMSNH, Morelia Michoacán, 58000. MEXICO*

*shamj21@gmail.com

This work exposes the synthesis of Cu_2O particles with cubic, octahedral, truncated octahedral and cubic truncated morphologies using a simple chemical reduction method at room temperature. The nanocrystals were synthesized directly in aqueous solution by varying the molar concentration of $CuCl_2$ precursor salt added to the sodium borohydride $NaBH_4$ as a reducing agent. The reaction was carried out by mixing 10 ml (15 mM-20 mM) of precursor salt and 12 ml (2.6 mM) of reducing agent at a speed of 0.348 cm/s under magnetic stirring. The solids obtained were characterized by ultraviolet-visible spectroscopy (UV-vis), X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). UV-vis absorption spectra coincide with those previously reported for the Cu_2ONPs. To confirm the crystal structure of the as-prepared Cu_2ONPs, X-ray diffraction (XRD) analyses were performed. Wherein all samples exhibit peaks at 29.60°, 36.45°, 42.34°, 52.53° and 61.40°. This angular distribution can be indexing to the planes (110), (111), (200), (220), (311) of the cubic structure of Cu_2O, respectively. These results confirm the presence of a pure oxide phase in the solids synthesized. SEM and TEM reveal particles with a cubic morphology at 15 mM $CuCl_2$, with an average particle size of 100 nm. Cu_2O particles are also grown in an octahedral shape at 16 mM of $CuCl_2$, having an average particle size of 150 nm. Finally, truncated octahedral and truncated cubic forms were produced for concentrations in the range of 17 to 20 mM with 100 nm of average size.

Key Words: Oxide materials, Chemical synthesis, Crystal structure, Scanning electron microscopy, SEM, transmission electron microscopy, TEM.

Hydroxyapatite/NPs Ag/ graphene oxide innovative composite, synthesis and characterization

Edith Bravo González[1], Yosemik Arjuna León Nataret[1], Aarón Israel Díaz Cano[1], Efraín Rubio Rosas[2]

[1]Instituto Politécnico Nacional UPIITA-IPN, Av Instituto Politécnico Nacional 2580, La Laguna Ticoman, 07340 Ciudad de México, CDMX
[2]Benemérita Universidad Autónoma de Puebla, 4 Sur #104; Col. Centro C.P. 72000; Puebla de Zaragoza, Puebla, México

aidiaz@ipn.mx

In the area of biomaterials different disciplines interfere due to the complexity that is required in the development of materials. A well-known and used material in this areas is the Hydroxyapatite, this material is one of the most attractive biomaterial for materials that replace bone parts damaged [1]. For this reason different synthesis methods and mixtures with different materials have been developed, an example of this is the incorporation of graphene which improves the mechanical properties and is used in biological sensors [2-4], finally the silver works as an antibacterial agent [5]. The precursors used were: calcium chloride dehydrate ($CaCl_2$. $2H_2O$), dibasic ammonium phosphate ($(NH_4)_2HPO_4$), silver nitrate ($AgNO_3$), Ethylene glycol ($C_2H_6O_2$), dimethylformamide (C_3H_7NO), and graphene oxide (GO). A solution of GO and $AgNO_3$ was dissolved in aqueous solution and was maintained in magnetic stirring by 2 hours, then $(NH_4)_2HPO_4$ on aqueous solution was made and mixed with the first solution, this solution was heated at 50 °C during 3 hours. Finally, the last solution of $CaCl_2$. 2H2O and (NH4)2HPO4 on Ethylene glycol was made, and mixed with the previous solution. These solution was poured on containers of teflon and before start the oven program, was added a dimethylformamide. Finally, the samples were cooled 20 min for his subsequent extraction and centrifuged at 3600 rpm for 10 min, washed with deionized water and dried at 60°C in air. Were used an X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and Fourier transformed infrared spectroscopy for study the structure, morphology and the functional groups of the compound.

Key Words: Biomaterials, Nanocomposite, Graphene Oxide, Hydroxyapatite.

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Custom-Tailored dielectric mirror prepared by thermal atomic layer deposition

J. Lopez[1 *], H. Márquez[2], A. Ortiz - Atondo[3], J. A. Huerta – Salcedo[4], H. Borbón - Nuñez[1], N. Abundiz[4], R. Machorro[4], M. Farias[4], H. Tiznado[4] and G. Soto[4]

[1]CONACYT - Centro de Nanociencia y Nanotecnología, UNAM, Ensenada, B.C. México, Km 107 Carretera Tijuana-Ensenada s/n, Ensenada, B.C., C.P. 22800, México.
[2]Centro de Investigación Científica y Educación Superior de Ensenada - CICESE, Km. 106 Carr. Tij-Ens, Ensenada C.P.22860, México
[3]Facultad de Ingeniería, Arquitectura y Diseño, UABC, Universidad Autónoma de Baja California campus Ensenada, Km. 106 Carr. Tij-Ens, Ensenada, C. P. 22800, México
[4]Centro de Nanociencia y Nanotecnología, UNAM, Ensenada, B.C. México. Km 107 Carretera Tijuana-Ensenada s/n, Ensenada, B.C., C.P. 22800, México

*javierlo21@cnyn.unam.mx

In this work we design and fabricate from n(λ) and k(λ) experimental data for both Al_2O_3 and TiO_2 single layer materials, an optical coating as “dielectric-mirror” following the stack formula $(HL)^8H$. Optical coating based on multilayer film on BK7 glass and Si(100) wafer substrates, was growth by atomic layer deposition (ALD) at 150 °C. The optical constants and optical properties of Al_2O_3 - TiO_2 multilayer stack for a single sample before and after thermal treatment at 450 °C were studied via spectroscopy ellipsometry and Uv – vis measures in the spectral range between 200 to 1100 nm, also similar samples were studied through TEM, SEM and AFM at room temperature in order to obtain information about the morphological properties. From optical studies, we found a rejected zone or “stopband region” between 369 - 464 nm with maximum transmission around of 1.16 % and cut - off points in 364 and 488 nm respectively. A high optical density value after thermal treatment was observed, which indicates a very low transmission of light around 0.01% and the presence of an acceptable bandwidth for rejected zone at λ_0 = 420 nm reference wavelength. Results opens possibility to fabricate a “dielectric-mirror” based on multilayer and propose new designs around these materials for the implementation of optical elements that are required in the industry.

Key Words: Optical coating; multilayers stacks; dielectric mirror atomic layer deposition

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Electrical and optical properties in ultrathin capacitors base on Al_2O_3 - Y_2O_3 growth via atomic layer deposition

J. López[1,*], J. Portelles[2], L. Alvarez[3], J. A. Huerta - Salcedo[4], N. Nedev[5], G. Soto[4], M. Farias[4] and H.Tiznado[4]

[1]CONACYT - Centro de Nanociencia y Nanotecnología, UNAM. Km 107 Carretera Tijuana-Ensenada s/n. B.C., C.P. 22800, México
[2]Facultad de Física, Universidad de La Habana, San Lázaro y L, La Habana 10400, Cuba
[3]Facultad de Ingeniería, Arquitectura y Diseño, UABC, Universidad Autónoma de Baja California campus Ensenada, Km. 106 Carretera Tijuana-Ensenada s/n. B.C., C.P. 22800, México
[4]Centro de Nanociencia y Nanotecnología, UNAM.. Km 107 Carretera Tijuana-Ensenada s/n, Ensenada, B.C., C.P. 22800, México
[5]Universidad Autónoma de Baja California, Instituto de Ingeniería, Blvd. Benito Juárez s/n, C.P. 21280 Mexicali, B.C., México

*javierlo21@cnyn.unam.mx

This work focuses on the study of the electrical and optical properties in ultrathin capacitors based on Al_2O_3 – Y_2O_3 bilayers. A set of 10 samples with a total thickness of about 10 nm were grown by means of thermal atomic layer deposition (ALD) on n-type (100) silicon substrates from Trimethylaluminum (TMA), Tris (methylcyclopentadienyl) yttrium ($(MeCp_3)_3Y$) and water as co-reactants. Thickness and optical parameters were studied via spectroscopic ellipsometry in order to obtain information about the refractive index and dielectric constant behavior. Ellipsometric data revealed an increase of the refractive index when the Y_2O_3 layer thickness varies between 1 and 9 nm. Electrical characterization from Capacitance-Voltage (C-V), Current-Voltage (I-V), capacitance - frequency (c-f), impedance - frequency (z-f) measurements was carried out in order to evaluate the potential of the MOS ultrathin capacitors for micro and nano electronic applications. Results demonstrate that electrical and optical parameters can be modulated by varying the Y_2O_3 layer thickness.

Key Words: MOS capacitors; electrical and optical properties; atomic layer deposition, impedance spectroscopy.

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Afterglow, TL and OSL characterization of Beta irradiated $SrAl_2O_4:Eu^{2+}$, Dy^{3+} combustion synthesized phosphor

N. J. Zúñiga-Rivera[1], R. Ruíz-Torres[2], R. García[3], V. Chernov[3], R. Meléndrez[3], M. Barboza-Flores[3*]

[1]Universidad de Sonora, Unidad Regional Sur, Navojoa, Sonora, México
[2]Departamento de Física, Posgrado en Nanotecnología, Universidad de Sonora, Hermosillo, Sonora 83000, México
[3]Departamento de Investigación en Física, Universidad de Sonora, Hermosillo, Sonora 83000, México

*mbarboza@cifus.uson.mx

Strontium aluminates co-doped with Eu^{+2} and Dy^{+3} were synthesized by the combustion synthesis method employing a highly exothermic redox reaction between the metal nitrates [$Al(NO_3)_3$, $Sr(NO_3)_2$, $Eu(NO_3)_3$ and $Dy(NO_3)_3$] and organic fuel carbohydrazide (CH_6N_4O). The $SrAl_2O_4:Eu^{2+}$, Dy^{3+} phosphors exhibited a distinct TL and OSL depending on the annealing treatment and beta radiation dose exposure. The afterglow, TL and OSL emission were measured depicting a wide emission band centered at 510 nm (green) related to Eu^{2+} ions. The presence of a variety of defects and aggregates were responsible for the observed broad 100 °C peaked TL glow curve of the irradiated sample which is composed of several overlapped TL peaks. The existence of multiple trapping levels, with different trapping/detrapping probabilities, is behind the particular features for the afterglow, TL and OSL emissions. It was demonstrated that in the $SrAl_2O_4:Eu^{2+}$, Dy^{3+} phosphors, the low temperature TL peaked around 30–75 °C is responsible for the long time decay afterglow emission and those around 100 °C were related to very stable trapping states which provide suitable radiation storage properties to be used as a passive TL/OSL radiation detector and dosimeter.

Key Words: Afterglow, TL, OSL, beta radiation, dosimetry.

Thermal impact on Light Emission and Structure of Er-doped Si-rich-HfO_2 films prepared by magnetron sputtering

Brahim El Filali[1*], Jorge L. Ramírez García[1], Tetyana V. Torchynska[2], Larysa Khomenkova[3,4] , Christophe Labbé[5], Xavier Portier[5] and Fabrice Gourbilleau[5]

[1]Instituto Politécnico Nacional, UPIITA, Av. IPN, México City, DF, 07720, México.
[2]Instituto Politécnico Nacional, ESFM, Av. IPN, México City, DF, 07338, México.
[3]V.Lashkaryov Institute of Semiconductor Physics, 45 Pr.Nauky, Kyiv 03028, Ukraine
[4]National University «Kyiv-Mohyla academy», 2 Skovorody str., Kyiv 04070, Ukraine
[5]CIMAP/CEA/CNRS/Ensicaen/UCBN, 6 Boulevard Maréchal Juin, Caen 14050, France

*braelf@hotmail.com

Undoped HfO_2, Si-rich-HfO_2 and Er-doped Si-rich-HfO_2 films with specific structural and spectroscopic properties have been prepared by radio-frequency magnetron sputtering. The effect of post-deposition thermal annealing on the film optical and structural properties was investigated by means of scanning electronic microscopy (SEM), Energy dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), Raman scattering and photoluminescence methods. Annealing was carried out at 900-1100oC for 10-60 min in nitrogen atmosphere.

It was observed that annealing treatment causes the phase separation process together with the formation of HfO_2, SiO_2, Er_2O_3 and pure Si phases. A light emission in the orange-red spectral range was observed from Si-rich-HfO_2 samples contrary to their pure HfO_2 counterparts. Photoluminescence was ascribed to carrier recombination in silicon clusters and host defects. The appearance of silicon clusters was also confirmed by the XRD study.

Additional argument for Si clusters' formation was obtained under investigation of Er doped Si-rich HfO_2 films. They demonstrated 1.54-μm Er^{3+} luminescence under non-resonant excitation originating from an energy transfer from Si clusters towards Er^{3+} ions. The phase separation mechanisms as well as the nature of radiative transitions were discussed.

Synthesis and characterization of MoS_2/GO/ZnO composites

Jeniffer S. Liahut-Lopez[1], Maria A. Hernandez-Perez[1*], Roberto Vargas-Garcia[1], Elvia A. Sanchez-Ramirez[2]

[1]*Instituto Politécnico Nacional, Departamento de Ingeniería en Metalurgia y Materiales, ESIQIE, CP 07738 CDMX, Mexico*
[2]*Instituto Politécnico Nacional, Departamento de Ingeniería Metalúrgica - UPIIZ, Zacatecas, CP 98160, Mexico*

*mhernandezpe@ipn.mx; angeleshp@yahoo.com

Increasing interest has been focused on the study of MoS_2 nanostructures due to its photocatalytic properties which can be improved by synergetic effect with GO and ZnO [1-2]. In this work we report the preparation of MoS_2/GO and MoS_2/GO/ZnO composites by the hydrothermal method. MoS_2/GO/ZnO materials have been obtained in a 1 or 2 step synthesis. L-cysteine and sodium molibdate solutions and commercial GO where sonicated and transferred into a Teflon lined autoclave. The reactor was then heated at 200ºC during 24 h. The results show that the obtained MoS_2 sheets are homogeneously distributed on GO surface. MoS2 and GO show poor crystalline quality while ZnO well crystallizes in wire and plate structures (Fig. 1). The efficiency of one step route is higher than that of two step route, however the stoichiometry of MoS_2 was not clearly defined by EDS and XPS analysis. Two step route synthesis produces micro-sized plates of ZnO. Cyclic voltammetry results indicate that these materials have high potential in H_2 evolution reaction.

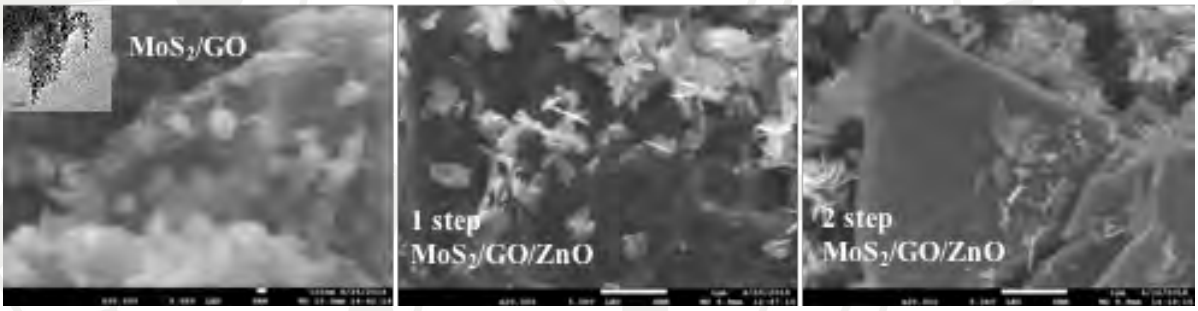

Figure 1 – SEM images of MoS_2/GO and MoS_2/GO/ZnO composites. The inset shows a TEM image of MoS_2 sheets.

Key Words: MoS_2/GO, MoS_2/GO/ZnO, nanocomposites, hydrothermal method

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Hydrophobic sorbents obtained from polymer waste for oil spills in water remediation

Cynthia Estephanya Ibarra Torres, Thelma Serrano Quezada, Boris Kharissov*

Universidad Autónoma de Nuevo León, Ave. Universidad, San Nicolás de los Garza, N.L., Mexico 66455.

*bkhariss@hotmail.com

Nowadays, there is a rising concern about the separation of oil-water mixtures to solve environmental problems. The oil spill accidents are an important problem because of they cause loss of energy and resources while they generate long-term environmental damage. Oil spill cleanup can be carried out by many methods and technics, being the sorbents the most attractive due to the possibility of collection and complete removal of the oil in situ from the water surface. On the other hand, another serious problem is the growing polymer production, because of between 10 and 20 million tons end up in the oceans every year.

In this project, sorbent materials were prepared from polymer waste (polyethylene terephthalate, PET and polyurethane, PU) using salt templates. Salt templates were form using NaCl with three different grain sizes (table salt, ground table salt and sea salt). To form salt templates, first salt is moistened, then placed in molds and left to dry 24 hours at room temperature, finally the templates were removed from the molds. To form porous materials, the salt templates were surrounded with PET or PET-PU mixture (maintaining constant temperature, 250-260°C), the polymer infiltrates the salt templates thanks to the capillary forces, once this process is completed, the salt templates were dissolved in water (at 50°C). For the formation of the PET-PU mixture, first it was necessary to prepare a suspension of PU in a solution of ethylene glycol and n-butanol (50 v/v%), this suspension was mixed with PET. Sorbents were hydrophobized using SiO_2 nanoparticles and commercial carbon nanotubes. SiO_2 NPs were synthesized by sol-gel method (molar ratio $[H_2O]/[TEOS]=25.13$). Hydrophobization of the porous materials were performed by the dip coating technique using a SiO_2 nanoparticles or carbon nanotubes suspension in THF.

Polymers were not degraded during the sorbents forming process, it was proved due to infrared spectroscopy. SEM images showed the porous sizes in the sorbents, demonstrating that porous size is related to grain size on salt template. Porous sizes were between 50 nm-3 µm using ground table salt template, 1 µm-5 µm using table salt template and 2 µm-18 µm using sea salt template. SiO_2 nanoparticles had particles sizes less than 100 nm but they were in clusters (according to SEM data) and amorphous (according to XRD data). Hydrophobicity was tested visually by dripping water on the hydrophobized sorbent; this way it was proved that the water is repelled.

Metal matrix composite containing ($TiC–Al_2O_3$) reinforcement

A. Santos-Beltran[1*], V. Gallegos-Orozco[1,2], I. Ronquillo-Ornelas[1], M. Santos-Beltrán[3], R. Carbajal-Sánchez[1], F. Paraguay-Delgado[3]

[1]Universidad Tecnológica de Chihuahua Sur, Carretera Chihuahua-Aldama Km 3, C.P. 31313, Chihuahua, Chih., México.
[2]Instituto Tecnológico de Chihuahua, Ave. Tecnológico #2909, CP 31310, Chihuahua, Chih., México.
[3]Centro de Investigación en Materiales Avanzados, Avenida Miguel de Cervantes Saavedra 120, Complejo Industrial, C.P31136 Chihuahua, Chih., México.

*asantos@utchsur.edu.mx

Engineering ceramics, such as TiC, Al_2O_3, TiB_2, B_4C, SiC, etc., are frequently used as reinforcement metal matrix composites. Among these ceramics, Al_2O_3 is one of the most important used in the engineering materials due to its high elastic modulus, high wear and its strength retention at high temperature. Consequently, the addition of TiC to Al_2O_3 matrix can be expected to increase the microhardness resistance of composite powder [1]. In this work Al_2O_3-TiC composites were fabricated through the powder metallurgical process (mechanical milling combined with sintering treatment) from powder mixtures of TiO_2, Al and C. The effect of different processing conditions (milling time, temperature and time thermal sintering) on the TiC phase dispersion on Al_2O_3 matrix were evaluated. Morphology and microstructure were studied by electron microscopy techniques and XRD techniques. XRD patterns were refined by Rietveld method to determine lattice parameters, percentage of phases, crystal sizes, phase determination and quantity of phases of the composite powder samples. The sample diffraction pattern of the Fig. 1 shows a widening of the diffraction peaks as a result of a decrease in the crystallite size, as well as the possible presence of microstrains. The crystallite size of the Al_2O_3 phase from Rietveld refinement was of about 50 nm. The presence of the nanocrystalline state present combined with the TiC phase dispersion in the powder has an important effect in the increase of mechanical properties.

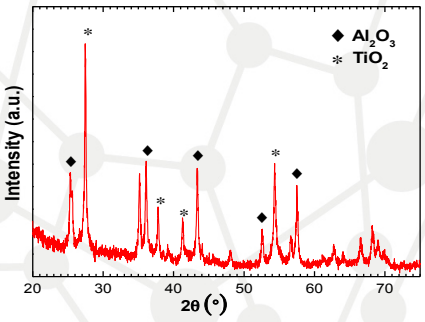

Fig.1 - XRD Pattern obtained from mechanically ground samples for 4 h and followed by 1 h of heat treatment at 1000 ° C.

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Superhydrophobic structures on the 304 steel surface by femtosecond LASER ablation

V. Gallegos-Orozco[1,2*], A. Santos-Beltran[1], R. Carriles-Jaimes[3], I. Ronquillo-Ornelas[1], F. Paraguay-Delgado[4], M. M. Santos-Beltrán[4]

[1]Universidad Tecnológica de Chihuahua Sur, Carretera Chihuahua-Aldama Km 3, C.P. 31313, Chihuahua, Chih., México.
[2]Instituto Tecnológico de Chihuahua, Ave. Tecnológico #2909, CP 31310, Chihuahua, Chih., México,
[3]Centro de Investigaciones en Óptica A.C., Loma del Bosque 115, Colonia Lomas del Campestre León, C.P. 37150 Guanajuato, México.
[4]Centro de Investigación en Materiales Avanzados, Avenida Miguel de Cervantes Saavedra 120, Complejo Industria,l C.P31136 Chihuahua, Chih., México

*vgallegos@utchsur.edu.mx

Micro and nanotechnology are advancing rapidly in recent years, which has opened a range of opportunities in the improvement of advanced surfaces by introducing characteristics which alter the surface properties drastically. The micro/nano structures can be manufactured by several methods, for example photolithography, X-rays, electron beam, particle beam and mechanical methods [1]. However, machining with micro-nano femtosecond laser has emerged as an effective technique to create scalable surfaces with micro and nanostructures. In this work, a nanostructuring was performed on a 304 steel surface using a pulsed femtosecond laser. The equipment used is a Ti: Sapphire laser that consists of a 'mode-locked' oscillator and a regenerative amplifier that generates pulses of 50 femtoseconds with a central wavelength of 800 nm and a repetition frequency of 1 kHz. Fig. 1 shows the laser ablated surface sample with aprox. 0.5 μm spacing of linear structure. The hydrophobicity (contact angle, CA test) of treated surface with laser ablated surface is shown in Fig. 2.

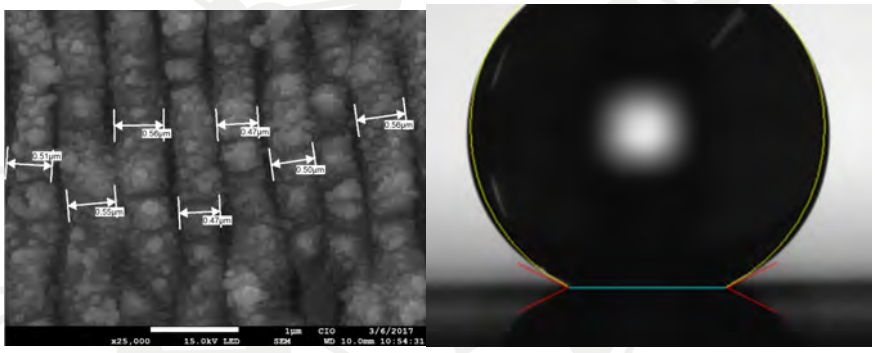

Fig. 1 - SEM image of nanostructured surface, using 20 mW of laser power.
Fig. 2 - Samples of CA measurements on laser processed substrate. CAavg= 153.2°

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Comparison of light emission and structure of Nd-doped Si-RICH-HfO_2 nanocrystal films prepared by magnetron sputtering in different atmospheres

Tetyana Torchynska[1*], Leonardo G. Vega Macotela[2], Georgiy Polupan[2], Larysa Khomenkova[3,4], Christophe Labbé[5], Xavier Portier[5] and Fabrice Gourbilleau[5]

[1]Instituto Politécnico Nacional, ESFM, Av. IPN, México City, DF, 07738, México.
[2]Instituto Politécnico Nacional, ESIME, Av. IPN, México City, DF, 07738, México.
[3]V.Lashkaryov Institute of Semiconductor Physics, 45 Pr.Nauky, Kyiv 03028, Ukraine
[4]National University «Kyiv-Mohyla academy», 2 Skovorody str., Kyiv 04070, Ukraine
[5]CIMAP/CEA/CNRS/Ensicaen/UCBN, 6 Boulevard Maréchal Juin, Caen 14050, France

*gpolupan85@yahoo.com.mx

Nd-doped Si-rich-HfO_2 nanocrystal films with specific emitting and structural properties have been prepared by radio-frequency magnetron sputtering using standard (pure argon plasma) and reactive (argon-nitrogen mixed plasma) approaches. The effect of post-deposition thermal annealing on film properties was investigated by means of scanning electronic microscopy (SEM), Energy dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), Raman scattering and photoluminescence methods. Annealing was carried out within the temperature range 800-1100℃ for 15 min in nitrogen atmosphere.

The SEM study revealed that the films obtained in pure argon plasma demonstrate nanocrystals with the grain size about 100 nm. Contrary to this, SEM images the films prepared in argon-nitrogen plasma presented clear unstructured film surface. It was observed that annealing treatment causes the phase separation process. In nitrogen-free samples, the formation of HfO_2, NdO_2, SiO_2 and pure Si phases detected by XRD and in Raman spectra. PL spectra these films are complex and demonstrate several PL bands centered at 380, 450, 550, 780 and 880 nm. Their contribution depends on the annealing temperature and governs the shape of total PL spectrum.

It was found that PL spectra of the films grown in argon-nitrogen plasma are featureless. Whatever the annealing temperature, they demonstrate broad unstructured PL band with the peak within 440-480nm. Peculiarities of PL spectra are analyzed and discussed together with the mechanism of phase separation.

Optical and structural characterization of ZnO Er nanocrystals prepared by spray pyrolysis

Tetyana V. Torchynska[1*], Brahim El Filali[2], Jorge L. Ramírez García[2], and Jose L. Casas Espinola[1]

[1]Instituto Politécnico Nacional, ESFM, México City, DF, 07738, México.
[2]Instituto Politécnico Nacional, UPIITA, México City, DF, 07320, México.

*ttorch@esfm.ipn.mx

Morphology, emission and structure of ZnO:Er nanocrystal (NC) films have been investigated by means of scanning electronic microscopy (SEM), energy dispersive spectroscopy (EDS), X-ray diffraction (XRD) and photoluminescence (PL) methods. ZnO:Er NC films were obtained by spray pyrolysis with different Er-doping (0, 1, 2, 3 and 5at%) and then thermal annealed at 400℃ in ambient air. SEM study has confirmed the nanocrystal (NC) structure of obtained ZnO and ZnO Er films. X-Ray diffraction has revealed the wurtzite crystal structure in ZnO and ZnO Er NCs. The XRD intensity of all XRD peaks monotonically decreases with Er concentrations PL spectra demonstrate the near band edge (NBE) and defect related PL bands in visible (2.0-3.0 eV) and infrared (0.80-0.85eV) spectral ranges: The PL spectra were studied in dependence on Er atom concentrations and at different temperatures within the range 10-300K for the identification the optical transition responsible for the emission bands.

PL and XRD results have shown that the crystal quality of ZnO:Er NC films can be improved at a small level of Er-doping (≤ 3at%) together with intensity enlarging the near band edge (NBE) emission and PL bands related to the inner-shell optical transitions in Er ions. In contrary, at high level of Er-doping (≥3at%) the ZnO:Er crystallinity falling down, the PL intensities of NBE and Er-related PL bands decrease, but the intensity of green PL band related to native defects enlarges. The mechanisms of mentioned processes are discussed as well.

Growth kinetics and thermal properties of gold nanoshell

Netzahual-Lopantzi Angel[1], Jiménez-Pérez José Luis[1], Sánchez-Ramírez José Francisco[2]

[1]Unidad Profesional Interdisciplinaria en Ingeniería y Tecnologías Avanzadas, Instituto Politécnico Nacional, Avenida Instituto Politécnico Nacional No. 2580, Col Barrio la Laguna Ticomán, Gustavo A. Madero, Ciudad de México, C. P. 07340.
[2]Centro de Investigación en Biotecnología Aplicada, Instituto Politécnico Nacional, Ex -hacienda San Juan Molino Carretera Tecuexcomac-Tepetitla Km 1.5, Tlaxcala C.P. 90700.

gelo89_@live.com.mx

In this work were development core@shell of silica@gold nanostructure. As first step, silica nanoparticles of 300, 150 and 90 nm were synthesized by Stöber method, over this nanospheres were attached gold nanoparticles and further a thin layer of gold were growth in precence more $HAuCl_4$. The results revealed a red shift of surface resonance plasmon of core@shell since the visible to near infrared around at 800 nm. Shells of 10 nm of thickness were observed by microscope TEM at all samples. Nanofluids containing core@shell of silica@gold inside water were made, the nanofluids were measurement by thermal len spectroscopy, the results show at increased of thermal diffusivity in agreement to increment of nanostructure into water.

Key Words: Thermal diffusivity, core@shell.

Study of the effect of the seed layer in the synthesis of ZnO nanorods by microwave-assisted technique

Magda Barajas Hernández[1], Jorge López Villarreal[2], Abel Fundora Cruz[3], Francisco Solís Pomar[2*], Eduardo Pérez Tijerina[2]

[1]Universidad Tecnologica Gral. Mariano Escobedo. Libramiento Noreste km 33.5, Escobedo Nuevo Leon C.P. 66050
[2]Universidad Autónoma de Nuevo León, Centro de Investigación en Ciencias Físico Matemáticas, Facultad de Ciencias Físico Matemáticas, Av. Universidad s/n. Ciudad Universitaria, C.P 66451 San Nicolás de los Garza, Nuevo León, México
[3]Instituto de Ciencias y Tecnología de Materiales (IMRE), Universidad de La Habana, San Lázaro y L, Vedado, CP 10400, Cuba.

*francisco.solispm@uanl.edu.mx

ZnO nanorods were prepared using a seed layer of zinc oxide deposited by RF Sputtering, using a constant power varying the Argon flow (Ar) and a deposit time of 5 minutes. For the synthesis of zinc oxide nanorods, the hydrothermal method assisted by microwave was used, using a solution of Hexamine ($(CH_2)_6N_4$) and zinc nitrate ($Zn(NO_3)_2$) with different concentrations and different reaction times. The effect of the seed layer in the synthesis of the nanorods was studied to determine the best conditions for they synthesis. The samples were characterized by X-ray diffraction (XRD), scanning electron microscopy and UV-Vis spectroscopy.

Key Words: ZnO; Nanorods; Microwave synthesis; RF Sputtering

Dye degradation based on TiO_2 nanostructures

Malinalli RAMIREZ[1*], Omar RODRIGUEZ[3], Wendy HERNÁNDEZ[2] Julio TINOCO[3], Andrea MARTINEZ[3]

[1]Fac. de Ciencias Químicas, U. V., Bv. Ruiz Cortines 455, C.P. 94294, Boca del Río, Ver., México
[2]Depto. de Física Aplicada, CINVESTAV-I.P.N., Antigua, Carr. Mérida-Progreso Km 6, C.P. 97310, Mérida, Yuc., México.
[3]MICRONA, U. V., Bv. Adolfo Ruiz Cortines 455, C.P. 94294, Boca del Río, Veracruz, México

*malinalliramirez@hotmail.com

Modern life style has induced strong water pollution. In our country, wastewater treatment methods are not always able to degrade some recalcitrant pollutants, for example, textile dyes. It has been demonstrated that anatase phase nanostructured TiO_2 can degrade organic pollutants through photocatalysis in the presence of UV light [1,2]. However, the release of TiO2 nanostructures to the environment could have negative effects [3]. In this work, commercial textile dye degradation using immobilized TiO_2 was studied. Two different samples were fabricated. The first one based on TiO_2 nanofibers obtained by electrospinning technique (TNM), and the second one based on TiO_2 nanoparticles deposited on a stainless-steel mesh by electrospray technique (TCM). Both samples were evaluated by testing "Rojo Granada" commercial textile dye degradation. Experiments were performed under solar light, and degradation percentage was evaluated by UV-Vis spectrophotometry. Overall results indicated that the use of TiO_2 allowed to degrade commercial textile dye without significant TiO_2 lost. TNM showed better performance than TCM, reducing dissolved dye concentration to 0.5236% of initial value in 1 hour. With TCM sample, dye degradation was slower, but after 6 hours concentration was reduced to 31.4136% of the original value.

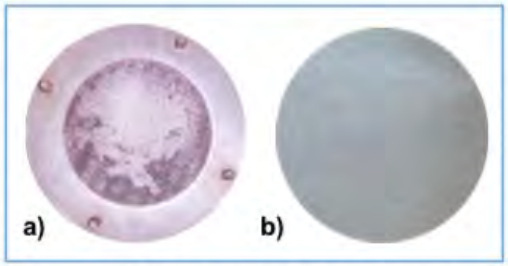

Figure 1. TNM (a) and TCM (b) samples

Figure 2. Original solution (left), solution degraded by TCM (center) and solution degraded by TNM (right).

Key Words: Titanium dioxide, nanofibers, nanoparticles, photocatalysis, electrospinning, electrospray.

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Study of the optical, electrochemical, and structural properties of semiconductor CdS1-xSex-ITO films growing by CBD

Elvia A SANCHEZ-RAMÍREZ[1], María de los Ángeles HERNANDEZ-PEREZ[2], Arturo MANZO-ROBLEDO[3], Fredy J. CASTILLO-PLATAS[2], Fernando SAUCEDO-SALAZAR[1]

[1]Departamento de Ingeniería Metalúrgica - UPIIZ, Instituto Politécnico Nacional, Zacatecas, 98160, Mexico, saraelan2411@hotmail.com
[2]Departamento de Ingeniería en Metalurgia y Materiales - ESIQIE, Instituto Politécnico Nacional, Ciudad de México, 07738, Mexico
[2]Departamento de Ingeniería Quimica - ESIQIE, Instituto Politécnico Nacional, Ciudad de México, 07738, Mexico

*saraelan2411@hotmail.com

Semiconductors II-VI are amply study in the last years and some papers are focused on the possible applications because their properties are tunable by changing the deposition conditions especially when these materials are ternary of doped. The deposition of CdS1-xSex films by chemical bath deposition (CBD) occurs if the ionic product of Cd+2, S-2 and Se-2 ions exceeds the solubility product of CdS and CdSe [1]. The main goal for this work were prepared and characterized CdS1-xSex thin films using CBD technique on ITO substrate at 90°C and 120 min, varying the atomic composition “x” and pH 9-10. Structural, morphological, optical and electrochemical properties were analyzed.

All the films are polycrystalline exhibit a hexagonal and preferential orientation on (002) plane [2-3]. The crystal size was 5-4 nm. It is observed a dense and flat surface as x increase density and flatness decrease until the surface is forming by semispherical grains. A well absorption edge was observe this indicating a good quality in all film and suggesting a solid solution. Eg were estimated using the Tauc’s relation, the value decreases with x (2.41-1.85 eV). CdS and CdSe exhibit a single phonon band, however in ternary compounds are observe two phonon bands. LO1 and LO2 modes linearly shift to lower and higher frequencies, depending of quantity of Se. PL band which is shifted to values in between those of CdS (2.30 eV) and CdSe (1.72 eV). Ternary materials show a good electrochemical responds for hydrogen evolution reaction (HER). Flat-band potential change from -1.5 to -0.5 V with Se. Best photoresponse was obtained on CdS films.

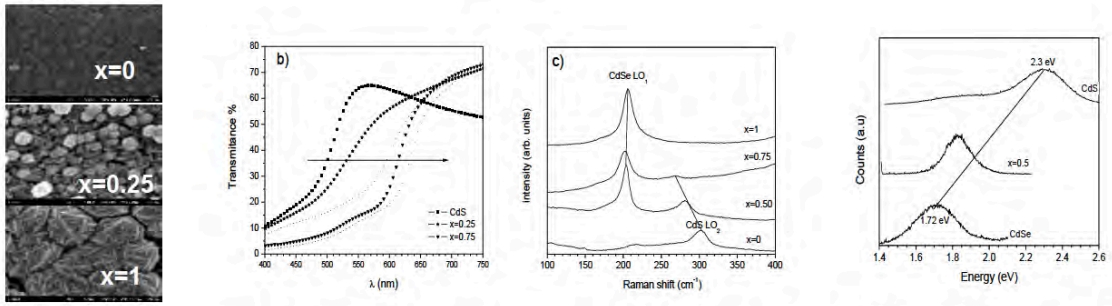

Fig 1. a)High resolution SEM micrographs b) Transmittance spectra c) Raman spectra d) Room temperature PL spectra of as grown $CdS_{1-x}Se_x$ films deposited at 90°C during 120 min.

Key Words: Semiconductors, ITO, CBD, Photoluminescence, Raman

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Synthesis, study and characterization of nanoforest-like carbon nanotubes decorated with fluorescent nanoparticles

Arquieta PATSY[1,2], Kharissova OXANA[1], Ortega BEATRIZ[1, 3], Galindo HUGO[1]

[1]Centro de Investigación en Ciencias Físico Matemáticas - Universidad Autónoma de Nuevo León. Pedro de Alba, Ciudad Universitaria, C.P. 66451 San Nicolás de los Garza, Nuevo León, México.
[2]Facultad de Ciencias Biológicas - Universidad Autónoma de Nuevo León. Pedro de Alba, Ciudad Universitaria, C.P. 66451 San Nicolás de los Garza, Nuevo León, México.
[3]Facultad de Ciencias Químicas - Universidad Autónoma de Nuevo León. Pedro de Alba, Ciudad Universitaria, C.P. 66451 San Nicolás de los Garza, Nuevo León, México.

patsy.arquieta.g@gmail.com

Multiwall Carbon Nanotubes (MWCNT's) is a nanomaterial that attracts the attention for research and development areas, due to its excellent properties, in particular in the area of biosensors design and development, in which the fluorescence property is one of the most important elements. In some biosensors, fluorescent property has been contemplated like the principal factor by its quick response. This property is fundamental for detection of some cancer cells and other bioelements. In previous investigations, Strontium Aluminate ($SrAl_{12}O_{19}$) presented a higher fluorescence being compared with other aluminates; we used it for the decoration process of CNTs. This research purpose is based on the synthesis, characterization and study of CNTs obtained by Spray Pyrolysis method, with fluorescent properties in one step. These MWCNTs was doped with five Lanthanides ions, Europium Oxide, Neodymium Oxide, Lanthanum Oxide, Samarium Oxide and Cerium Oxide. The method, used to obtain the CNTs, allowed obtaining three-dimensional (3D) structures formed by these nanostructures, called nanoforests. This Nanoforests were growth in the surface of five optical fibers, which were used like the substrate. The decoration process is held on the surface of the forest, and the obtained materials were analyzed by UV-Vis Spectroscopy, FTIR Spectroscopy, Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM), to study the decoration process.

Key Words: Carbon Nanotubes, Fluorescence, Nanoforest, FTIR Spectra, UV-Vis Spectra

Silver nanoparticles incorporated in epoxy resin as colorimetríc sensor

Miguel Angel Gonzalez Cruz[1], Alexa Carrillo Mercader[1], Celso Velásquez Ordoñez[1], Víctor Rentería Tapia[1*]

[1]Centro de investigación en Nanociencias y Nanotecnologías, Centro Universitario de los Valles, Universidad de Guadalajara, Carretera Guadalajara-Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México.

*victor.renteria@profesores.valles.udg.mx

Silver nanoparticles incorporated in epoxy resin were prepared for applications as colorimetric sensor of organic solvents and glucose dispersed in water. The electronic transmission microscopy images show dispersed spherical particles of average size 8 nm and plasmonic resonance located at 425 nm. These particles were very efficient and sensitive for colorimetric identification of acetone, DMF, toluene, and aqueous solutions of glucose. Colloidal solutions are sensitive to these analyses at concentrations from 10 mg / dL to 500 mg / dL and the colorimetric response is instantaneous. In this regard, changes in the position, intensity and width of the surface plasmon were observed [1]. The results carried out by dynamic light scattering and UV-vis spectroscopy showed that the organic solvents and glucose dispersed in water rapidly induce silver nanoparticles aggregation. The transformation of the particle shape due to the interaction of the analyses generates a awesome change of color in the solution at 500 mg / dl, observed with the naked eye. It is argued that the proposed nanosensor offers the possibility of generating a highly sensitive and specific assay at very low cost and can be applied to a wide variety of analyses of complex nature.

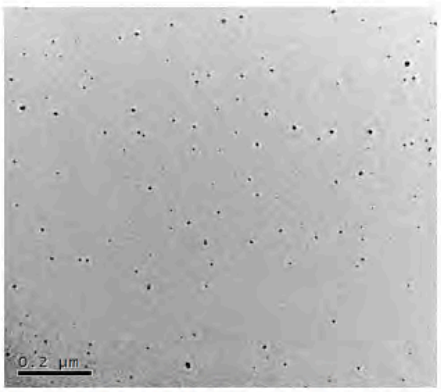

Figure 1–TEM image of spherical particles of average size 8nm.

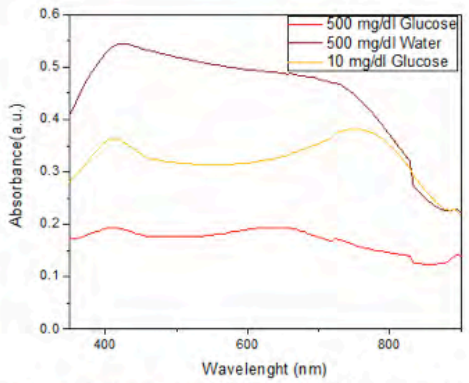

Figure 2- Plasmonic resonance of silver nanoparticles to glucose solutions.

Key Words: Silver nanoparticles, epoxy resin, colorimetric sensor, plasmonic

resonance.

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Nanoemulsions of Limonene

Janneth BERNARDO LINO[1,2], Andrea LÓPEZ MARTÍNEZ[1,2], Abril FONSECA GARCIA[2], Reyna Araceli MAURICIO SÁNCHEZ[2], Luz Ma. Reina AVILÉS ARELLANO[2], Gabriel LUNA BERCENAS[2]

[1]Universidad Tecnológica Fidel Velázquez, Emiliano Zapata s/n, col. El tráfico, 54435 Villas Nicolás Romero, Estado de México, e-Mail: janny509@hotmail.com.
[2]Centro de Investigación y de Estudios Avanzados del I.P.N, Unidad Querétaro, Querétaro, 76230, México.

*gabriel.luna@cinvestav.mx

In this work, nanoemulsions of limonene were prepared by high energy. Limonene is an essential oil, which possess exceptional properties to medical applications such as the absorption of drugs subcutaneously, and a great bactericidal potential [1]. Also, its smell is unpleasant for insects [2], with this properties this essential oil can be used as a repellent and take care of infection derivate of pinch of insect. For these reasons the goal of this work was to develop nanoemulsions with a good stability for their application as an insect repellent for humans. In addition, silver nanoparticles (Npa Ag) were added at non-cytotoxic concentration for humans (less than 10 µg/l) to optimize the antibacterial effect. The limonene was stabilized by two kinds of emulsions, oil-in-water (O/W) and water-in-oil (W/O). Tween 80 is the surfactant used in the preparation of these emulsions. Both emulsions, O/W and W/O showed a stability, being monitored along 4 weeks. Infrared spectroscopy was performed to characterize the essential oil and Tween 80.

Key Words: Nanoemulsion, Limonene, Essential oil, oil-in-water, water-in-oil..

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Microstructural characterization of food proteins by microscopy techniques

Liliana Edith Rojas-Candelas[1], Juan Vicente Méndez Méndez[2], José Jorge Chanona-Pérez[1], Claudia Albany Resendiz-Mora[1], Felipe Cervantes-Sodi[3], Jocelyn Madrigal-Acevedo[1], Pedro López-Ordaz[1]

[1]Instituto Politécnico Nacional, Escuela Nacional de Ciencias Biológicas, Av. Wilfrido Massieu s/n C.P. 07738. Gustavo A. Madero, México
[2]Centro de Nanociencias y Micro y Nanotecnologías - Instituto Politécnico Nacional. Unidad Profesional Adolfo López Mateos, Luis Enrique Erro s/n, C.P. 07738 CDMX
[3]Universidad IberoamericanaProlongación Paseo de la Reforma 880 Lomas de Santa Fe, C.P. 01219

lrojasc0802@alumno.ipn.mx

The study of the structure and mechanical properties of proteins at nanoscale is an interesting topic to food nanotechnology [1,2]. The aim of this work was to study of the microstructure of ovalbumin and casein by SEM (scanning electron microscopy) and AFM (atomic force microscopy). Overall morphology and topography of ovalbumin and casein were studied by SEM (Hitachi, SU3500 I) and AFM (Bruker, Bioscope Catalyts ScanAsyst, USA).

Figure 1. Scanning electron microscopy images of powder a) ovalbumin and b) casein

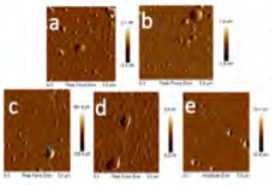

Figure 2. AFM images ovalbumin a) pH 4.6, b) pH 5.6 and casein c) pH 4 d) pH 5 and e) pH 6

Fig. 1 shows SEM images of powder proteins, where the ovalbumin particles have a spherical form (Fig 1a), while casein is like amorphous agglomerates (Fig. 1b), these morphologies corresponds to its obtention process, spray drying and crystallization respectively. Then, proteins solutions were observed under AFM at different pHs (Fig. 2), casein at its isoelectric point (5.0) and at ±1 pH unit and ovalbumin at 4.6 (isoelectric point) and 5.6. Ra (arithmetic roughness) was obtained from scanning area of 5x5 µm. At pH 5 Ra for casein was 8.023 ± 5.28 nm, while that at pH 4 was 1.56 ± 0.58 nm and pH 6 was 2.59 ± 0.84 nm. To ovalbumin, at pH 4.6 the Ra was 4.05 ± 2.60 nm, whereas at pH 5.6 its Ra was 2.59 ± 0.84 nm. Thus the proteins in its isoelectric point showed a largest Ra values due to the agglomeration of proteins. This preliminary study of morphology and topography of proteins by microscopy techniques provided an initial overview to establishing the dispersion conditions and pHs to study its mechanical properties by nanoindentation with AFM.

Key Words: Protein, roughness, isoelectric point, microstructure.

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Antibody N1C1-functionalized graphene oxide for the effective detection of neurodegenerative diseases

Arianee Sainz-Vidal, Araceli Solís Gómez, Daniel Matatagui, Roberto Sato Berrú, J. M. Saniger

Instituto de Ciencias Aplicadas y Tecnología (ICAT), Universidad Nacional Autónoma de México (UNAM), Circuito Exterior S/N, Ciudad Universitaria, Ciudad de México 04510, México.

arianee.sainz@icat.unam.mx

The development of biosensors has a growing scientific activity now days due to its effectiveness in the diagnosis and treatment of diseases such as neurodegenerative and cancer. The performance of a biosensor depends in a great extent on the material that is used as a substrate and on the use of a method for modifying its surface that guarantees the adequate anchoring of the biomolecules without losing their bioactivity. Graphene oxide (GO) is a good substrate material due to its biocompatibility, its abundance of hydrophilic groups, its extensive surface area and its outstanding solubility in water. In this work we conjugated GO with polyclonal antibody N1C1 that binds to tyrosine hydroxylase (TH) with high specificity and affinity. We used TH as a target molecule for its potential as biomarker of oxidative stress in brain that is a process observed in neurodegenerative diseases like Parkinson and Alzheimer. N1C1 was covalently conjugated to GO via the formation of the amide between the –COOH group of GO and the $–NH_2$ moiety at N1C1 by EDC-NHS chemistry. The conjugation of N1C1 on GO was confirmed by FTIR and Raman spectroscopy.

Key Words: Antibody, Functionalization, Graphene oxide, tyrosine hydroxylase

Acknowledgment
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Catalysis of organic waste with Co_2FeO_4 nanoparticles for biogas obtention

Nava ERICK[1], Topete JUAN[1], Palacios CRISTIAN[1], Santiago ALAN[1], Flores JOSE[1], Martínez BEATRIZ[1]

[1]Universidad Politécnica del Valle de México, Av. Mexiquense s/n, Col. Villa Esmeralda, C.P. 54910, Tultitlán, Estado de México, México.

cae06ciencias@gmail.com

Currently, biogas is used throughout the world as a source of fuel both industrially and domestically, its exploitation has contributed to boost sustained economic development and has provided a renewable alternative energy source to coal and oil. Because the cobalt ferrite nanoparticles Co_2FeO_4-NPs have catalysis properties of organic products [1], were used in the present work for the catalysis of organic waste in the biogas production. A bioreactor prototype was designed for the production of biogas through the reaction of fermentation reactions and/or degradation of organic waste catalyzed by Co_2FeO_4-NPs. Also Co_2FeO_4-NPs-NPs were synthesized by precipitation and solvothermal techniques. A bioreactor prototype was designed (Figure 1) to perform the biogas production reactions. 250g of organic waste was placed at the start to carry out the reaction. Tests were performed with the addition of 0.25 and 0.5 ml of Co_2FeO_4-NPs. The volume of biogas obtained was measured. The tests were performed in triplicate. We obtained an increase in the production of biogas through the catalysis reaction of the fermentation / degradation of organic waste with Co_2FeO_4-NPs.

Fig. 1. Bioreactor prototype for obtaining biogas.

Key Words: Catalysis, Organic, Waste, Nanoparticles, Biogas.

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Plasmon modes in layered graphene structures

G. Gonzalez de la Cruz

Departamento de Fisica, CINVESTAV-IPN Apartado postal 14-740,07000, CDMX, Mexico

*bato@fis.cinvestav.mx

In recent years, graphene plasmonics, has attracted significant interest motivated by graphene´s unique high carrier mobility, electrically or chemically tunable carrier density, long-lived and strong plasmon excitation confinement. In the context of optoelectronics and nanophotonics, graphene is considered as promising plasmonic material working in the mid-infrared and terahertz spectral windows. However, in a single layer graphene, the electromagnetic energy has a limited capability to plasmon excitations. To obtain a more powerful capacity of excite plasmon resonance, one can employ multilayer graphene structures as possible solution. In this work, we find an analytical expression for the dielectric function of the N-layer graphene structure solving a recurrence relation between the electric potential at different graphene layers. We also find that the highest energy of the plasmon oscillations supported by the multilayer graphene stacks at long wavelength correspond to electrons in each plane oscillating in phase. In addition, a surface plasmon mode emerges at certain finite wave vector outside the bulk plasmon band and it is Landau damping in the continuous interband single particle excitation with increasing wave vector.

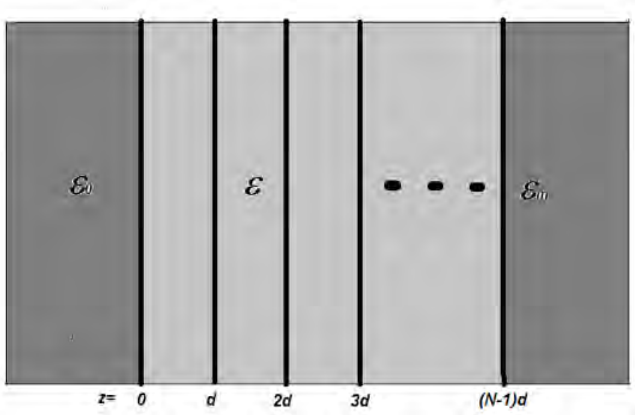

Figure 1 Schematic representation of a N graphene layers embedded in a material with dielectric constant ε surrounded by two substrates with dielectric constant ε_0 (left) and ε_m (right), respectively.

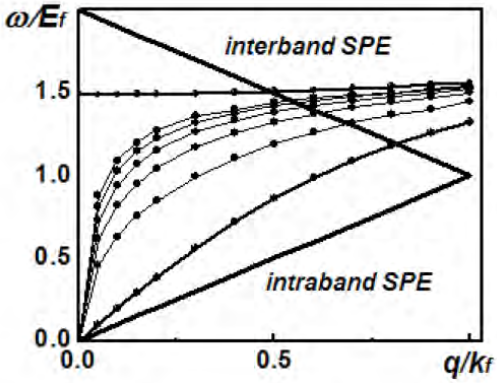

Figure 2 Energy plasmon dispersion for a freestanding multilayer graphene for N=5 and $\varepsilon = \varepsilon_0 = \varepsilon_m = 1$. These electron collective excitations are free Landau damping in the region $\gamma q < \omega < 2E_f - \gamma q$, otherwise they decay generating a electron-hole pair in the single particle continuum. The edges of bulk plasmon band for infinite graphene superlattice are also shown with white circles. The value of the parameters are $n = 1\ 10^{-12}\ \mathrm{cm}^{-2}$, $d = 100\ \text{Å}$.

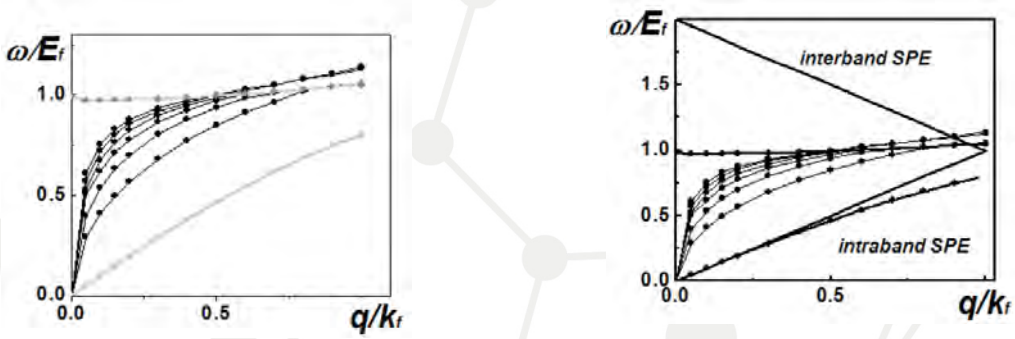

Figure 3 - Plasmon dispersion relation for a finite system of graphene layers with $\varepsilon = \varepsilon_0 = 4, \varepsilon_m = 1$. The surface plasmon is shown in Fig. 3a rising at finite values q/k_f above the bulk plasmon band, as the wave vector increases, is expected that eventually the dispersion relation of the surface mode decays into the continuum single particle excitation, Fig. 3b.

Key Words: Graphene; Plasmons in finite superlattices; Recursive approximation

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TiO_2 films as a photocatalyst of hydrogen reduction reaction

Maria GALLARDO[1*], Ana BALBUENA[2], Gonzalo GALICIA[2], Aida MEDINA[3], Andrea MARTINEZ[4], Julio TINOCO[4]

[1]Fac. de Ciencias Químicas, UV; Adolfo Ruíz Cortines 455, Costa Verde, 94294 Veracruz, Ver.
[2]Instituto de Ingeniería, UV; Av. Juan Pablo II S/N, Costa Verde, 94292 Boca Del Rio, Ver
[3]ININ; Carretera México Toluca-La Marquesa s/n, Ocoyoacac, Estado de México. C.P. 52750
4MICRONA, UV; Adolfo Ruíz Cortines 455, Costa Verde, 94294 Veracruz, Ver.

*maria.galca712@gmail.com

Nuclear power industry has implemented several methods in order to control metallic degradation. Between them, the electrochemical corrosion potential (ECP) is currently a major indicator for the Intragranular stress corrosion cracking (IGSCC) susceptibility of stainless steel (SS) components in boiling water reactors environments. Hence, this industry has developed environment improvements of the water in contact with the internal components of the reactor; one of these is the Noble Metal Chemical Addition program which involves injecting platinum and rhodium compounds into the reactor water during an outage. These metal particles incorporated catalyze the hydrogen recombination that in turn reduces the ECP [1,2]. However, there are several aspects that do not guarantee the protection of the components of the reactors against the IGSCC, so the investigations are being directed to the search of methods and materials that make efficient the protection and reduce the economic cost of these. In this work, Titanium dioxide coatings [3,4] has been obtained by two methodologies over SS 316L in order to evaluate the effect of the surface in the catalytic properties of hydrogen reduction reaction by using electrochemical techniques.

Key Words: TiO_2, Photocatalysis, Hydrogen reaction, Intergranular stress corrosion cracking

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WEDNESDAY

Influence of chitosan degree of acetylation and molecular weight on DNA/chitosan nanoparticles formation

K. G. FERNANDEZ[1,2,3], J. ROSSELGONG[1,2], F. CARVAJAL[4], M. RINAUDO[5], L. M. BRAVO-ANAYA[1,2*]

[1]University of Bordeaux, LCPO, UMR 5629, F-33600, Pessac, France.
[2]CNRS, LCPO, UMR 5629, F-33600, Pessac, France.
[3]Centro Universitario UTEG, Héroes Ferrocarrileros #1325 44460, Guadalajara, Jalisco, México
[4]CUTonalá, Departamento de Ingenierías, Universidad de Guadalajara, Nuevo Periférico # 555 Ejido San José Tatepozco, C.P.45425, Jalisco, México.
[5]Biomaterials applications, 6 rue Lesdiguières. 38000 Grenoble, France.

*monik_ayanami@hotmail.com

Polyelectrolyte complexes present different and interesting physicochemical properties combined with a high biocompatibility, very useful for biomedical applications. DNA, in its double helical structure is a long and locally cylindrical polyelectrolyte chain. Cationic polymers interact electrostatically with negatively charged DNA forming polyplexes. These positively charged polymers have been widely studied as non-viral vectors for their applications in gene therapy. Chitosan, a polysaccharide very abundant in nature, is considered as one of the most attractive vectors due to is biocompatibility and its biodegradability [1]. DNA chitosan complexes are formed due to electrostatic interactions between DNA phosphate group and chitosan protonated amine group in acidic conditions (Figure 1). Here we study the influence of chitosan molecular weight (MW) and its degree of acetylation (DA) on chitosan-DNA polyelectrolyte complexes formation and characteristics. Seven chitosan samples were firstly studied through different techniques (conductivity, IR, 1H NMR and SEC) to determine their DA, MW and protonation behavior. Then, the formation of DNA /chitosan nanoparticles was monitored in terms of the variation of the zeta potential and the hydrodynamic radio (RH) as a function of the charges ratios between the chitosan and the DNA ([NH3+]/[P-]). A set of nanoparticles was prepared at different charges ratios, giving to RH values ranging from 25±5 nm to 80±10 nm before the isoelectric point (IP) and from 60±10 nm to 150±20 nm after the IP. Figure 1 – DNA/chitosan complexes formation scheme and AFM image taken for a [NH3+]/[P-]=5.

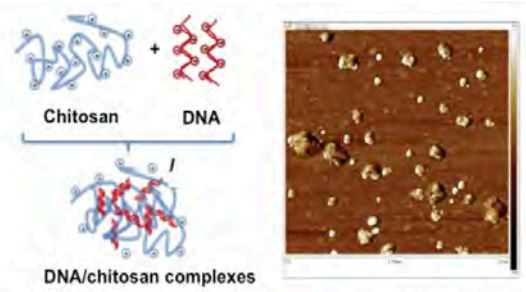

Figure 1 – DNA/chitosan complexes formation scheme and AFM image taken for a $[NH_3^+]/[P^-]=5$.

Key Words: DNA, chitosan, electrostatic complex, DA, molecular weight, stability

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Degradation of polychlorinated biphenyls through iron, zirconium and titanium oxide nanoparticles using visible light

Guzmán-Islas JOSÉ ÁNGEL[1*], Rodríguez-Huerta JESSICA MARIANA[1], Yáñez-Valerio ZAIDA ROCÍO[1], Martínez-Dueñas MARCELO[1], Huerta-Aguilar CARLOS ALBERTO[1]

[1]División de Nanotecnología, Universidad Politécnica del Valle de México, Avenida Mexiquense s/n, 54910, Tultitlán, Estado de México, México.

*josean1206@live.com.mx

Polychlorinated Biphenyls (PCBs) have a great negative impact on the environment as a result of their toxicity. The physicochemical properties of PCBs, as well as their toxicity, depend directly on the structure that the compound presents, therefore its analytical determination is very important. The behavior of these compounds in the presence of metal oxide nanoparticles has been little studied. However, due to the application of these materials in the degradation of other refractory contaminants, it was considered that they can be efficient in the degradation of PCBs [1, 2]. In this work, the presence of chlorinated aromatic compounds was observed in the samples under study. These contaminants were characterized by analytical techniques (FTIR and UV-Vis spectrophotometry). Moreover, this project seeks to degrade polychlorinated biphenyls through the use of nanoparticles of iron (Fe_3O_4), zirconium (ZrO_2) and titanium (TiO_2) oxides as photo catalysts under visible light. These materials are sought to prove that they can be applied in the degradation of chlorinated aromatic contaminants, which are difficult to degrade by conventional methods. Within this research work, PCBs obtained from obsolete electrical devices were exposed to artificial visible and solar irradiation using a parabolic cylindrical solar collector (PCC) previously calibrated and positioned, both in the presence of Fe_3O_4, ZrO_2, and TiO_2 in constant stirring. The degradation kinetics for each catalyst were determined in order to know the speed and removal efficiency. On the other hand, the results have been corroborated with theoretical computational studies of DFT in order to have and insight the mechanism of degradation of these compounds.

Key Words: polychlorinated biphenyls, degradation, visible light, photocatalyst.

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Organic nanoparticles from natural plant extracts and its application as bug repellents

C. A. Huerta-Aguilar[a, b*], M. C. Solís-Pacheco[a], C. I. Xolio-Cortés[a], J. Narayanan[a], T. J. Ariza-Ortega[a], P. Thangarasu[b]

[a]Division of Nanotechnology, Universidad Politécnica del Valle de México, Tultitlán, 54910, México.
[b]Faculty of Chemistry, Universidad Nacional Autónoma de Mexico, Coyoacán, 04510, México.

caha_09@comunidad.unam.mx

During 20th century, there was a trend for development and utilization of synthetic chemicals in many areas ranging from food additives to drugs. However, man made products are usually non-biodegradable which has as consequence ecosystems degradation once these products are liberated to the environment. To overcome this issue, the new trends in pharmaceutical and food science seek for application, modification and commercialization of natural products according to human needs. Among natural products with potential applications, essential oils have gained attention due to its low toxicity, availability and bioactive components; nowadays, many commercial products derived from these molecules are found elsewhere. For example, the extracts from certain plants have shown good efficiency as bug repellents due to the presence of biomolecules such as phenolic acids, flavonoids and terpenes. The development of effective and low cost repellents is of great concern in developing and tropical countries with large touristic flow and vulnerable population due to the presence of harmful insects that spread serious diseases such as malaria, dengue and yellow fever. In the present study, we present the obtainment of essential oil and later formation of organic nanoparticles (ONPs) through microemulsion method from three plant extracts: Syzygium aromaticum, Rosmarinus officinalis, Cymbopogon nardus. Obtained extracts were characterized though FTIR and prepared ONPs were studied in its morphology and size through Atomic Force Microscope (AFM) and Dynamic Light Scattering (DLS) showing round shapes ranging from 60 to 250 nm. Effectiveness as bug repellent was tested using a modification of World Health Organization (WHO) method where Syzygium aromaticum ONPs showed superior performance among all tested materials. The future applications of these extracts and its applications as ONPs allow the commercial production at low costs and avoiding the utilization of harmful products such as N, N-Diethyl-meta-toluamide (DEET) which is the main bug repellent worldwide.

Key Words: organic nanoparticles, bug repellents, Syzygium aromaticum, Rosmarinus officinalis, Cymbopogon nardus

Removal of contaminants from water based on a super-hydrophobic-magnetic sponge

Jesús Iván Tapia[1*], Elizabeth Alvarado[2], Armando Encinas[1]

[1]*Instituto Potosino de Investigación Científica y Tecnológica A.C., Camino a La Presa de San José 2055, Lomas 4 sección, 78216 San Luis, S.L.P., México*
[2]*Universidad Autónoma de San Luis Potosí, Alvaro Obregon 64, Centro, 78300 San Luis, S.L.P., México*

*jesus.tapia@ipicyt.edu.mx

Water contamination by oils and heavy metals is an important problem, since environmental, economic and health issues can be caused. It can mainly damage the aquatic ecosystem as well as the biodiversity of the land, affecting the long-term health of population who live near to affected regions [1]. Furthermore the emission sources are multiple such as oil spill from oils platforms and the discharge of organic chemicals from industrial activities. Therefore, it is necessary to implement simple and non-expensive methods for the removal pollutant oils from water [2,3].

In this sense, we studied the use of Luffa sponge, a naturally occurring porous structure, and a natural organic hydrophobic coating in order to develop a super-hydrophobic porous material (Figure 1) with high absorption capability. The material was also functionalized with magnetic nanoparticles. This material has potential applications to remove oils and toxic heavy metals from water using magnetic separation techniques. The material obtained was characterized using Scanning Electron Microscopy, Fourier Transform Infrared, Ultraviolet–visible spectroscopy, water contact angles and oil-metal absorption properties.

Figure 1. A water droplet as a spherical shape trace on the surface of the modified luffa sponge

Key Words: Luffa, super-hydrophobic, magnetic-nanoparticles, water, oil.

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Surface modification of magnetite nanoparticles with γ-aminobutyric acid

Rosales-de los Santos S.[1*], Cervantes-Arreola O.[1], Topete A.[2], Cano M. E.[3], Pérez B. V.[1], Bárcena-Soto M.[1], Casillas N.[1]

[1]Universidad de Guadalajara, Blvd. Marcelino García Barragán 1421, C. P. 44430, Guadalajara, Jalisco, México
[2]Universidad de Guadalajara, Sierra Mojada 950, C. P. 44340, Guadalajara, Jalisco, México
[3]Universidad de Guadalajara, Av. Universidad 1115, C. P. 47820, Ocotlán, Jalisco, México

*saray_r_s87@hotmail.com

The γ-aminobutyric acid (GABA) is a inhibitory neurotransmitter in the central nervous system and is a multifunctional molecule that has different situational functions in the central nervous system, the peripheral nervous system, and some nonneuronal tissues [1]. The purpose of this work is to surface modify magnetite nanoparticles, produced by the coprecipitation method, with GABA hydrochloride. The ultimate goal of the project is to produce a magnetically addressable vehicle to specific sites of the cerebral cortex. The advantage of the use of magnetite nanoparticles lies in their superparamagnetic properties, biocompatibility and saturation of magnetization, which makes them useful in biomedical applications, as a radiological contrast medium, hyperthermia treatment or as a carrier of active principles [2]. In structural terms, magnetite is a mixed oxide with a reverse spinel structure in which the Fe^{+2} ions occupy the octahedral positions of the network and the Fe^{+2} ions the octahedral and tetrahedral positions [3]. Functionalization of the magnetite surface with GABA is carried out by sonication by reaction with amino or carboxylic functional groups. The results presented include nanoparticles magnetite size and distribution by TEM and the characterization by FTIR and vibrating sample magnetometer (VSM) of functionalized magnetite samples.

Key Words: Magnetite, coprecipitation, neurotransmitter and γ-aminobutyric acid.

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Different loading methods on the encapsulation capacity of ibuprofen into MCM-41

Josué Castillo N[1], Laura Estrada[1], Miguel Ojeda M[1], Celso Velasquez O[1], Ma. Luisa Ojeda M[1]

[1]Universidad de Guadalajara, Centro de Investigación en Nanociencia y Nanotecnologías, CUVALLES Carretera Guadalajara-Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México

*jochess507@gmail.com

The synthesis of ordered mesoporous silicas has received extensive attention due to the possibility to obtain an ordered arrangement, large surface area, and chemical stability [1, 2]. The pore size and pore volume of these materials make them suitable potential matrices for hosting. MCM-41, which is a member of the M41S family with a highly hexagonal arrangement of parallel mesopores [3]. The objective of the present study was to encapsulate ibuprofen into MCM-41 using different loading methods. Ibuprofen (IBU) with a molecular size about 1.0 nm was selected for encapsulation into MCM-41 with diameter around of 3 nm. The loading of IBU was done by three methods, which are known as suspension, soaking, and immersion (membrane) method. Characterization of the loaded MCM-41 was done by DRX, UV-Vis with diffuse reflectance, FT-IR and TEM. IBU was successfully encapsulated into MCM-41, without affecting the mesoporous structure.

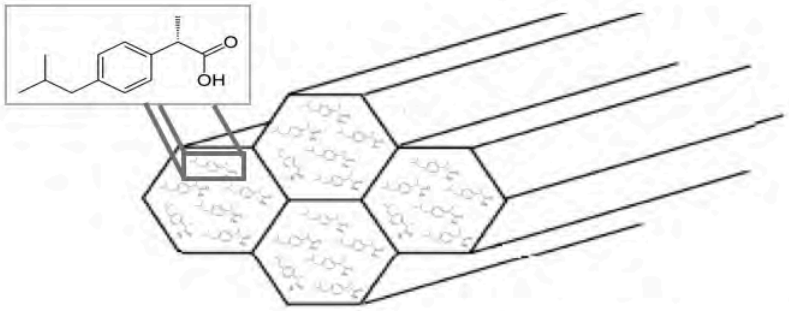

Figure 1 Schematic representation of IBU loading in MCM-41

Key Words: mesoporous, encapsulation, ibuprofen, loading.

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Development of a nanostructured biosensor of TiO_2 doped Ag to measure ascorbic acid

Jorge Ebisai Sanchez Alvarez[1]*, M. G. Garnica-Romo[2], M. Romero Arcos[3], T. Hernández Quiroz[2], J. Hernández-Torres[1], L. Zamora Peredo[1] and L. García-González[1]

[1]Centro de Investigación en Micro y Nanotecnología, Universidad Veracruzana, Calzada Adolfo Ruiz Cortines 455, C.P. 94294, Boca del Río, Veracruz, México
[2]Facultad de Ingeniería Civil, Universidad Michoacana de San Nicolás de Hidalgo, Santiago Tapia 403, C.P. 58000, Morelia, Michoacán, México.
[3]Cinvestav unidad Querétaro. Laboratorio de nanomateriales y electroquímica, Norponiente 2000 C.P 76230, Querétaro, Qro. México

jor_91_3@hotmail.com

In the current work an ascorbic acid biosensor was developed, using thin films of TiO_2 doped Ag over glass coating with ITO. The synthesis of nanostructured TiO_2/Ag was obtained by sol-gel method, the reactive used were Titanium Isopropoxide (IV) TIP Sigma Aldrich, Nitric Acid (HNO_3), deionized water, 2-propanol, all the chemicals were analytical grade with no further purification. The deposition of TiO_2/Ag was done by spin coating, the spin speeds at 2000 and 5000 rpm for 30s. Afterward heat treatment was carried out at 500°C for 1 hour. To study of the nanostructured matrix of TiO_2/Ag was characterized by these means method Raman spectroscopy obtaining the characteristic 143, 396, 514 y 636 cm-1 of anatase, these results were corroborated by X-ray diffraction, as identifies that the crystalline phase was anatase with preferred orientation (101), (004), (112), (112), (200), the presence of Ag was identified in 2θ =38.61, 50.37, 66.75, 72.67); The crystal size calculated for the crystalline phase of TiO_2 by the Debye-Scherrer method was from 13 to 15 nm. Film thicknesses were obtained in SEM between 100-250 nm and in AFM a pore size between 50-120 nm with a uniform topography. The cyclic voltammetry and amperometry tests show the hysteresis cycle of the system, with enzyme percentages of 10, 20, 30 cm^{-1}. showing a response in the range of 10 µM-150 µM / L ascorbic acid per minute and 15-50 mV / mM sensitivity, this response in the middle range of this type of sensors.

Keys words: Titanium isopropoxide, sol-gel, sping-coating

Environmental impact of nanoparticles of calcium phosphate by chemical synthesis

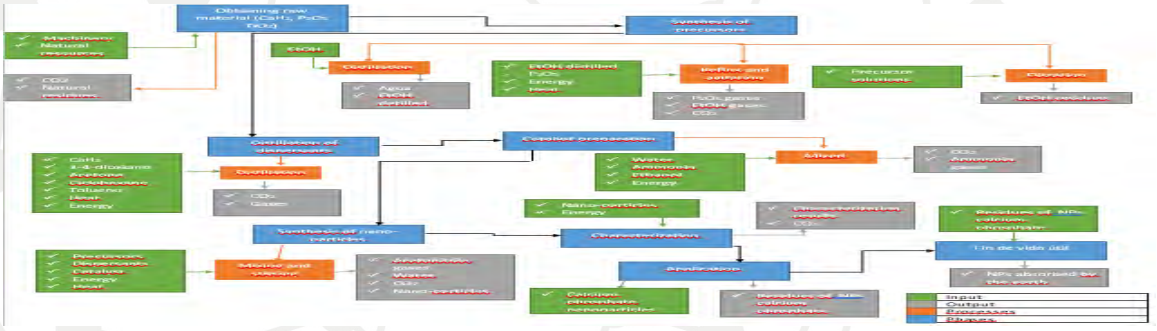
Lugo CAROLINA, López MIGUEL, Pablo DANIEL, Sánchez YAVAZUL, Huerta CARLOS, Narayanan JAYANTHI, Martínez BEATRIZ

Avenida Mexiquense s/n, esq. Universidad Politécnica, Col. Villa Esmeralda, Tultitlán. C.P. 54910, Estado de México

*nano.pm801@gmail.com

Introduction: Currently, it is known that conventional fertilizers generate a large amount of contaminant residues once they finish their operation. The 50% of the world's population depends on chemical fertilizers, as the organics are overstretched [1]. Erosion and the sterilization of the earth are some of the consequences present. With the synthesis of these nanoparticles is intended to give an alternative friendly to the environment to perform the same functions but with a lower rate of contamination.

Objective: To evaluate with a torn LCA the phases of the synthesis of nanoparticles of calcium phosphate as well as its viability for use as fertilizer. Methodology: Was considerate the ISO Normativity as 14040, 14041, 14042, 14043 and 14044 to do the LCA (Figure1) of the sol gel synthesis [1] and can be assessed the environmental impact of each phase of the synthesis and determine which generates the most amount of contaminants.



Results: It is obtained because of the LCA that the preparation phase of the catalytic converter is where you will find the most significant contaminant (ammonia), it is estimated to obtain 53.1 microliters of ammonia.

Conclusions: Thanks to the LCA is analyzed the phases of the synthesis of the NPS and determine possible improvements to such synthesis and determine which of the phases presents a greater contamination (phase of preparation of the catalytic converter).

Key Words: LCA (life cycle assessment), Fertilizers, Sol-Gel.

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Micro-contact printing of low molecular weight polydimethylsiloxane oligomer thin films and their application in materials processing

J. A. Rangel Castillo[1*], E. Araujo[2], A. Encinas[1]

[1]*Instituto Potosino de Investigación Científica y Tecnológica (IPICYT), Camino a la Presa San José # 2055., Col. Lomas 4 sección, CP. 78216. San Luis Potosí, S.L.P., México.*
[2]*Instituto Tecnológico y de Estudios Superiores de Occidente (ITESO), Periférico Sur Manuel Gómez Morín # 8585, C.P. 45604 Tlaquepaque, Jalisco, México.*

*jorangelcas@gmail.com

Polydimethylsiloxane (PDMS) is an elastomer that is widely employed both in research as well as in well-established applications. It received a great deal of attention in the last two decades due to its applications in soft-lithography techniques [1] an in microfluidics technology [2]. An interesting property of these PDMS elastomers is that depending on the degree of cross-linking there is an amount of un-cured PDMS chains free within the elastomeric network. Among these, low molecular weight cyclic oligomers (LMWCO) are highly mobile, abundant and diffuse freely through the elastomer structure. These properties have been exploited to use these LMWCOs as a highly hydrophobic ink that can be transferred onto a wide variety of substrates by simply putting in contact PDMS with the surface [3]. In this work, we use the transfer of the LMWCO ink using micro-contact printing to study its applications in materials fabrication and processing. We show that the ink allows to fabricate chemical wettability patterns on a wide variety of surfaces which combined with other techniques such as thin film evaporation or chemical etching allow fabricating materials with patterned physico-chemical properties.

Key Words: Oligomers, soft-lithography, hydrophobic ink.

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NPs-Cu Bifunctional use: as an electrochemical sensor and catalyst in a μFC using Chol as fuel.

I. Murillo-Borbonio[1], R. A. Escalona-Villalpando[1], J. Ledesma-García[2], M. P. Gurrola[*1], L. G. Arriaga[*1]

[1]Centro de Investigación y Desarrollo Tecnológico en Electroquímica, Parque Tecnológico Querétaro s/n Sanfandila, C.P. 76703, Pedro Escobedo, Querétaro.
[2]División de Investigación y Posgrado, Facultad de Ingeniería, Universidad Autónoma de Querétaro, Carretera Chichimequillas s/n, Ejido Bolaños, C.P. 76140, Santiago de Querétaro, Querétaro.

*larriaga@cideteq.mx

Materials development that can be used in more than one application, has been the research focus in recent years, calling them as bifunctional materials [1]. In this sense, the present work is dedicated to the electrodes modification with lower added value materials than the conventional ones in the market (NiO, Au-Pt) [2, 3], opting for an economic metal and with high selectivity to the proposed fuel (cholesterol) as Copper [4]. Copper was synthesized as nanoparticles (NPsCu), which were used to develop a non-enzymatic electrochemical cholesterol sensor (NECS) and the cholesterol (Chol) application of as energy source, evaluating the Cu-NPs in a micro-fuel cell (µFC). As an electrochemical sensor, a calibration curve was constructed with the different electrochemical processes (Reduction and Oxidation), obtaining an R^2 = 0.9632, with them, the limits of detection (LOD) and quantification (LOQ) were calculated, which presented values of up to 99.97% lower than conventional electrodes, reducing the error for the detection of Chol concentrations lower than 1mM. On the other hand, the evaluation of Chol as an energy source was carried out in the µFC used by Escalona et al [5], where the flows applied in the cathode, as well as the anodic zone, are schematized, in this case best results were for the [C] < 0.4 mM, due to the saturation of the electrode by the vesicles of Triton® X-100 used as a surfactant.

Key Words: Bifunctional, non-enzymatic, selectivity, cholesterol, sensor, micro-fuel cell.

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Synthesis and characterization of biocomposite materials based on corn husk dyed with magnetic of FE_3O_4 nanoparticles in a polimer matrix

Daniel Camacho, Armando Encinas

Instituto Potosino de Investigación Científica y Tecnológica A.C., Camino a La Presa de San José 2055, Lomas 4 sección, 78216 San Luis, S.L.P., México

*daniel.c2694@hotmail.com

Due to the increasing demand on materials with tailored properties and the need to find different approaches to satisfy industrial as well of social needs, an important research effort has been given to find novel approaches to use and re-use renewable and abundant natural resources to develop materials that can either provide solutions to specific needs or replace other materials that are more scarce or expensive. In this sense, this study aims to develop a methodology for the synthesis of a material based on corn husk residues collected of small street markets in the locality. The samples were first cleaned, sun dried, to later be chopped in small fibers. The fibers were then chemically treated with NaOH in order to increase the porosity and the hardness of the fibers by removing lignin contents. Using of the volume left after lignin removal Fe_3O_4 magnetic nanoparticles were synthetized by the co-precipitation method. The magnetic corn fibers where then used to make a composite material in a polymeric matrix. The composites were characterized using optical and electronic microscopy and their magnetic and mechanical properties are discussed.

Key Words: Corn husk, Biocomposite, Magnetic Fibres, magnetic nanoparticles

Life cycle analysis of titanium oxide nanoparticles through the method of chemical synthesis and its toxicity in the environment

Chávez BRENDA, Morales JOSE, Hernandez JESUS, Martínez BEATRIZ

Universidad Politécnica, Col. Villa Esmeralda, Tultitlan. C.P. 54910, Estado de México.

*jesus.hernandez-maravilla@outlook.com

Titanium dioxide (TiO_2) is a white and insoluble mineral. It is found naturally in three minerals: rutile, anatase and brookite. In cosmetics it is used as a physical sunscreen for its ability to reflect sunscreens. Today there are sunscreens with TiO_2 nanoparticles. However, there are no reported studies on the environmental impact of this type of product. However, it is vital to know the future impact of this type of products. To develope the LCA of the titanium dioxide nanoparticles (Nps TiO_2) and determine the risk of environmental impact they exert through a chemical synthesis method (Figure 1). The LCA of sunscreens was developed with TiO_2, based on ISO 14040, 14041, 14042, 14043, 14044 regulations.

The recognition of the emissions of the reagents and their possible damages, as well as the study of the LCA, provided clear information on their impact, demonstrating that they have greater influence in the manufacturing area. An LCA will be performed to determine the impact and possible damage of the TiO_2 NPs in them application as sunscreens.

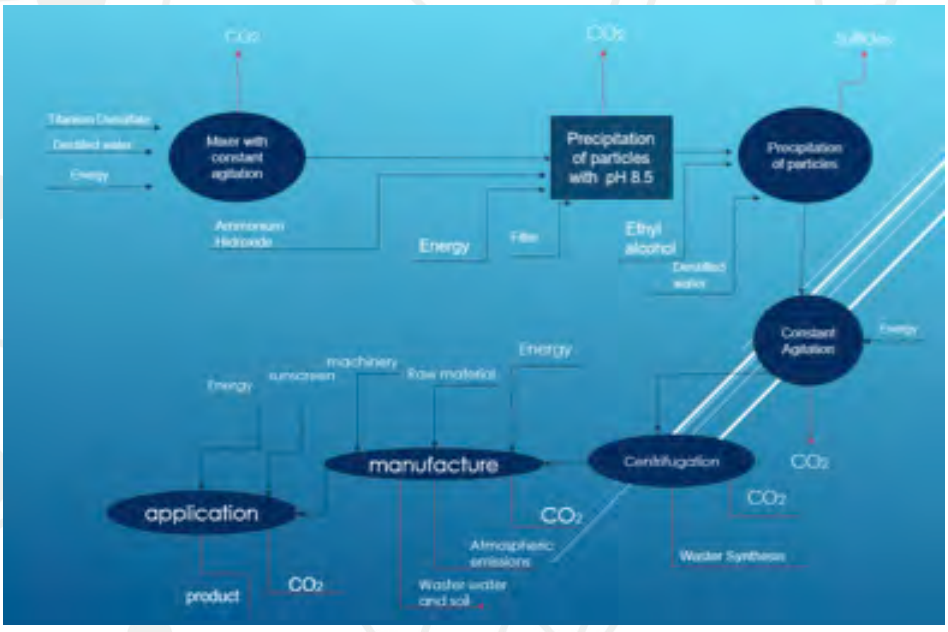

Figure 1- LCA of sunscreens with TiO_2 nanoparticles.

Key Words: Sunscreens, Nanoparticles, Life cycle analysis (LCA), Titanium dioxide, Carbon dioxide.

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Synthesis of nanocapsules of retinol for a cosmetic application

Valle RICARDO[1], Hernandez DIANA[1], Maldonado MANUEL[1], Martinez BEATRIZ[1]

[1]Universidad Politecnica del Valle de Mexico, Division of Nanotechnology Engineering Mexiquense Avenue s / n, esq. Universidad Politecnica, Col. Villa Esmeralda, Tultitlan. C.P. 54910, State of Mexico.

ricardovalle.upvm@gmail.com

INTRODUCTION: Dermic care in topical products with antioxidants, are considered one of the most promising strategies to maintain a healthy state in the skin [1], however most of these products show physical-chemical unfavorable properties, excessive lipophilic or hydrophilic, chemical instability and Low penetration limits the effectiveness of these products, so it is necessary to look for more efficient means of diffusion [2]. Retinol nanocapsules are a good solution to keep skin healthy and have more favorable properties than current products.

OBJECTIVE: Prepare retinol nanocapsules for use in cosmetic formulations.

METHODOLOGY: The nanocapsules were prepared by the method of emulsion and solvent evaporation: In phase a, 150 mg of polyexiloncapilactrona, 50 mg of Vitamin A and 10 mg of soy lecithin were weighed. All was dissolved in 10 mg of ethyl acetate by magnetic stirring at 400 rpm. For phase b, 50 ml of 3% Peg 40 solution was prepared. Subsequently, phase a in phase b was added dropwise and kept in evaporation.

RESULTS: Polymeric nanocapsules of Vitamin A were obtained between 200 and 300 nm. With a 60% encapsulation efficiency.

Key Words: Polymer nanocapsules in cosmetology, retinol, soy lecithin, polyexiloncapilactrona, emulsification, solvent evaporation.

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Impact of complex formation protocol and charge ratio on the characteristics of carrier/DNA polyplexes

R. A. NAVARRO GRAJEDA[1], F. CARVAJAL[1], G LANDAZURI[2], L. M. BRAVO-ANAYA[3,4*]

[1]CUTonalá, Departamento de Ingenierías, Universidad de Guadalajara, Nuevo Periférico # 555 Ejido San José Tatepozco, C.P.45425, Jalisco, México.
[2]Universidad de Guadalajara, Departamento de Ingeniería Química. Blvd. M. García Barragán #1451, Guadalajara, Jalisco, C.P. 44430, México.
[3]University of Bordeaux, LCPO, UMR 5629, F-33600, Pessac, France.
[4]CNRS, LCPO, UMR 5629, F-33600, Pessac, France.

*monik_ayanami@hotmail.com

DNA compaction and decompaction are two of the most important steps in gene therapy [1]. The compaction of DNA into small nanoparticles can facilitate cell uptake and can protect DNA from degradation by nucleases. Then, DNA decompaction and release inside the cells allows recovering DNA properties and proceeding to the transcription. DNA compaction is a reversible coil to globule transition favored by electrostatic interactions between cationic vectors and negatively charged DNA phosphate groups. When the number of neutralized charges reaches a critical value, DNA undergoes a localized twist, which enables the formation of complexes having sizes in the range of nanometers, much smaller than that of the DNA coil conformation (microns). Chitosan is a polysaccharide that has been identified as a safe and efficient cationic carrier possessing suitable characteristics for gene delivery. In this work we analyze the impact of experimental conditions on the resulting DNA/LMW-Chitosan complex characteristics. We show the influence of the carrier/DNA charge ratio, the medium where they are prepared and the protocol of complex formation, on DNA/LMW-Chitosan complex sizes and stability.

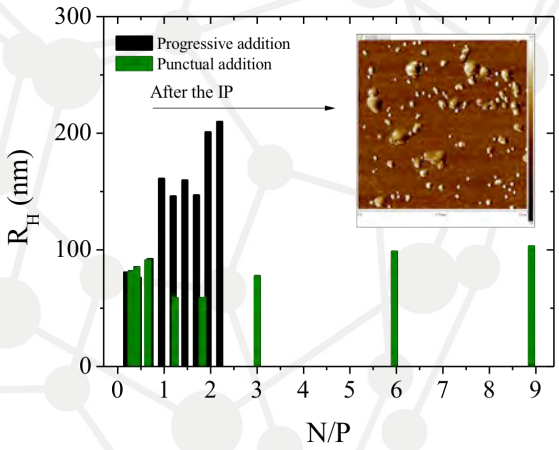

Figure 1 – RH of the obtained nanoparticles as a function of the N/P ratio. Insert: AFM images of LMW Chitosan/DNA complexes formed at a charge ratio (N/P) of 3.

Key Words: DNA, compaction, charge ratio, isoelectric point, chitosan.

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Band-Aid of chitosan hydrogel with silver nanostructures and calendula extract

Erika Fabiola Hernández Elizarrarás[1], Esmeralda Dhamar Rayas Urdiano[1], Susana Elizabeth Rocha González[1], Aurelio Galván Martínez[2], Hugo Getzael Rodríguez Acosta[2], Jose Maria Tapia Rivera[2], Yadira Guadalupe Sanchez Toscano[3], Adriana Cavazos Garduño[4], Ernesto David García Bustos[5], Adalberto Zamudio Ojeda[6]

[1]Licenciatura en Ciencias de los Materiales, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México.
[2]Ingeniería de Nanotecnología, Centro Universitario de Tonalá, Tonalá, Jalisco, México.
[3]Coordinación de investigación de básica biomédica, Universidad Guadalajara LAMAR, Campus Vallarta, Guadalajara, Jalisco, México.
[4]Departamento de farmacobiología, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México.
[5]Cátedras Conacyt, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México.
[6]Departamento de Física, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México.

kika.faby@live.com

Chitosan [1] is a cationic linear polysaccharide, which has antibacterial properties, is a biopolymer biocompatible, biodegradable, non-toxic and bactericide, it is used in medicine, cosmetics, the food industry and more. In this project we have create a hydrogel [2] with a chitosan base that it is elastic and when it gets dry, it crystalizes. Through a chemical process with silver nitrate and sodium citrate we have created silver nanostructures [3] which help to destroy bacteria. To make the chitosan hydrogel, we use triethanolamine, acetic acid, chitosan and we add silver nanostructures and calendula extract; this creates a solid elastic material, because of the chitosan and the silver nanostructures increase the bactericidal properties and the calendula extract help as natural healing. This will be tested in bacteria E. Coli. The obtained materials will be analyzed by the following characterization process: XRD, UV-Vis, and SEM. The chitosan hydrogel with silver nanostructures can be used as a Band-Aid, come other biomedical applications.

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Evaluation of DNA/chitosan complex stoichiometry

S. LOPEZ ALVAREZ[1], F. CARVAJAL[1], E.R. MACIAS BALLEZA[2], L. M. BRAVO-ANAYA[3,4*]

[1]CUTonalá, Departamento de Ingenierías, Universidad de Guadalajara, Nuevo Periférico # 555 Ejido San José Tatepozco, C.P.45425, Jalisco, México.
[2]Universidad de Guadalajara, Departamento de Ingeniería Química. Blvd. M. García Barragán #1451, Guadalajara, Jalisco, C.P. 44430, México.
[3]University of Bordeaux, LCPO, UMR 5629, F-33600, Pessac, France.
[4]CNRS, LCPO, UMR 5629, F-33600, Pessac, France.

*monik_ayanami@hotmail.com

Nanotechnology is currently used in the development of new strategies for the release of genes and therapies against cancer [1]. A large number of characteristics that benefit the release of genes are found only in some available natural polycations, capable of compacting DNA molecules [2]. The mechanism of formation of DNA-polycation complexes is a key step before the transfection of DNA into the nucleus of the cell to achieve its ultimate goal (Figure 1) [3]. Chitosan is a polysaccharide of low immunogenicity and high biocompatibility capable of protecting DNA from degradation by nucleases and transferring it within several cell types. In this work, the stoichiometry during the formation of nanoparticles constituted by chitosan and DNA was studied for improving the protocols of DNA/chitosan complexes formation for gene delivery purposes. Electrophoretic mobility (ζ-potential) and Dynamic Light Scattering (DLS) measurements were used to determine the effect of the amount of chitosan in the formation of the nanometric complexes resulting from DNA compaction process. The effect of variation of DNA concentration and ionic concentration on the complex stoichiometry was also evaluated in this work in order to determine the best experimental conditions to obtain stable polyplexes in size and charge.

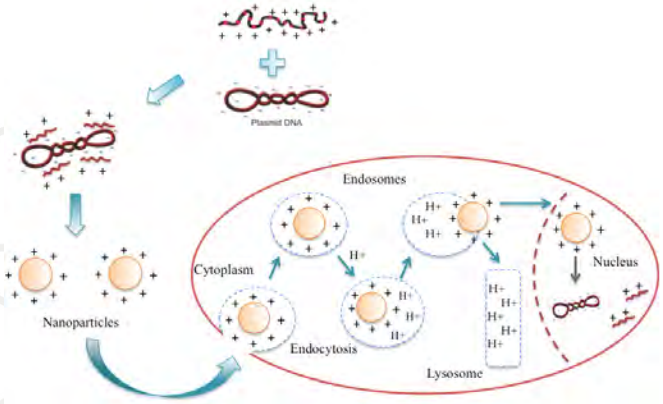

Figure 1 – Schematic representation of DNA compaction process and it´s transfection into a cell.

Key Words: DNA, stoichiometry, net charge, chitosan, electrostatic interactions, complex formation.

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Isolation of cellulose from banana raquis

V. Flores Velazquez[1*], C. G. Espinosa-González[2], F. Ortíz Chi[2], S. Godavarthi[2], J. G. Torres-Torres[1]

[1]Universidad Juárez Autónoma de Tabasco. Carretera Cunduacán-Jalpa Km 1 Col. La Esmeralda, CP. 86690, Cunduacán, Tabasco, México.
[2]Cátedras CONACYT- Universidad Juárez Autónoma de Tabasco. Carretera Cunduacán-Jalpa Km 1 Col. La Esmeralda, CP. 86690, Cunduacán, Tabasco, México.

*vale_2_02@hotmail.com

In the present work, cellulose from banana rachis was isolated. For this purpose, a combination of soft chemical treatments was used so that, cellulose fibers were obtained. For the obtaining procedure the lignocellulosic material the technique established by Escamilla et al., was used. The procedure is as follows: lignocellulosic material was obtained from the banana rachis, and then, it was cut in small pieces, and then these were washed with abundant water and finally dried at room temperature. After that the material was dried, cellulose was extracted with the methodology used by Zuluaga et al. The procedure is as follows: an extraction with a toluene-ethanol solution (2:1, v/v) was done by Soxhlet during 6 h, and then a treatment with alkaline solution containing 1.5 wt % H2O2 was carried out, adjusting pH at 12 using NaOH 12 M, and stirring for 14 h at 45 °C. Finally, the insoluble residue was treated with 80% acetic acid (v/v) and 70% (v/v) nitric acid at 120 °C for 15 min. To verify desired material, X-ray diffraction (XRD) was used. The results are shown in figure 1. In diffractograms can be observed a shoulder in range of 14-16 of 2q associated with an amorphous part of polymer, and others peaks close to 22 and 34 of 2q represent a crystalline structural phase characteristic of cellulose. It can be concluded that the material was actually obtained, moreover, that the technique is effective for isolation of cellulose.

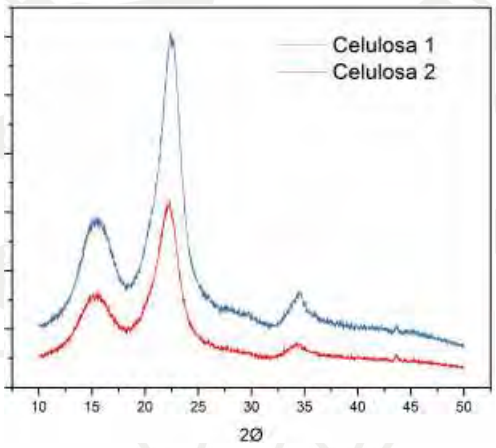

Figure 1 - Difractograms corresponding to Cellulose obtained from banana raquis; samples 1 and 2.

Key Words: Rachis, Celullose, Soft treatment, Amorphous part.

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Life cycle analysis of iron nanoparticles applied to the elimination of dyes in environment aqueous

Alpizar MISAEL, Castro DIANA, Rodriguez ITZEL, Martinez BEATRIZ

Universidad Politécnica del Valle de México, Av Mexiquense s/n, esq Av Universidad Politécnica, Villa Esmeralda, 54910 Tultitlán de Mariano Escobedo, Estado de México, México

misael1221@hotmail.com

INTRODUCTION: According with Iago Neira Garcia of the Faculty of Sciences at the University of Coruña, oxide nanoparticles of iron (FeNPs) have high potential in the use of adsorption of organic compounds such as dyes. Synthesis processes involving NPs-Fe redox. So far it not determined the environmental impact of the synthesis of NPs-Fe or use. [1-2]

OBJECTIVE: To determine the Life Cycle Analysis (LCA) of REDOX synthesis focus on obtaining NPs Iron (Fe) and so know the environmental impact of these nanoparticles.

METHODOLOGY: the LCA of NPs-Fe was elaborated for its use as adsorbents dye contaminants. The methodology was followed according to the ISO 14040, 14041, 14042.14043, 14044 and 14045 normativity's.

RESULTS: Through this synthesis, a Life Cycle Analysis (LCA) of the Fe NPs was performed, starting from obtaining the raw material, synthesis, application and the disposal of NPs as shown in the following table and figure below.

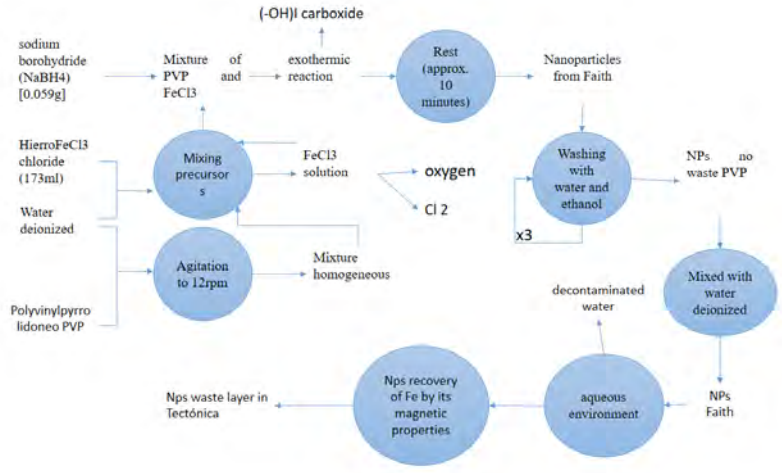

Figure 1 - LCA of NPs-Fe.

Key Words: Nanoparticles of Fe, dyes, life cycle analysis

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Preparation of surfaces with plasma coatings in wood

Britany Hernández Rosas

Academic Division of Environmental Technology and Nanotechnology, Fidel Velázquez Technological University, Emiliano Zapata Avenue S / N, Colonia el Tráfico, Nicolás Romero, C.P. 54400, State of Mexico. Mexico.

hilaryhr@hotmail.com

The present work develops the method of application of plasma-polymerization technology under the APPJ technique where the experimentation of preparation of plasma coatings is carried out with the projection of the solution of precursors; the human being has tried to imitate some characteristics that are they find in nature to improve their daily life. Such is the case of the hydrophobic properties of some plants that allow them to remain dry and clean as they are able to repel practically any liquid so that a hydrophobic coating is developed by means of the new technologies that is applied in surfaces of soft wood [1].

Key Words: Preparation of surfaces, plasma polymerization APPJ, Softwood, superhydrophobic surfaces.

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Synthesis of silver nanoparticles with sodium citrate and sugar as reducing agent under UV light

Gabriel Maxemin Ramírez[1], José Juan Gonzales Reséndiz[2], Diego Alberto Lomelí Rosales[3], Sara Angélica Cortéz Llamas[3], Adalberto Zamudio Ojeda[4], Juan Pablo Moran Lázaro[5]

[1]Ingeniería en instrumentación electrónica y nanosensores (IIEN), Centro Universitario de los Valles, Ameca, Jalisco, México.
[2]Ingeniería en nanotecnología, Centro Universitario de Tonalá, Tonalá, Jalisco, México. Guadalajara, Jalisco, México.
[3]Departamento de Química, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México.
[4]Departamento de Física, Centro Universitario de Ciencias Exactas e Ingenierías, Guadalajara, Jalisco, México.
[5]Departamento de ciencias computacionales e ingeniería, Centro Universitario de los Valles, Ameca, Jalisco, México.

gabmax4@gmail.com

Nanoparticles are very important in developing sustainable technologies for the future, for humanity and the environment. Most of the conventional methods for chemical synthesis have an impact on the environment and they are more expensive in comparison than those that use components found abundantly in nature, this is for the chemical reagents that are used in synthesis of materials and that is why it is important to make efficient methods in which can synthesize in a friendly way with the environment [1]. Sugar as normally known can be defined as sucrose which is a disaccharide formed by glucose and fructose, one of the most notable proprieties is the solubility in water. In this project we used sugar and sodium citrate witch in addition to water we make a solution which was expose under black light and we do this because it is normally used thermal sources (heating or microwave racks) to accelerate the reaction processes, but in this case for the light process we can carried out at room temperature [2].This chemical methods allow an easy synthesis of silver nanoparticles in solution. These metal nanoparticles have a great potential for biomedical applications as antibacterial agent, antifungal, biosensor, antiviral or wound healing [3]. For the characterization of the nanoparticles we use UV vis spectroscopy, SEM and TEM.

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Polarization and charge density variations, due to Arsenic in heme proteins

P. G. Nieto-Delgado[1*], A. J Rangel-López[2] and A. A. Vértiz-Hernández[2]

[1]Departamento de Físico-Matemáticas, Universidad Autónoma de San Luis Potosí (UASLP), Niño Artillero s/n, Zona Universitaria Poniente, 78290 San Luis Potosí, SLP, México.
[2]Coordinación Académica Región Altiplano, Universidad Autónoma de San Luis Potosí (UASLP), Carretera a Cedral Km 5+600, Ejido San José de las Trojes, 78700 Matehuala, SLP, México

guillermo.nieto@uaslp.mx

Cytochrome P450 (CTP 450) is a large family of heme proteins present in the mitochondrial cytoplasmic membrane, hepatic peroxisomes and the endoplasmic reticulum of many species, including mammals[1]. Associated with this complex we find the heteroenzyme CYP2C8, which is one of the most important in the metabolism of drugs. The heme-iron center of these is fundamental in the process of metabolism based on the electric charge exchange with the environment. Therefore, experimental data in the current literature reveal that this metabolic process is affected by the presence of arsenic [2,3]. Within this context, the objective was to determine the effects on charge density and polarization for the CYP2C8 heteroenzyme model by arsenic through the Density Functional Theory (DFT). The heteroenzyme was modeled from its crystallographic structure [4], including several amino acids in the around, and the iron-coupled atom. Thus, in several models we calculated charge density and polarization by means of the DFT in the presence and absence of arsenic. Our results demonstrate slight movement of iron in the presence of arsenic, and likewise, it changes its charge density importantly, also the iron reduces drastically the polarization due to the arsenic presence. In conclusion, our data suggest that the iron nucleus changes its electrical charge and polarization properties in the presence of arsenic.

Key Words: electronic density, polarization, CYP P450.

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Life cycle assessment for gold nanoparticles chemical synthesis

Gutierrez JOSUE[1], Estrada MANUEL[1], Martínez BEATRIZ[1]

[1]*Universidad Politécnica del Valle de México, División de Ingeniería en Nanotecnología, Col. Villa Esmeralda C.P 54910, Tultitlán Edo. de México, México.*

gut715@gmail.com

Manofacturing Nanomaterials (NNM´s) for biomedical applications has been researched since the last few years although there are not enough data about how its use could affect* our planet or health. To obtain information about how Au NP´s interact with the enivirоment and by suggesting methodologies to allow us evaluate each part a product´s life cycle [1,2]. Based on ISO 14000 norvativities the environmental impact of gold nanoparticles was analized with Life Cycle Assessment (LCA). This methodolgy was applied trough the next parts of their life cycle : Chemical-reduction synthesis, stabilization, use in cancer therapy, and, end of life. The diagram showed on the figure (Figure 1) includes inputs and outputs used for the LCA. In order to calcucate CO_2 and other emitions experimental procedure was done. We concluded that most environmental impact part of process was Synthesis owing to stabilizers and precursors toxicity.

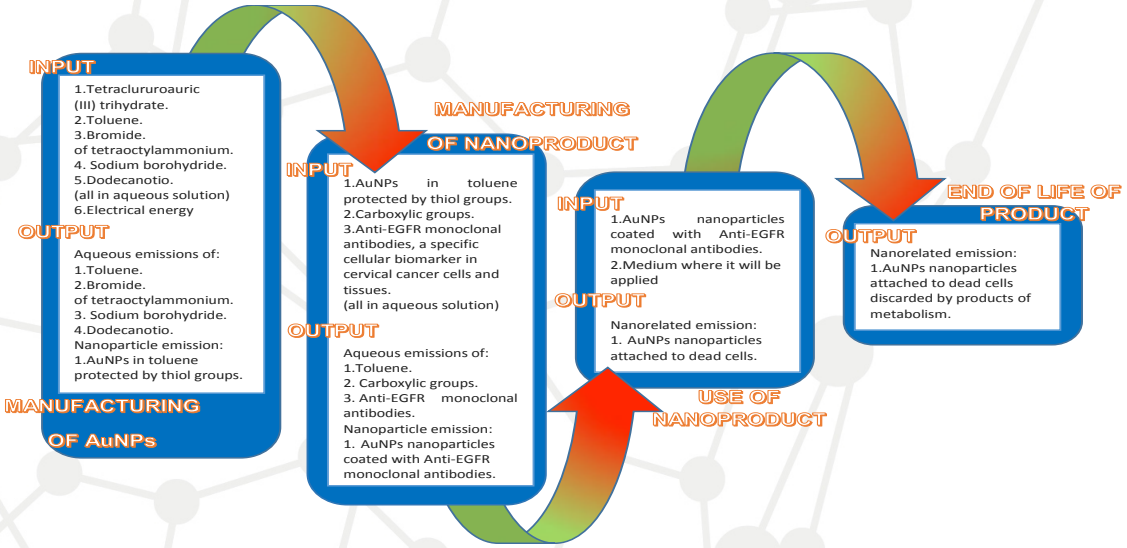

Figure 1 – Parts of Au NP´s Life cycle.

Key Words: Au Nanoparticles, Environmental Impact, Life Cycle Assessment, Toxicity.

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Chitosan-based thermosensitive nanoparticles as a carrier for hepatocyte targeted

Daniel Fernández-Quiroz[*1], J. Loya Duarte[1], A. Sarabia-Sainz[1], E. Silva-Campa[1], W. Argüelles-Monal[2], A. Lucero-Acuña[1], A. Burgara-Estrella[1], M. Pedroza-Montero[1]

[1]Universidad de Sonora, Blvd. Luis Encinas y Rosales S/N, CP. 83000, Hermosillo, Sonora, México. 2 Centro de Investigación en Alimentación y Desarrollo, 83304, Hermosillo, Sonora, México.

*daniel.fernandez@unison.mx

Cancer is the leading cause of death around the world. The current therapeutic approaches are still insufficient for successful treatments, and the overall survival rates for cancer patients is still very low [1]. Thus, the tissue-specific nanocarriers from thermo-sensitive biopolymers constitute an evolving therapeutic approach of controlled and directed drug delivery to tumor regions. In this sense, chitosan-graft-poly(N-vinylcaprolactam) (Cs-g-PVCL) biopolymer exhibits advantageous properties to biomedical applications, such as a dual pH- and thermo-sensitive close to physiological conditions [2]. Additionally, in the specific case for liver cancer, specific transporters can be obtained because the hepatocytes present an asialoglycoprotein receptor, which recognizes structures with galactose [3]. Toward that end, we reported the development of lactose-decorated Cs-g-PVCL nano-formulations able to be bio-recognized by the asialoglycoprotein receptor in liver cancer. Nanoparticles were prepared by ionotropic gelation and were characterized by DLS and AFM. The biorecognition tests were evaluated by riccinus comunis agglutinin I (RCA), and were performed using cancer cells from liver ($HepG_2$). The results showed that Cs-PVCL-Lac nanoparticles were highly recognized by RCA I. Moreover, the specific interaction of the nanoparticles with $HepG_2$ cells, demonstrating that they could be used as transport for an antitumor drug. Accordingly, this nanomaterial offers very interesting properties for the development of smart chemo-drug controlled delivery and tissue-specific carrier, which is an alternative potential to treat liver cancer.

Key Words: chitosan derivatives, stimuli-responsive polymers, biorecognition.

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Chitosan/PVA:ZnO doped nanofibers synthesis for possible applications in osteointegration

Del-Rio, J. Ignacio[1]. Estrada-Villegas, G. Mayeli[*2]. Arizmendi, Ana[3]. Elizalde-Peña, Eduardo[4]

[1]Universidad Autónoma de Querétaro, Carretera a Chichimequillas S/N, Ejido Bolaños, 76140, Santiago de Querétaro, Querétaro, México.
[2]CONACYT-Centro de Investigación en Química Aplicada, Alianza Sur 204, 66629, Parque de Investigación e Innovación Tecnológica, Apodaca, Nuevo León, México.
[3]Centro de Investigación en Materiales Avanzados, 66629, Parque de Investigación e Innovación Tecnológica, Apodaca, Nuevo León, México.
[4]División de Investigación y Posgrado de la facultad de ingeniería, Universidad Autónoma de Querétaro, Carretera a Chichimequillas S/N, Ejido Bolaños, 76140, Santiago de Querétaro, Querétaro, México.

*mayeli.estrada@ciqa.edu.mx

Chitosan-PVA electrospun nanofibers doped with ZnO nanoparticles were synthesized as the first stage of a novel electrospun core-shell fiber for prothesis osteointegration. Prothesis osteointegration is a desirable characteristic for which different coating materials are being developed. The main properties of these coating materials must have a high level of biocompatibility to avoid rejection or failure, antimicrobial functions to prevent infection during implantation and also promote bone formations for a full osteointegration on the prothesis [1]. These first two properties are addressed with the use of chitosan due to the excellent biocompatibility properties that it possesses [2], and the use of ZnO nanoparticles which at nanometric scale, acts as an antimicrobial agent and also presents biocompatibility [3]. First, different ratios of chitosan-PVA were tested for elecrospun ratios of 1:1 and 7:3 chitosan/PVA were tested. ZnO nanoparticles were synthesized by hydrothermal method [4] and characterized by SEM to obtain particles in the range of 50-100 nm. The ZnO nanoparticles were embedded by direct approach onto the fibers up to a concentration of 10%. Afterwards, fibers were electrospun at constant RH and temperature of 30°C. Parameters as a voltage, flow rate, and distance were evaluated in order to observe its effects on fiber size diameter, morphology, ZnO nanoparticles dispersion, and defect formation. The resulting fibers were characterized by SEM for morphology, XRD, and IR-ATR. The results show the differences between morphology and diameter sizes of the obtained fibers. The next step of this research will be the incorporation of PCL fiber as a core of the fiber to obtain CS/PVA:ZnO-PCL core-shell electrospun fibers and evaluate its osteointegration properties.

Key Words: electrospinning, nanofibers, ZnO NPs

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PTFE-CNT hybrid acaffold functionalization with 1,5 diamino naphthalene

Mariana Ailed Osorio Mejía, Edgar Alvarez Zauco

Facultad de Ciencias, Universidad Nacional Autónoma de México (UNAM), Circuito Exterior C.U. 04510, México, D.F., México

marianaosorio@ciencias.unam.mx

In the present work a hybrid scaffold was synthesized with carbon nanotubes and polytetrafluoroethylene (PTFE-CNT) by microwave irradiations [1], it was functionalized using gas-phase functionalization with 1,5 Diamino naphthalene (DAN), said material has potential electronic and biomedical applications due to the affinity between the electron cloud of the nanotubes and the cells. The adhesion of the functional molecule was controlled by the reaction time, observing that the DAN's aromatic nature maintains a similar thermal stability as the PTFE-CNT, but increases its conductivity in almost three orders [2]. The resulting material was characterized by FTIR and Raman spectroscopy, which allowed to observe characteristic bands of the amine group and PTFE-NTC-DAN, respectively, showing that the structures of PTFE and CNT have no covalent bonding. It means that the scaffold was generated by incrustation of the CNT. About DAN functionalization it was added by covalent bonds between CNT and amine groups.

Key Words: Carbon nanotubes, 1,5 Diamino naphthalene, gas-phase functionalization.

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Spectroscopic study on PTFE-CNT template functionalized with 1,8 diamino octane

Daniel Alberto Arcos Santiago, Edgar Alvarez Zauco

Facultad de Ciencias, Universidad Nacional Autónoma de México (UNAM), Circuito Exterior C.U. 04510, México, D.F., México

arcossantiagodaniel@ciencias.unam.mx

In this work, a hybrid material was synthesized (based on PTFE+CNT) for optoelectronic and biomedical applications. This scaffold was functionalized with 1,8 Diaminooctane (DO), regulating the added amine concentration, through gas-phase functionalization. The obtained products were characterized through out it's synthesis, by Raman spectroscopy, in which all the characteristic bands of PTFE and CNT can be seen without any apparent change, indicating the structural preservation of the precursor materials, and the absence of covalent bonds between them. As to the adhesion of the functional molecule, DO, it was found that the aliphatic nature of the molecule inherited the electric insulator behavior [1]. However this bond increases directly both the thermal and mechanical stability, generating a more stable template. It's proposed that the change in the superficial structure of the template it's due to the amine functional groups bonding with the carbon nanotubes, giving place to a molecular croos-linking [2].

Key Words: Carbon nanotubes, 1,8 Diaminooctane, gas-phase functionalization,

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Synthesis of triclosan liposomes for acne treatment

Cruz-Guerrero SARA; Godoy-Zaragoza MARIO ALBERTO; Gómez-Cruz ABDEL MANUEL; Vargas-Quijada JOSELIN IVETH; Chávez-Yuen WAN YIN; Vega-Jasso SAMANTHA; Lazaro-Becerril ISRAEL; Martinez-Pérez BEATRIZ

Universidad Politécnica del Valle de México, División de Ingeniería en Nanotecnología, México. Av. Mexiquense s/n esquina Av. Universidad Politécnica, Col. Villa Esmeralda, Tultitlán, C.P. 54910, Estado de México

cae06ciencias@hotmail.com

INTRODUCTION: Acne represents 43.2% of dermatoses more frequent in dermatological consultations [1]. Liposomal systems are lipid vesicles composed of a lipid bilayer that surrounds its aqueous core [2]. Conventional formulations, in addition to not achieving complete penetration of the drugs, can also generate adverse effects such as irritation, dryness, erythema and burning of the skin. AIM: Prepare and characterize triclosan loaded liposomes for the treatment of acne.

METHODOLOGY: Liposomal particles were prepared with Double solvent displacement based technique: PEG-40 was added to an ethanol phase containing phospholipids and triclosan to 750 rpm of magnetic agitation during 2 minutes. Next, the previous mixture was added to a glycerin aqueous solution. Particle size and Z potential were determined by photon correlation spectroscopy, using a Nanosizer® Coulter (Beckman, USA). Encapsulation efficiency was evaluated as follows: freeze-dried loaded and placebo liposomes were dissolved in ethanol, and suitable dilutions were performed until achieving an acceptable triclosan concentration. Quantification was performed by spectrophotometry at 285 nm, using an UV–Vis spectrophotometer. The antibacterial activity of triclosan was evaluated by determining the minimum inhibitory concentration (MIC) against Propionibacterium acnes.

RESULTS: An encapsulation efficiency of 75% of triclosan was obtained. The particle size was 120 nm and Z potential of -33.5 mV. MIC of triclosan methanolic solution was 450 mcg/ml and 150 mcg/ml for triclosan loaded liposomes evaluated against P. acnes.

CONCLUSIONS: The liposomal system offers an alternative treatment to acne dermatoses.

Key Words: Biomedical materials to drug delivery, Acne treatment, Liposomal triclosán

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Antibacterial activity of ZnO powders according to their particle size reduced by high-energy milling

Beatriz MARTÍNEZ-PÉREZ[1], Gustavo SANTANA DE LA CRUZ[1*], Omar IZQUIERDO-RAMÍREZ[1], Sandra CORTEZ-GATICA[1], Myriam PAREDES-OLGUÍN[1], Ricardo CISNEROS-TAMAYO[1], Fidel ALARCÓN-HERNÁNDEZ[2]

[1]UPVM, Av. Mexiquense s/n, esq. Universidad Politécnica, Col. Villa Esmeralda, C.P. 54910, Tultitlán, Estado de México.
[2]Escuela de Estudios Superiores de Xalostoc, UAEM, Av. Nicolás Bravo s/n, Parque Industrial Cuautla, C.P. 62717 Xalostoc, Morelos.

*ovat4@hotmail.com

Zinc oxide (ZnO) is a metal oxide characterized by their photocatalytic and photo-oxidizing ability against chemical and biological species. This fact has attracted much attention due to their potential utility in biological applications as an antibacterial material. In this study, the high-energy ball milling (HEBM) technique was used to produce micro and nanoparticles of ZnO. Four samples were milled for 1, 3, 5 and 7 hours, respectively. The structural and optical modifications induced in these powders were determined by X-ray diffraction (XRD), scanning electron microscopy (SEM), atomic force microscope (AFM), and photoluminescence emission spectra (PL). Microscopy results show a gradual decrease in particle size from around 250 μm to ~80 nm, with increased milling time. XRD analysis showed ZnO in a hexagonal structure, broadening in the diffracted peaks and going from larger to smaller particles along with a relaxation in the lattice constant c. PL result showed that the intensity of excitation wavelengths increases as the particles size decreases. The antibacterial activity of ZnO nanoparticles was evaluated by determining the minimum inhibitory concentration (MIC) against Candida Albicans showing an improved antibacterial potency with the decrease in ZnO particle size due to the increase in the c value, suggesting that the HEBM technique is quite suitable for process ZnO for this purpose.

Key Words: ZnO nanoparticles, antibacterial, HEBM, AFM, XRD, photoluminescence.

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Preparation and evaluation of biodegradable microfibers for open wound treatment

Munguía-Huerta JORGE EDUARDO; Gutiérrez-López JUAN PABLO, Olivano-Esquivel DANIELA; Perea-Jacobo ROCÍO NICTEHA; Martinez-Pérez BEATRIZ

Universidad Politécnica del Valle de México, División de Ingeniería en Nanotecnología, México. Av. Mexiquense s/n esquina Av. Universidad Politécnica, Col. Villa Esmeralda, Tultitlán, C.P. 54910, Estado de México

cae06ciencias@hotmail.com

INTRODUCTION: The utility of polymer biomaterials has become a very interesting area for research, due to the large number of applications that are attributed to them. A clear example of the multiple applications are the polymer microfibers, which have been used in tissue engineering, biosensors, pharmaceutical, electronic devices, filters and drug delivery [1]. Polymeric, uniaxial poly-ε-caprolactone, biocompatible and biodegradable polymer, and triclosan were synthesized. Polymeric microfiber has diversity applications for example to treatment of open wound. AIM: The objective of this research was to obtain a prolonged delivery drug system of poly-e-caprolactone loaded with triclosan as antiseptic film to treatment of open wound.

METHODOLOGY: Electrospinning device: The system was ensemble with recycled pieces from televisions and printers. Synthesis of microfibers: 0.2g of poly-e-caprolactone was dissolved with 0.25 g of triclosan in 3 mL of acetone. The prepared solution was filled into a glass syringe and pushes it down with a constant flow and a voltage of 10 kV. Microfibers were collected from an aluminium sheet. Microbicidal activity was evaluated against Staphylococcus aureus and Candida Albicans.

RESULTS: A polymeric film of triclosan was obtained. The mean diameter of microfiber was of 4 µm. Microbicidal and antifungal activity was more efficient than the triclosan-methanolic solution.

CONCLUSIONS: The electroespinning technique allowed us to synthesize a polymeric film as an alternative for the treatment of open wounds.

Key Words: polymeric microfibers, open wound fil, biomedical materials

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Metallic nanoparticles in graphene oxide: synthesis, characterization and antimicrobial activity

Laura M. Aguirre-Gómez[a], Lorena G. Pelayo-Arreola[b], Diego A. Lomelí-Rosales[a], Adalberto Zamudio-Ojeda[c*], Gilberto Velázquez-Juárez[a]

[a]Departamento de Química, [b]Departamento de farmacobiología, [c]Departamento de Física. CUCEI. Universidad de Guadalajara. Blvd. Marcelino García Barragán 1421, 44430, Guadalajara, Jalisco, México

*nanozam@gmail.com

Develop materials with antibacterial properties is a potential issue in the application of medical and industrial treatments creating an alternative to antibiotic resistance. A key research area in this field is the synthesis of nanoparticles with different chemical compositions, sizes, shapes, and controlled dispersities [1,2]. It has been shown that some metal nanoparticles are microbicides agents that inhibit and prevent the growth of bacteria interacting with membranes in gram-negative and gram-positive bacteria [3]. In this work a general methodology for the preparation of nanoparticles of gold (AuNPs), silver (AgNPs) and palladium (PdNPs) anchored in oxide Graphene is presented. It is pretend to evaluate the effects of this nanomaterials on Gram (+) Staphylococcus aureus and Gram (-) bacteria Serratia marcescens. The characterization of the surfaces was performed by different techniques: UV-Vis spectroscopy, Infrared Spectroscopy (FTIR), scanning electron microscopy (SEM) and transmission electron microscopy (TEM).

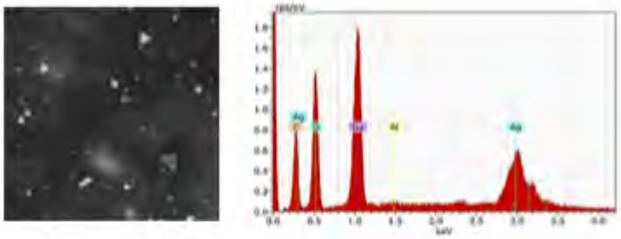

Figure 1. SEM image obtained for AgNPs.

Key Words: metal nanoparticles, morphology, graphene oxide, antimicrobial activity.

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Toxic effects of metallic nanoparticles and graphene oxide in boar semen

Guerrero, Andrea[1], Rojas,Citlalli[1,2], Padilla, Víctor Rubén[1,2], Serrano-Niño, Julio C.[5], Cavazos, Adriana[5], Velázquez-Juárez, Gilberto[6], Carvajal, Gregorio G.[6], Sánchez, Jorge M.[4], Ramírez, Daniel[2], Sánchez, David R.[1,3], Zamudio, Adalberto[4]

[1]Médico Veterinario Zootecnista, Centro Universitario de Ciencias Biológicas y Agropecuarias, Camino Ramón Padilla Sánchez 2100, Nextipac, 44600 Zapopan, Jal.
[2]Posgrado en Fisicomatemático, Centro Universitario de los Valles, Carretera Guadalajara-Ameca Km. 45.5, 46600 Jal.
[3]Departamento Producción Animal, Centro Universitario de Ciencias Biológicas y Agropecuarias, Camino Ramón Padilla Sánchez 2100, Nextipac, 44600 Zapopan, Jal.
[4]Departamento de Física, Centro Universitario de Ciencias Exactas e Ingeniería, Boulevard Marcelino García Barragán 1421, Olímpica, 44430 Guadalajara, Jal.
[5]Departamento de Farmacobiología, Centro Universitario de Ciencias Exactas e Ingeniería, Boulevard Marcelino García Barragán 1421, Olímpica, 44430 Guadalajara, Jal.
[6]Departamento de Química, Centro Universitario de Ciencias Exactas e Ingeniería, Boulevard Marcelino García Barragán 1421, Olímpica, 44430 Guadalajara, Jal.

mvzandrea8@hotmail.com

[2] Nowadays, the nanomaterials have had great acceptance in different technology areas, like, medicine, alimentary industry, cosmetology and others. However, is missing a lot of investigation in secondary consequences and the effects that cause this nanostructure when they are in the environment or consumed by living beings. [3] One of the main application at the moment is, to be a biocidal in different types of microorganisms causing damage in their membrane; in fact, it has been decided to tried in germinal cells, like in spermatozoids. [1] Based on this, they are studies that are related with nanoparticles of silver (AgNPs) interaction with semen of mouse, rat and human; each sample has different characteristics; in conclusion, the nanoparticles caused toxic effects in the animals, but in the sample of the human being showed more resistance to them. The objective of this investigation was to make an evaluation of dose-response using nanoparticles of silver (AgNPs), gold(AuNPs) and graphene oxide (GO) to evaluate the loss of motility in the boar spermatozoids. We used AgNPs and AuNP, which were synthesized by chemical reduction with metal salts and a reducing agent, in this case was sodium citrate; the GO was synthetized with modified Hummers method. Each sample was tested in different concentrations and time with the boar semen, the dilution with the same concentration of semen and AgNPs showed 100% absence of motility in 12 minutes; we observed at the electron microscope. In each case the characterization of the nanoparticles that we use it would be with Scanning and transmission electron microscopy (SEM and TEM) and spectrometry UV. The nanoparticles could be use as an alternative form in different animals sterilization.

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Green synthesis of gold, silver and copper nanoparticles using bromelia plumieri extract

Jorge GONZALEZ[1*], Adalberto ZAMUDIO[2]

[1]Colegio de Estudios Científicos y Tecnológicos del Estado de Jalisco Plantel 15, Calle Sor Juana Inés de la Cruz S/N, El Salate, 44760, Guadalajara, Jal.
[2]Departamento de Física del Centro Universitario de Ciencias Exactas e Ingenierías, Boulevard Marcelino García Barragán 1421, Olímpica, 44430 Guadalajara, Jal.

*georgemorrigan@outlook.com

Nanotechnology is a science that has had a great boom in recent years with the opportunity to develop new products at scales not previously possible [1]. The conventional physical and chemical methods to obtain nanoparticles are expensive, the chemicals used are toxic and in some cases are carcinogenic. High temperatures and pressure are used, having a great cost of energy and necessary specialized laboratory equipment to reach the optimal measures and morphologies [2,3]. The green synthesis of nanoparticles presents a great advantage compared to physical and chemical methods, these turn out to be less expensive, non-toxic, they do not require high temperatures or specialized laboratory equipment, friendly to the environment, easily reproducible and capable to elaborate it on a large scale [4]. The initial hypothesis was the morphology and dispersity will be affected by the metal salt concentration of silver nitrate, copper sulfate and tetrachloroauric acid interacting with the concentration of reducing sugars extracted from the Bromelia plumieri. Base on the results of this project, nanoparticles were synthesized with optimal dispersity of metallic salts, and characterized on Scanning Electron Microscope and UV-Vis Spectrophotometer.

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Bio-synthesis of Fe_3O_4 nanoparticles: magnetic properties and catalytic behavior in methylene blue reduction

Álvaro de Jesús Ruíz-Baltazar[1], Simón Yobbany Reyes-López[2], María de Lourdes Mondragón-Sánchez[3], Anel Ivonne Robles Cortés[3] and Ramiro Pérez[4]

[1]CONACYT-Centro de Física Aplicada y Tecnología Avanzada, Universidad Nacional Autónoma de México. CP 76230.Juriquilla, Querétaro, México.
[2]Instituto de Ciencias Biomédicas, Universidad Autónoma de Ciudad Juárez, Estocolmo s/n, Ciudad Juárez, Chihuahua, México C.P. 32300.
[3]Tecnológico Nacional de México/Instituto Tecnológico de Morelia. Posgrado en Metalúrgia. Av. Tecnológico 1500, col. Lomas de Santiaguito. C.P. 58120, Morelia MICH, México
[4]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Av. Universidad s/n, Col. Chamilpa, Cuernavaca, MOR, 62210, México

aruizbaltazar@fata.unam.mx

The synthesis of Fe_3O_4 nanoparticles by green synthesis route was carried out. The Fe_3O_4 nanoparticles were obtained using, mixture of ($FeCl_3$)/($FeCl_2$) as precursor. The Fe ions reduction were carried out by the antioxidant component presents in the cynara scolymus leaf extract. This green synthesis route, offer a novel and environmental friendly alternative to obtaining of iron oxides nanoparticles. The structural characterization of the Fe_3O_4 nanoparticles were carried out by scanning electron microscopy (SEM), X-ray diffraction, techniques (XRD). Additionally, FT- IR and Raman spectroscopy support the Fe_3O_4 characterization. Posteriorly, Fe_3O_4 nanoparticles were evaluated on the methylene blue degradation. Magnetic properties were determinates by a vibrating sample magnetometer (VSM) at different temperatures (10, 100, and 300 K). Kinetic adsorption model were performed in order to establish the behavior during the methylene blue degradation process. Pseudo first order, Pseudo second order, Intraparticle diffusion and Elovich Models were calculated based on the experimental data obtained. Calculations as the correlation factor indicates the best linear fit between the theoretical models and the experimental data obtained during the blue methylene degradation.

Polymeric nanofibers of collagen and sodium ascorbate for tissue regeneration

Hernández FERNANDO[1], Gastellu CHRISTOPHER[1], Grada JESSICA[1], Narayanan JAYANTHI[1], Martínez BEATRIZ[1]

[1]Universidad Politécnica del Valle de México, Av. Mexiquense s/n, C.P. 54910, Tultitlán, Estado de México, México

feralva297@gmail.com

A Nanofibers manufactured by electrospinning have been suggested to develop novel applications, including the controlled release of drugs, and supports or scaffolds for the growth of cells or tissues [1,2]. In this work, polymeric nanofibers of collagen and sodium ascorbate were synthesized and characterized by UV-Vis spectroscopy. A polymeric film of collagen was obtained and the diameters of nanofiber were less than 4 μm.

Key Words: Polymeric, Nanofibers, Collagen, Tissue, Regeneration.

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Lipase enzymes on graphene oxide support for high-efficiency reusable nanobiocatalysis of biodiesel

B. Guzmán Martinez*, J. Wang, R. Limas Ballesteros and Lifang Chen

Escuela Superior de Ingenieria Química, Instituto Politécnico Nacional, Avenida Wilfrido Massieu s/n., esq. Manuel I. Stampa, 07738, México City

bguzmanmartinez@gmail.com

Here, we demonstrate that stability and activity of the enzymes can be enhanced by their immobilization on graphene oxide. In this study we report the use of functionalized carbon-based nanomaterials, such as amine-functionalized graphene oxide (GO) by using sieved graphite flakes (300-500 meshes) as the starting materials produced using an improved Hummers method without using $NaNO_3$. This method decreases the cost and environmental duty of GO production. This Hummers method for eco-friendly synthesis of graphene oxide does not decrease the yield of product. Structural and biochemical characterization have revealed that the curvature of the nanomaterial affect the immobilization yield, the catalytic behavior and the secondary structure of enzymes. Infrared spectroscopy study indicates that the catalytic behavior of the immobilized enzymes is correlated with their a-helical content. The covalently immobilized enzymes exhibited comparable or even higher activity compared to the physically adsorbed ones, while they presented higher operational stability. The enhanced catalytic behavior observed for most of the hydrolases covalently immobilized on amine-functionalized indicate that these functionalized nanomaterials are suitable for the development of efficient nanobiocatalytic systems.

We report the immobilization of several lipases (LPP, CAL, JCL)of biotechnological interest on graphene oxide, investigating the influence of carbon-based nanomaterials properties on the immobilization efficiency, function and structure of enzymes. Enzymes were immobilized on GO derivatives via two different methods: [1] physical adsorption and [2] covalent linkage with amine functionalized carbon based nanomaterials. The resulting novel hybrid biocatalysts were characterized by SEM, Spotlignt FTIR, Confocal, X-ray photoelectron spectroscopy (XPS), and MALDI TOF Mass Spectrometry.

Key Words: Graphene, lipase, nanobiocatalysis, biodiesel

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Effects of finite size systems in enzyme catalysis without cooperation modelled using Hopfield neural networks

J. M. Castellanos[1*], A. Castellanos[1], A. Corella[1]

[1]*Universidad de Sonora, Blvd. Luis Encinas J. & Calle Av. Rosales, Centro, C.P. 83000, Hermosillo, Sonora, México.*

*jmiguelcastellanosj@gmail.com

This work studies the effects of finite size in enzymatic catalysis when cooperativity is not present. This corresponds to the regime where the Michaelis-Menten model is applicable. The effects caused by finite sized systems can present themselves in nano scaled devices where the volume is reduced to the point that random fluctuations become important. The treatment is based on a Hopfield neural network. In this model each active site (occupied or unoccupied) of the enzyme is modelled as a formal neuron that sends a signal or not at time t. This is a model first introduced by Elena Agliari et. al., with the addition of the consideration of a finite neural network. The cornerstone of this approach is that the substrate concentration is constant, and the random nature of the phenomenon is allotted to the temperature of the neural network. The problem is approached using computer simulation.

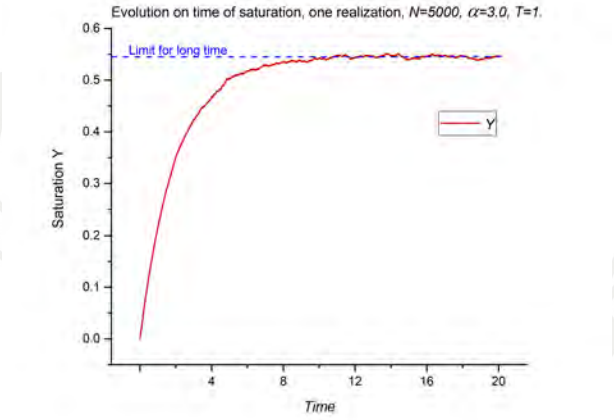

Figure 1. Evolution of the saturation Y of a single realization, with N=5000, α=3.0, T=1. Each unit of time is 1⁄N. The neural network evolves to an equilibrium state. For a long period of time, this produces one point in the Michaelis-Menten saturation curve.

Key Words: Stochastic process, Neural networks, Enzymatic catalysis, Computer simulation.

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Bimetallic Ag@Pt core-shell nanoparticles and their catalytic activity: a green approach

F. Mares-Briones[1], R. Esparza[2], G. Rosas[1]

[1]*Instituto de Investigación en Metalurgia y Materiales, UMSNH, edificio U, ciudad universitaria. C.P. 58060, Morelia Michoacán, México.*
[2]*Centro de Física Aplicada y Tecnología Avanzada, Universidad Nacional Autónoma de México, Boulevard Juriquilla 3001, Santiago de Querétaro, Querétaro, C.P. 76230, México.*

*fabianmares@gmail.com

In this work, we presented the biosynthesis of the silver@platinum nanoparticles by aqueous extract of Schinus molle L. leaves. The biosynthesis was carried out in two steps; first, seeds of Ag nanoparticles varying the ratio of plant extract/$AgNO_3$-precursor salt were obtained. Second, different H_2PtCl_6 precursor salt concentration was added to form a platinum shell in the Ag seeds, with no more plant extract addition. The structural characterization of the products was performed using UV-vis spectroscopy (UV-vis), X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). From the UV-vis spectra, it was noted that the typical AgNPs absorption band depressed with the addition of the H_2PtCl_6 precursor that indicates the Ag@PtNPs formation. XRD analysis revealed that the as-synthesized Ag@PtNPs have a face-centered cubic structure. SEM and TEM observations showed that most of the obtained particles were irregular morphology, like dendrites having particle sizes in the range of 20-100 nm, most of them with an average size of about 45nm. Finally, the nanoparticles exhibited an excellent catalytic activity in the degradation of the methylene blue dye.

Key Words: Ag@Pt Bimetallic Nanoparticles; Biosynthesis; Schinus Molle L; Structural Characterization; Catalytic Activity.

Fast synthesis of a composite powder consisting of a graphitic carbon matrix with embedded iron carbide and silver nanoparticles

G. Soto[1], J.M. Aguilar-Torres[2,3], L. A. Arce-Saldaña[2,3], A. Portillo-López[3], S. González-Martínez[3], M.E. Gómez[4], E. Vargas-Viveros[3], J. López[5], D. Dominguez[1] and H. Tiznado[1]

[1]Universidad Nacional Autónoma de México (UNAM), Centro de Nanociencias y Nanotecnología, Km 107 Carretera Tijuana-Ensenada s/n, Ensenada B.C., México. C.P. 22800.
[2]Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE), Km 107 Carretera Tijuana-Ensenada s/n, Ensenada B.C., México. C.P. 22800
[3]Universidad Autónoma de Baja California (UABC), Facultad de Ingeniería, Arquitectura y Diseño; Facultad de Ciencias. Km 107 Carretera Transpeninsular Ensenada-Tijuana 3917, Ensenada B.C., México. C.P 22860
[4]Thin film Group, Universidad del Valle , Cali – Colombia. C.P. 25360.
[5]CONACYT – Centro de Nanociencias y Nanotecnología, Km 107 Carretera Tijuana-Ensenada s/n, Ensenada B.C., México. C.P. 22800.

*javierlo21@cnyn.unam.mx

In this study, we report the composite powder synthesis that consisting of an amorphous carbon matrix with embedded Fe_3C and silver nanoparticles (AgNPs). The synthesis method is straightforward: ferrocene, silver nitrate and polyethylene glycol loaded in a combustion tube and pyrolysed under vacuum conditions by microwave plasma. The synthesized material is a black powder, similar to graphite in texture, but magnets can attract it. Several analytical techniques were carried out, including X-ray photoelectron, energy-dispersive X-ray spectroscopies; transmission and scanning electron microscopies; as well X-ray diffraction and vibrating sample magnetometer. The material shows a homogeneous dispersion of metallic particles in the carbon matrix. Due to the addition of AgNPs it has antibacterial effect, as it was tested on E. coli bacteria. We conclude that the magnetic behavior attraction combined with the antibacterial property make this material a possible vehicle for environmental purposes, for example as wastewater treatment, using magnetic separation procedures.

Key Words: core-shell magnetic nanostructures; Fe_3C; activated carbon; magnetic separation; wastewater treatment; antibacterial material.

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Influence of magnetite particles on electrical properties of a porcine heart tissue

Michelle Solis Rojas[1*], Gustavo Moreno González-Terán[2], Marysol García Pérez[2], Christian Gómez Solis[2], María del Rosario Galindo González[3], José Marco Balleza Ordaz[2]

[1]Universidad Politécnica del Bicentenario, Carretera Silao-Romita Km. 2, C.P. 36283, Silao, Guanajuato, México.
[2]División de Ciencias e Ingenierías, Universidad de Guanajuato, Loma del Bosque 103, Col. Lomas del Campestre, C.P. 37150, León, Guanajuato, México.
[3]División de Ciencias Naturales y Exactas, Universidad de Guanajuato, Noria Alta S/N, C.P. 36050, Guanajuato, Guanajuato, México.

*mich250112@gmail.com

Electrical bioimpedance (EB) is a technique that allows to characterize the electrical properties of tissues. EB is composed by two parameters: impedance-module and phase. The first parameter determines the changes of volume tissue and the second one the changes of cellular structure [1]. This study analyzed the electrical properties of a porcine heart tissue under the influence of two types of nanomagnetite. Objective. To characterize the electrical properties of a porcine heart tissue by electrical impedance spectroscopy (EIS) using a magnetite particles suspension as medium contrast. Material and methods. a) EIS device: A BioLogic Science Instruments SP-150 was used. b) Biological tissue: It was analyzed a porcine heart with a weight of 380g. c) magnetite particles: Two types of magnetite were used. The first type (NM1) was synthetized by coprecipitation method and the second one (NM2) was synthetized by combustion method. The materials were characterized by X-ray diffraction (DRX) and scanning electronic microscopy (SEM). Both materials have shown a typical peak characteristic of magnetite, however, the sample NM1 showed hematite phase which has an important influence in the impedance response. d) Procedure: The EIS device was connected at each ventricle through four hypodermic needles (38mm). 5 measures at basal biological stage by EIS were obtained. Left and right ventricle was injected with NM1 and NM2 particles, respectively. Subsequently, 5 more impedance measurements were acquired for each ventricle. e) All data was analyzed by Bode graphics (impedance and phase) at 50kHz frequency. Results. The mean value of impedance (phases) at basal biological stage of left and right ventricles were of 287.7 Ω (-53.12°), and 421.8 Ω (-65.3°), respectively. The mean value of impedance-module and phases in the left ventricle with NM1 and right ventricle with NM2 were of 156.36Ω (-60.24°) and 141.8Ω (-57.90°), respectively. Conclusion. The changes of the electrical properties of tissues were detected by both parameters of impedance vector (module and phase).

Key Words: biological tissue, electrical impedance spectroscopy, nanomagnetite.

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Characterization of muscle tissue by electrical impedance spectroscopy (EIS) using different nanomaterials

Gustavo Moreno González-Terán[1*], Michelle Solis Rojas[1], Mariana Villagómez Mora[1], Roberto Santos Silva[2], Andrea Ceja Fernández[1], Christian Gómez Solis[1], María del Rosario Galindo González[3], José Marco Balleza Ordaz[1]

[1]División de Ciencias e Ingenierías, Universidad de Guanajuato, Loma del Bosque 105, C.P. 37150, León, Gto., México.
[2]Centro Universitario de los Valles, Universidad de Guadalajara, Carretera Guadalajara-Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México.
[3]División de Ciencias Naturales y Exactas, Universidad de Guanajuato, Noria Alta S/N, C.P. 36050, Guanajuato, Gto, México.

*gustavo.moreno.gt@gmail.com

The electrical impedance spectroscopy is a technique that allows to characterize the electrical properties of tissues by detecting the changes of volume and the variations of cellular structure of them [1]. In this study, it was analyzed the changes of electrical properties of three chicken breasts were injected with three different types of nanoparticles (1mg of particles in a 1ml of solution). Objective. To characterize the changes of the parameters of impedance vector (module and phase) in three chicken breasts under the influence of three different nanoparticles. Material and methods. a) EIS device: A BioLogic Science Instruments SP-150 was used. b) Biological tissue: Three chicken breasts (345.9g, 349.5g and 270.0g) were analyzed. c) Nanoparticles: Three different particles were analyzed (two types of nanomagnetite and a sample of Gold particles). The first (NM1) and the second (NM2) sample of nanomagnetite were synthetized by coprecipitation and combustion method, respectively. Meanwhile, the Gold particles (GNP) were synthetized by Turkevich method. d) Procedure: Four needles (38mm) were placed in each chicken breasts to connect the EIS device. Five measurements were obtained form each chicken breast at: I) basal stage II) after being injected with nanoparticles. e) Data analysis: All parameters of impedance vector were determined at a 50 kHz frequency. These were analyzed by Bode graphics (module and phase). Results. The mean value of impedance-module (phase) at basal stage and under the influence of three chicken breast were for breast 1 (NM1): 244.1Ω (-58.47°) and 147.5Ω (-47.8°), for breast 2 (NM2): 141.4Ω (-47.7°) and 138.9Ω (-47.6°), for breast 3 (GNP): 130.9Ω (-38.1°) and 132.9 (-39.1°), respectively. Conclusion. The major changes of electrical properties of chicken breast were evidenced by using NM1 and GNP.

Key Words: electrical impedance spectroscopy, nanomagnetite, gold nanoparticles, biological tissue.

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Monocytes as nanocarriers of complexed nanoparticles, chitosan, and pDNA for specific tumoral-targeted delivery

de la Hoz Camacho–Rafael[1], Luna Cruz–Itza[1], Alcocer González–Juan[1], Gómez-Flores Ricardo[1], Valadez Lira-Alberto[1], Rodríguez Padilla-Cristina[1]

[1]Universidad Autónoma de Nuevo León, Pedro de Alba, S/N, Ciudad Universitaria, San Nicolás de los Garza, Nuevo León.

Rafael.delahozcamacho@gmail.com

The main objective of this research was developing a microbot to focalize and control the delivery and expression of genes in target tissues such as tumors, using cells as a carrier complexed with magnetic fluorescent nanoparticles, chitosan and, pDNA. Methods: Magnetic nanoparticles were complexed with chitosan and pDNA (pHRE, contains a promoter that responds to Hypoxia) following Calvo and Cols (1997) ionic gelation method [1]; nanocomplexes were characterized by size, Z potential, Atomic Force Microscopy and, cytotoxicity by XTT. Cells were obtained of peripheral blood, monocytes were isolated using density gradient and cultured in RPMI medium at 37°C under a humidified atmosphere of 5% CO2. After two hours, cells were detached using StemPro Accutase. Microbots were produced by adding 1x106 monocytes into a suspension containing 50 µg of the nanocomplexes. Finally, female 6-week old C57BL/6 mice with subcutaneous tumor previously induced [2,3] were divided into 4 groups of three mice each. After administrating the microbot, nanocomplexes, or PBS as a control a magnetic field (3 T) was placed in the tumor. One group of mice with microbots was not exposed at magnetic field, to demonstrate de chemotactic power of the monocyte. After 48 hours, animals were killed following the MX-NOM-062-ZOO-1999. Lungs, liver, kidneys, spleen, heart, and tumor were aseptically removed, after which they were frozen and macerated to determinate the efficiency of delivery by fluorescence and gene expression efficiency by luminescence.

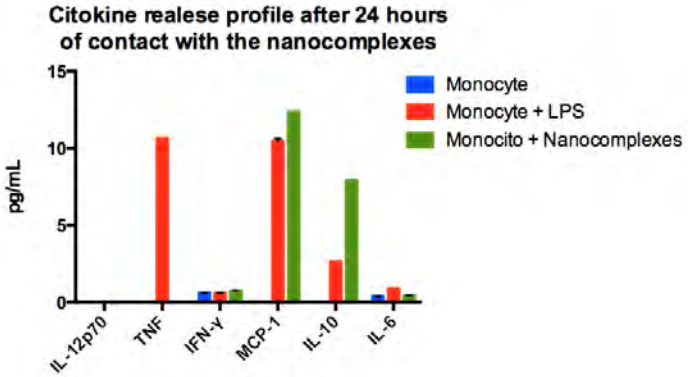

Figure 1. Citokine realese profile after 24 hours of contact with the nanocomplexes.

Key Words: Nanotechnology, nanomedicine, tumor specific delivery system.

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Preparation of ceramic membranes of nanofiltration by nano-deposition to be used in the purification of impacted effluents with diferent contaminants

Irlanda Grisel-Cruz Reyes

Instituto Politécnico Nacional-ENCB Unidad Profesional Adolfo López Mateos, Av. Wilfrido Massieu Esq. Cda. Miguel Stampa s/n, C.P. 07738 Delegación Gustavo A. Madero, Ciudad de México.

irlandahu@hotmail.com

In the present work, deep eutectic naturals solvents (NADEs) were synthesized from glucan derivatives such as sacarose and urea. These solvents have been developed as a type of ionic liquid and have demonstrated the great utility they have in the decomposition of pollutants discharged into storm water. They were synthesized using 1:3 molar, being characterized as dynamic light scattering, Spectroscopy Infrared, Viscosity and Mass Spectroscopy. Getting a catalyst, biodegradable, economical and environmentally friendly.

Key Words: ionic liquid, deep eutectic solvent, glucans

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Cytotoxic effects of silver nanoparticles on mice primary cultures

Blanco-Salazar ALBERTO[1*], Espinosa-Villalpando MARÍA FERNANDA[1], Santiago-Solís ALBERTO[1], Rodríguez-Marino LUIS RICARDO[1], Mendoza-Ávila JOSE MARCO[1], Meneses-Sagrero SALVADOR[2], González-Vega JESÚS GABRIEL[3], Pestryakov ALEXEY[4], Toledano-Magaña YANIS[4*], García-Ramos JUAN CARLOS[4], Bogdanchikova NINA[1]

[1]CNyN-UNAM, Carretera Tijuana-Ensenada Km. 107, C.P. 22860, Ensenada, Baja California, México.
[2]UNISON – División de Ciencias Químico Biológicas, Blvd. Luis Encinas y Rosales S/N, C.P. 83000, Hermosillo, Sonora, México.
[3]UABC – Facultad de Ingeniería Arquitectura y Diseño, Carretera Transpeninsular Ensenada-Tijuana No. 3917, C.P. 22860, Ensenada, Baja California, México.
[4]Tomsk Polytechnic University, 30 Lenin Avenue, Tomsk Polytechnic University, Tomsk, Russia, 634050.
[5]CONACyT-UNAM-CNyN, Carretera Tijuana-Ensenada Km. 107, C.P. 22860, Ensenada, Baja California, México.

*g6_blan17@cnyn.unam.mx

Nowadays, AgNPs are present in various healthcare products but without official regulation for their use. This emphasizes the need for identifying their toxicological effects in order to prevent possible adverse effects in human exposed [1]. Because of their dimensions, nanoparticles may bypass natural mechanical barriers, disrupting the structure and function of several cellular structures and interfere with very important metabolic processes [2]. Hence the importance of knowing the toxicological profile. The cytotoxicity of AgNPs has been evaluated using in vitro models but there is still a lack of consistent and reliable data [3]. Primary cells isolated from target tissues are desirable for cytotoxicity evaluation, as the first step to simulate more closely the in vivo environment [2]. In this work we evaluate the cytotoxic response of commercially available AgNPs against healthy BALB/c mice primary culture cells (kidney, liver, bone marrow, spleen, aorta and heart). In general, no cytotoxic effects were observed at the AgNPs concentrations evaluated in the mice primary cultures selected for this study, but a different effect for each tissue was observed. In our knowledge, this is the first time that cytotoxicity of AgNPs is evaluated in mice heart primary culture and remarkably, with no cytotoxic effects.

Key Words: Silver nanoparticles, cytotoxic effect, primary culture, mice.

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Use of polyurethane foam and carbon nanoparticles for cleaning oil mixtures on water surface

Hugo Galindo[1,2], Oxana Kharissova[1,2], Eliezer Flores[1,3], Jordán Coronado[1,3], Emiliano Quiroz[1,4], Beatriz Ortega[1,2], Romeo Selvas[1,2]

[1]Centro de Investigación en Ciencias Físico Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL 66455, México
[2]Facultad de Ciencias Físico Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL 66455, México
[3]Facultad de Ciencias Biológicas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL 66455, México
[4]Facultad de Agronomía Universidad, Autónoma de Nuevo León, San Nicolás de los Garza, NL 66455, México

patsy.arquieta.g@gmail.com

Actually exist methods for identify viruses, ranging from immunological to molecular techniques. The immunological techniques have a relatively short time and less complicated procedures, but his disadvantage is that they aren't sensitive to low concentrations on the sample. In other way, the molecular tests are sensible to low concentrations, but is required a longer time and need a qualified staff for perform the tests. Is necessary a test that removes these disadvantages and get a high sensibility combined with a simple system. This project consists in the development of a biosensor for the detection of influenza antibodies. We functionalize carbon nanotubes with viral proteins to perform the immunological reaction with the antibodies that we are detecting. It is possible to characterize the reaction even at very low concentrations that current methods fail to detect.

Development of a prototype for characterization of nanostructured materials using infrared photothermal radiometry (PTR)

[1]Verónica Ofelia Torres Guerrero, [1]Rubén Velázquez Hernández, [2]Minerva Robles Agudo, [1]José de Santiago Luna, [1]Ignacio Rojas Rodríguez, [1]Miguel Ángel Pérez González, [1]Mario Antonio Rojas Mérida, [1]Edgar Daniel Martínez Orduña

[1]Universidad Tecnológica de Querétaro, Querétaro, Qro., C.P. 76148, México.
[2]Cátedra CONACYT-UTEQ

veronica.otg24@gmail.com

Infrared Photothermal Radiometry (PTR) is a non-destructive and non-contact technique that can be applied to characterize properties in metals and semiconductors materials, such as: defects, thermal properties, thermoelectronics, thicknesses in nanometric coatings and thin layers. In PTR, a low energy modulated laser is used to scan the surface of the sample and simultaneously record the infrared radiation emitted by the surface of the material. The principle of PTR is Boltzman's blackbody law and Plank Radiation. In this work we present the advances obtained in the development of a Photothermal Radiometry prototype for the characterization of nanostructured materials. Compared with other radiometry systems, this prototype has a compact opto-mechanical system whose design allows in-situ measurements in metallic materials or nanostructured semiconductors. The parameters obtained by this technique are related to physical properties of the material such as diffusivity and thermal conductivity, diffusion coefficient and life time of minority carriers. We can also distinguish mechanical defects, and structural properties in the sample. Measurements of the pore distribution in nanostructured materials have been obtained, especially in the case of porous silicon, which shows that it is possible to use the PTR technique for this type of applications.

Key Words: Infrared Photothermal Radiometry (PTR), in-situ, COMSOL Multiphysics.

Development of non-invasive colorimetric glucose biosensor with nanoparticles

Iñiguez Saldaña M. M.[1*], San Martín Martínez E.[1], Quintana Zavala D.[1]

[1]*Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada del Instituto Politécnico Nacional, Legaria 694. Colonia Irrigación, 11500 CDMX; México*

*muzikart@hotmail.com

Currently diabetes is a disease that affects thousands of people around the world, being one of the diseases with the highest mortality rate, since not only implies a single condition, but a series of associated disorders as they are, diabetic foot, diabetic nephropathy, peripheral neuropathy, strokes, heart attacks, etc. With all this, it is very important to have an adequate control of glucose monitoring in the body, these sensors currently require the taking of blood making it more difficult to monitor in people [1,2]. In this project it is proposed to develop a prototype of a non-invasive biosensor, based on polymeric nanofibers, which helps the easy detection of glucose in saliva and improve the way of monitoring of people with diabetes.

Key Words: Diabetes, biosensor, polymeric nanofibers, non-invasive.

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Nanoparticles of chitosan derivatized loaded with Carvacrol

López-Mata M. A.[1*], Luna-Verdugo M.[1], Juárez Josué[2], Quihui-Cota L.[3], Valdez-Covarrubias M.[2], Valbuena-Gregorio E.[1], Valdez-Melchor R G.[1]

[1]Departamento de Ciencias de la Salud, Universidad de Sonora. Blvd. Bordo Nuevo s/n, Antiguo Providencia, Cd. Obregón, Sonora.
[2]Departamento de Física, Universidad de Sonora, Unidad Centro, Hermosillo, Sonora.
[3]Departamento de Nutrición Pública y Salud, Coordinación de Nutrición, Centro de Investigación en Alimentación y Desarrollo, Hermosillo, Sonora.

*marco.lopezmata@unison.mx

Chitosan (Qs) is a biopolymer capable to form films and, micro and nanoparticle systems [1] and chemical modification of Qs is an alternative to improve and develop novel biological biomaterials with exceptional physicochemical properties [2]. The aim of this study was to synthetized chitosan nanoparticles as well as their capability to entrap carvacrol into chitosan matrix (CAR-NPs). Firstly, CH was modified with octanoic acid (Aoc-Qs), using activated ester to couple chains of 8 C with 15% of saturation. CH modified was utilized to prepare CAR-NPs at 25.0, 50.0 and 75 % (w/w) for ionic gelation method, using tripolyphosphate as crosslinker. Hydrodynamic radius, Z potential and atomic force microscopic (AFM) were utilized to characterize the NPs. The CAR-NPs 25% were the smallest (87 ± 2.0 nm) and the nanoparticle size increased as the amount of CAR was increased (until 487± 2.0 nm for NPs-CAR 75%). The Z potential observed for the CAR-NPs prepared at 25 and 50% of CAR remained constant (13.06 to 13.33 mV, respectability) compared with the control NPs (13.56 mV) (NPs-Aoc-Qs), however the CAR-NPs 75% shows a reduction of the surface charge (7.09 mv). The images of AFM show NPs of size of ≈200 nm.

Key Words: Chitosan, carvacrol, crosslink, nanoparticle.

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Mechanical and electrical properties of chitosan-MWCNT

Alejandro Gomez Sanchez[1*], Evgen Prokhorov[1], Gabriel Luna-Barcenas[1], Araceli Mauricio Sánchez[1], Yuriy Kovalenko[2], Eric M. Rivera-Muñoz[3], Maria Grazia Raucci[4], Giovanna Buonocore[4]

[1]Cinvestav, Libramiento Norponiente 2000, C.P. 76230, Querétaro, México.
[2]University of Aeronautics of Queretaro, Carretera Estatal 200 Querétaro – Tequisquiapan 22154, C.P. 7627, Querétaro. México.
[3]CFATA, UNAM, Blvd. Juriquilla 3001, C.P. 76230, Querétaro, México.
[4]Institute for Polymer, Composites and Biomaterials, Via Paolo Gaifami 18, 9 -95126 Catania, Italy.

*alejandrogomez@cinvestav.mx

Percolation phenomena include mechanical properties; herein, a polymer nanocomposite exhibit a sharp increase in mechanical properties with increasing the volume fraction of fillers due to formation connected percolated microstructure [1]. Above the percolation threshold concentration there appears saturation of conductivity and mechanical properties [2,3]. In general, percolation phenomena strongly depend upon the aspect ratio of the MWCNTs, concentration, degree of dispersion, and their interaction with polymer matrix (formation of an interfacial layer) [3]. It is noteworthy that the interface between the polymer matrix and the MWCNTs is directly influenced by the development of an interfacial layer with variable thickness; this layer affects percolation thresholds (both electrical and mechanical), maximum values of conductivity, Young's modulus and hardness of nanocomposites. Consequently, the proper study of this interfacial layer is of utmost importance since it dominates nanocomposite's properties and performance. Therefore, the objective of this work is to probe CS-MWCNT nanocomposite's electrical and mechanical properties by taking advantage of the presence of interfacial layer.

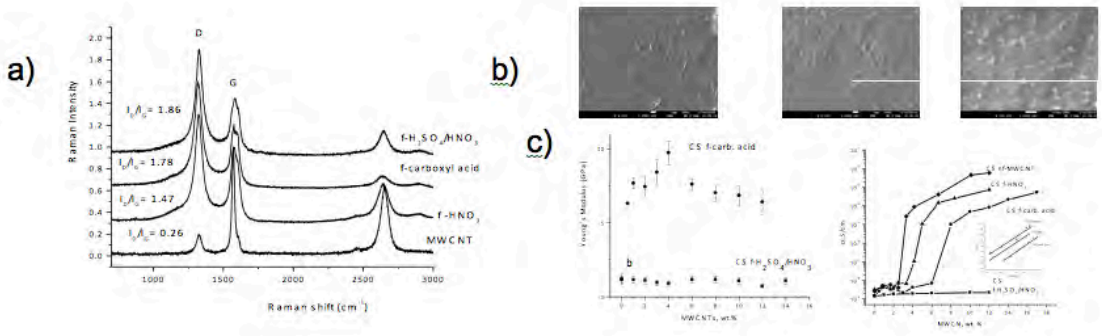

Figure 1 – a) Raman spectra of MWCNT b) SEM CS-f-MWCNT with 1, 8 and 10 wt.% of MWCNTs, c) CS- f-MWCNT Mechanical and electrical properties (Young´s Modul and conductivity).

Key Words: Multiwall carbon nanotubes, Chitosan, mechanical and electrical properties.

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