INTERNATIONAL MULTIDISCIPLINARY JOINT MEETING

Nanoscience and Condensed Matter Physics

2013

- 2do Congreso Anual de la División de Materia Condensada, SMF
- 7th Annual Meeting of DINANO, SMF
- 10th International Topical Meeting on Nanostructured Materials and Nanotechnology (NANOTECH)
- 6to Encuentro Internacional e Interdisciplinario en Nanociencia y Nanotecnología (NANOMEX'2013)

Morelia, Michoacan Mexico

International Multidisciplinary Joint Meeting

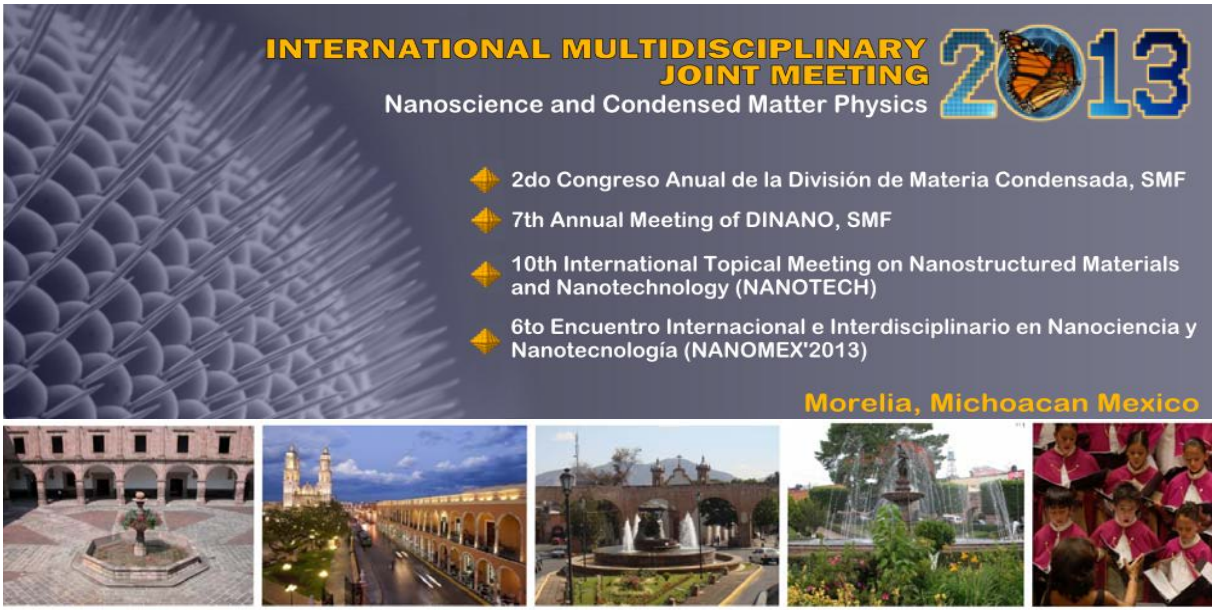
Nanoscience and Condensed Matter Physics

May 15 - 17, 2013

Escuela de Materia Condensada y Nanociencia

13 y 14 de Mayo, 2013

ABSTRACTS BOOK



CONTENTS

International Multidisciplinary Joint Meeting 2013

Nanoscience and Condensed Matter Physics

2do CONGRESO ANUAL DE LA DIVISIÓN DE MATERIA CONDENSADA

7th ANNUAL MEETING OF DINANO-SMF

10th INTERNATIONAL TOPICAL MEETING ON NANOSTRUCTURED MATERIALS AND NANOTECHNOLOGY (NANOTECH)

6to ENCUENTRO INTERNACIONAL E INTERDISCIPLINARIO EN NANOCIENCIA Y NANOTECNOLOGÍA (NANOMEX'2013)

ESCUELA DE MATERIA CONDENSADA Y NANOCIENCIA

Morelia, Michoacán
Unidad Académica y Cultural
Universidad Nacional Autónoma de México
Campus Morelia
13 - 17 May, 2013

Editors
Yesenia Arredondo León
Oracio Navarro
Alan Dierick Ortega Gutiérrez

Abstracts Book

The accuracy of the submitted *abstracts* is the *responsibility* of the *author*(s)

Welcome Address

Condensed Matter Physics, Nanoscience and Nanotechnology are areas of interdisciplinary study investigating the properties of matter at the micro- and nanoscale, which hold many of the phenomena that determine the macroscopic behavior we see in our daily lives. Particularly, the scientific progress that has been developed from the interaction between these fields has had great impact on society finding applications in the fields of medicine and pharmaceutics, chemistry, telecommunications, recording systems, among others.

Training of scientists able to understand, develop technologically new materials and processes, and analyze the implications of scientific advances is key to the development of our societies. Hence the importance of forums such as the Congress of the Condensed Matter Division (DMC-SMF), the School of Condensed Matter and Nanoscience, the Congress of the Division of Nanoscience and Nanotechnology (DINANO-SMF) of the Mexican Physical Society and the International and Interdisciplinary Nanoscience and Nanotechnology (NANOMEX), which pursue to foster, support and organize various scientific and academic events nationally and internationally, where their members (researchers, teachers and students at various levels, affiliated to different national institutions) have the opportunity to present, discuss and learn from the latest developments in Condensed Matter Physics, Nanoscience and Nanotechnology.

As part of the program of activities for 2013, the Mexican Physical Society together with the National Autonomous University of Mexico (UNAM), the University of La Ciénega of the Michoacán de Ocampo State (INAT-UCM), the Optics Research Center (CIO) and NANOMEX organized the joint meeting of the 10th edition of the International Topical Meeting on Nanostructured Materials and Nanotechnology (NANOTECH), the 2nd edition of the Condensed Matter Annual Congress and the National School Condensed Matter, the 7th Annual Meeting of DINANO-SMF, and the 6th International Conference and Interdisciplinary in Nanoscience and Nanotechnology. This event will be held on 13-17 May 2013, in the city of Morelia Michoacán at the Academic and Cultural Unity of UNAM, Campus Morelia. This event represents a fundamental space in which information on new materials and their various technological applications will be found throughout the lectures and presentation of current research. Topics of broad scientific interest will be taught by academics and researchers of international renown on different issues in Condensed Matter Physics, Nanoscience and Nanotechnology.

We wish you a fruitful meeting and a pleasant stay in Morelia.

Oracio Navarro Chávez
Chairman

CHAIRMAN

Oracio Navarro Chávez - IIM, UNAM

LOCAL ORGANIZING COMMITTEE

Yesenia Arredondo León - IIM, UNAM
Milton Muñoz Navia - INAT, UCM
Alan Dierick Ortega Gutiérrez – IIM, UNAM

ORGANIZING COMMITTEE

Elder de la Rosa – CIO, SMF
Takeuchi Noboru - CNyN, UNAM
Gian Carlo Delgado Ramos – CEIICH, UNAM
Rodolfo Zanella – CCADET, UNAM
Claudia Gutiérrez Wing – ININ
José Luis Rodríguez López - IPICyT

Sponsors


CONACYT


CENTRO DE INVESTIGACIONES
EN OPTICA, A.C.


Universidad de La Ciénega del Estado de Michoacán de Ocampo


cecti
Consejo Estatal de Ciencia, Tecnología
e Innovación de Michoacán


SMF
Sociedad Mexicana de Física


morelia


JEOL


PerkinElmer
For the Better


hielscher
Ultrasound Technology

	Monday 13	Tuesday 14	Wednesday 15		Thursday 16	Friday 17
09:00 - 10:00	Procesos de fabricación de celdas solares de películas delgadas de CdTe de alta eficiencia Juan L. Peña Chapa (CINVESTAV-Merida, Mexico)		09:00 - 09:30	*Conference Opening*	Miguel A. García-Garibay	Saw Wai Hla
10:00 - 11:00			09:30 - 10:30	Julio Mendoza	Karen Hallberg	Marek Przybylski
11:00 - 11:30	*Coffee*		10:30 - 11:30	Marco Buongiorno	*Coffee*	
11:30 - 12:30	Coherent diffraction imaging and its application to the characterisation of nanoscale materials Grant van Riessen (La Trobe University, Australia)		11:30 - 12:00	*Coffee*	Zahid Hasan	Rafael Vázquez Duhalt
12:30 - 13:30			12:00 - 13:00	Ignacio Garzón	Juan Luis Peña	José Lemus
13:30 - 14:30	*Lunch*		13:00 - 14:00	Rafael Baquero	Grant van Riessen	
14:30 - 15:00			*Lunch*			
15:00 - 16:00	Caracterización óptica de materiales semiconductores Ma. Lucero Gómez Herrera (FI-UAQ, Mexico)					
16:00 - 17:00			Sandra E. Rodil		L. Alberto Lightbourn	
17:00 - 17:30	*Coffee*		**Poster Session** Poster code: Wed-01 to Wed-100		**Poster Session** Poster code: Thu-01 to Thu-100	
17:30 - 18:00	Raman Spectroscopy Claudia Hernández, Bernabé Rico (Perkin Elmer de Mexico, S. A.)					
18:00 - 19:00						
19:00 - 20:00						
20:00 - 21:00			Welcome Cocktail †			

† The welcome cocktail will take place at the Centro Cultural - UNAM located between Av. Acueducto and Calzada Fray Antonio de San Miguel, Col. Centro

Guest Lectures

Juan Luis Peña Chapa
(CINVESTAV-Mérida, Mexico)
Procesos de fabricación de celdas solares de películas delgadas de CdTe de alta eficiencia
Monday 13 & Tuesday 14
09:00 – 11:00

Ricardo F. Aroca
(University of Windsor, Canada)
Raman spectroscopy
Monday 13 & Tuesday 14
11:30 – 13:30

Gran van Riessen
(La Trobe University, Australia)
Coherent diffraction imaging and its applications to the characterization of nanoscale materials
Monday 13 & Tuesday 14
15:00 – 17:00

Ma. Lucero Gómez Herrera
(FI- Universidad Autónoma de Querétaro, Mexico)
Caracterización óptica de materiales semiconductores
Monday 13 & Tuesday 14
17:00 – 19:00

Plenary Conferences

Wednesday 15

Julio Mendoza Álvarez
(CINVESTAV, Mexico)
Crecimiento de nanopartículas semiconductoras de los tipos II-VI y III-V y sus aplicaciones
Wednesday 15
09:30 – 10:30

Marco Boungiorno Nardelli
(University of North Texas, USA)
Recent advances in molecular transport from first principles
Wednesday 15
10:30 – 11:30

Ignacio Garzón Sosa
(Instituto de Física - UNAM, Mexico)
Computational nanoscience
Wednesday 15
12:00 – 13:00

Rafael Baquero Parra
(CINVESTAV, Mexico)
Grafeno y superconductividad
Wednesday 15
13:00 – 14:00

Sandra E. Rodil Posada
(IIM-UNAM, Mexico)
Nanocomposite thin films
Wednesday 15
16:00 – 17:00

Thursday 16

Miguel A. García-Garibay
(UCLA, USA)
Amphidynamic crystals, molecular rotors, and molecular machines
Thursday 16
09:00 – 10:00

Karen Hallberg
(CAB-IB, Argentina)
Correlations, quantum entanglement and interference in nanoscopic systems
Thursday 16
10:00 – 11:00

Zahid Hasan
(Princeton University, USA)
Topological surface states: Discovery and recent results
Thursday 16
11:30 – 12:30

Juan Luis Peña Chapa
(CINVESTAV-Mérida, Mexico)
Studies of the thin film CdS/CdTe solar cells of high efficiency
Thursday 16
12:30 – 13:15

Grant van Riessen
(La Trobe University, Australia)
Coherent diffraction imaging for nanostructure analysis using synchrotron radiation
Thursday 16
13:15 – 14:00

L. Alberto Lightbourn Rojas
(Instituto de Investigación Lightbourn A.C. & BIOTEKSA S.A. de C.V., Mexico)
Fulvalene, rotaxane and catenane nanocompounds: Bioremediation and ultraviolet radiation effects on plants
Friday 17
16:00 – 17:00

Friday 17

Saw Wai Hla
(Ohio University, USA)
Imaging atomic spin orbit to operating nanomachines
Friday 17
09:00 – 10:00

Marek Przybylski
(AGH University of Science and Technology, Poland)
Magnetic anisotropy, exchange bias effect and orthogonal spin configuration in FM/AFM bilayers
Friday 17
10:00 – 11:00

Rafael Vázquez Duhalt
(Instituto de Biotecnología-UNAM & UCSD, USA)
Cytochome P450, pseudoviral nanoparticles, and chemoteraphy
Friday 17
11:30 – 12:30

José Lemus Ruiz
(IIM-UMSNH, Mexico)
Interfacial behavior during bonding of silicon nitride to stainless steel AISI-304
Friday 17
12:30 – 13:30

Guest Lectures

Procesos de fabricaciónde celdas solares de películas delgadas de CdTe de alta eficiencia

Juan Luis Peña Chapa
CINVESTAV Mérida, Mexico

Raman spectroscopy

Ricardo F. Aroca
Windsor University, Canada

Coherent diffraction imaging and its application to the characterisation of nanoscale Materials

Grant van Riessen
ARC Centre of Excellence for Coherent X-Ray Science, Department of Physics,
La Trobe University, Melbourne, Australia
Email: g.vanriessen@latrobe.edu.au

X-rays enable a versatile visualization of materials properties. Diffraction from crystals plays a particularly important role in elucidating structure with very high resolution. However, the structure of amorphous and disordered materials, including biomolecules that cannot be crystallized, is inaccessible by this method. A promising method for overcoming this limitation called coherent diffraction imaging (CDI) uses highly coherent X-ray beams and allows the reconstruction of two and three-dimensional images of nanoscale structures from the measured intensity of their far-field diffraction patterns. The reconstruction process employs algorithms to retrieve the phases of the (oversampled) coherent diffraction pattern. Free from the limitation of image-forming lenses, CDI can achieve very high spatial resolution, limited only by the numerical aperture of the scattered Xrays that are detected. CDI depends on the coherence properties of an X-ray beam, but retains all the fundamental advantages of utilising a weakling interacting probe that is both penetrating and (relatively) non-destructive, and which can couple to various order parameters, including internal structure, chemical bonding, orbital orientation and magnetism.

In these lectures, organised in four parts, the development of coherent diffraction imaging and related methods for studying nano- and mesoscale materials science will be reviewed. In the first part, the nature of x-ray interactions with matter will be briefly reviewed with a view to understanding how the properties and behaviour of condensed matter can be discovered and characterised. The development of experimental methods that make use of the coherence properties of synchrotron X-ray beams will then be introduced. In particular, the principles, development and techniques of coherent diffraction imaging (CDI) will be explored.

The second part will focus on experimental aspects of coherent diffractive imaging and its application to the study of complex materials in two- and three-dimensions. The dedicated instruments required for CDI experiments depend on high-brightness, highly coherent light sources and generally include nanofabricated optics, nanopositioning and nanometrology technology, and state-of-the-art detectors. The design and implementation of such an instrument that was recently installed at a soft X-ray elliptically polarising undulator beamline of the Australian Synchrotron will be presented as a case study to illustrate some of the experimental challenges in coherent diffractive imaging.

In the third part, we will explore contemporary applications of coherent X-ray diffraction imaging and related techniques to the study of materials properties, including nanoscale morphology and composition, magnetism, and the internal strain distribution of thin films and

individual nanocrystals. A variety of examples of synchrotron CDI experiments from groups around the world will be considered.

In the final part, we will examine a completely new generation of coherent X-ray scattering experiments that make use of the recent availability of ultrashort X-ray pulses from X-ray freeelectron lasers (X-FEL). The dramatically higher coherent flux available with an XFEL allows improved spatial and energy resolution and access to new domains of dynamical processes. In this part we revisit the basic concepts of the interaction of X-rays with matter to understand the implications for ultrafast imaging and structure determination.

Application of optical spectroscopies to the study of semiconductors

M.L. Gómez-Herrera
Faculty of Engineering, Autonomous University of Queretaro
Cerro de las Campanas s/n, Santiago de Querétaro, Qro. C.P. 76010 Mexico.
E-mail: lucero.gomez@uaq.mx

Most of the major technological advances have been linked to the development of new materials and processes. By understanding the similarities and differences between these kinds of materials you can choose properly their applications within the challenges of current and future technology. The properties of a material are related to its structure, hence the importance of understanding the processing details and how its parameter modification affects its structure. Semiconductor materials of high importance in the manufacture of the optoelectronic industry with a special importance in optical communications are manufactured and processed with the most advanced growth techniques in which there is a precise control on the composition and structure allowing their reproducibility.

The study of the interaction of electromagnetic radiation with matter provides valuable information concerning the properties and processing of semiconductors. The optical spectroscopies have been useful and important in the characterization of physical, chemical and biological processes. Optical spectroscopy is a large branch of science which comprises, from the various methods for obtaining spectra, their measurement and applications, up to their deepest theoretical interpretation related to the atomic and molecular structure of the material. Particularly in semiconductors, this interaction with light give information of specific parameters such as band gap energy, states within the band gap such as excitons, defects, impurity levels, phonon energy, grain size, crystal quality, lattice parameters, etc. From the point of view of the interaction of electromagnetic radiation with matter, a spectrum can be thought as a graphical representation of the intensity distribution of the electromagnetic radiation emitted or absorbed by a material as a function of the wavelength (or frequency) of this radiation. A spectrum depends in principle on the separation between different types of energy levels. Therefore, we can distinguish different types of spectra depending on the energy levels involved and the experimental techniques used for their observation.

There are several optical characterization techniques such as photoluminescence, photoreflectance, thermoreflectance and electroreflectance, which are complementary to each other. They are usually non-destructive techniques, in samples comprising bulk materials, thin films, microstructures, nanostructures, quantum dots. The fundamentals, analysis and implementation criteria of optical spectroscopy techniques for the characterization of semiconductors will be discussed during the presentation of this course.

Plenary Conferences

Crecimiento de nanopartículas semiconductoras de los tipos II-VI y III-V y sus aplicaciones

Julio G. Mendoza Álvarez

Departamento de Física, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Mexico

Los efectos de confinamiento cuántico predichos a nivel teórico desde comienzos del siglo XX, encontraron sus primeras demostraciones prácticas hacia inicios de los años 70's cuando se pudieron fabricar las primeras estructuras de pozos cuánticos basadas en los semiconductores III-V como el arseniuro de galio (GaAs), los cuales consistían de capas con espesores menores al radio de Bohr del excitón; esto es, para el GaAs espesores menores a 20 nanómetros. A partir de entonces dio inicio una enorme avalancha de investigación sobre éste nuevo tipo de materiales de dimensionalidad reducida, con nuevas propiedades estructurales, mecánicas, ópticas y eléctricas, resultado de los fenómenos de confinamiento cuántico. A la fecha, el campo de las nanociencias y la nanotecnología es quizás el de mayor actividad y desarrollo, y muchos dispositivos basados en materiales nanoestructurados están ya en el mercado.

En el Grupo de Estado Sólido del Cinvestav, unidad Zacatenco, desde el año de 1996 se inició el estudio de semiconductores nanoestructurados al reportar el crecimiento de películas delgadas nanoestructuradas de CdNiTe (Journal of Applied Physics, Vol. 80, pp. 2833-2837, 1996).

En este trabajo reportamos el crecimiento de puntos cuánticos semiconductores de CdS (de la familia II-VI), y de InP (de la familia III-V), usando técnicas de crecimiento del tipo baño químico.

Las nanopartículas (NP's) de CdS se embebieron en almidón como agente estabilizador funcionalizando la superficie del semiconductor con grupos polares como el SO^{3-} y el OH^{-}. Se presentan resultados de la influencia del pH de la solución de crecimiento, sobre la absorción óptica, la fotoluminiscencia, y el tamaño de los nanocristales semiconductores.

En el caso de las NP's de InP, éstas se sintetizaron por medio de un método químico de un solo paso con calentamiento a bajas temperaturas. Se variaron los parámetros a fin controlar el tamaño de los nanocristales con el objeto de poder variar la energía de banda prohibida del InP en todo el rango del espectro visible; además se pasivó la superficie de los nanocristales de InP con ZnS a fin de incrementar la eficiencia de luminiscencia, para su posible uso como marcadores fluorescentes en la biomedicina. Se presentan resultados sobre la caracterización estructural y óptica de éstas NP's de InP.

Recent advances in molecular transport from first principles

Marco Buongiorno Nardelli

University of North Texas, USA

Molecular spintronics envisions the construction of molecular spin states that will control spin injection, transport, and manipulation for new high speed, low-power devices through designed synthesis. Not only can molecular spin states be designed as key components of new molecules, these spin states can also be designed to be *switchable* using external stimuli via a process known as spin crossover. In this talk I will review recent advances in the study of molecular spintronics with first principles techniques and discuss recent results on the electronic/spintronic/thermal transport properties of a variety of molecular systems. These include but are not limited to: molecular organization at surfaces and transport behavior of metal phthalocyanine, Co-based valence tautomers and Fe spin crossover compounds.

Prof. Buongiorno Nardelli is a pioneer of the development and applications of Density Functional Theory computational methods in the study of electronic/spintronic/thermal transport in nanostructured materials. A fellow of the APS and IOP, he is currently Professor of Physics and Chemistry at the University of North Texas.

Computational nanoscience

Ignacio L. Garzón Sosa

Instituto de Física
Universidad Nacional Autónoma de Mexico
México, D. F., Mexico
E-mail: garzon@fisica.unam.mx

Computational nanoscience is a fundamental area of Nanoscience and Nanotechnology since it allows the prediction, understanding, and confirmation of novel properties existing in matter at the nanoscale. By developing theoretical and simulation methods it had been possible the calculation of a large variety of physical and chemical properties of nanoparticles and other nanostructures. These calculations are based on diverse methodologies going from semiempirical (atomistic) approaches to quantum-mechanical first principles, *ab initio* descriptions.

In this talk, we present as a useful example of the predictive capability of the computational nanoscience, an overview of the results obtained by my research group at UNAM, on the physicochemical properties of bare and ligand-protected metal clusters and nanoparticles.
In particular, we will discuss recent results on the chiroptical properties of small ligand-protected gold nanoclusters [1,2], and on the vibrational properties of metal nanoparticles with size 0.5 – 4 nm [3]. In addition, a discussion of the relation of these theoretical results with experimental data and possible applications in Nanotechnology will be presented.

[1] A. Tlahuice, I. L. Garzón
"On the Structure of the $Au_{18}(SR)_{14}$ Nanocluster"
Phys. Chem. Chem. Phys. **14**, 3737 (2012).

[2] A. Tlahuice, I. L. Garzón
"Structural, electronic, optical, and chiroptical properties of small thiolated gold clusters: the case of Au_6 and Au_8 cores protected with dimer $[Au_2(SR)_3]$ and trimer $[Au_3(SR)_4)]$ motifs"
Phys. Chem. Chem. Phys. **14**, 7321 (2012).

[3] H. E. Sauceda, D. Mongin, P. Maioli, A. Crut, M. Pellarin, N. del Fatti, F. Vallée, I. L. Garzón
"Vibrational properties of metal nanoparticles: atomistic simulation and comparison with time-resolved investigation"
J. Phys. Chem. C **116**, 25147 (2012).

Grafeno y superconductividad

R. Baquero Parra

Departamento de Física, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Mexico

Uno de los materiales que ha llamado la atención en los últimos tiempos es el carbono en sus múltiples configuraciones, C_60, tubos de carbono, grafito, y, en particular, en los últimos dos o tres años, el grafeno. La altísima conductividad propiciada por una dependencia lineal de las bandas alrededor del punto K que resulta en una ecuación que tiene la misma forma que la de una partícula relativista de masa cero ha llamado mucho la atención. Tratare este punto. La investigación actual se ha dirigido a volver al grafito por intercalación y al grefeno por deposición, superconductores. Sus temperaturas son relativamente pequeñas (alrededor de 10K). Sin embargo, un tratamiento de grafeno en agua ha sido publicado donde se reporta la presencia de superconductividad (obtenida por medios magnéticos) a temperaturas del orden de las ambientales. En esta charla analizaré este reporte para concluir que, si como se manifiesta, la superconductividad en este material es por interacción electrón-fonón, un análisis a la luz de la teoría de Eliashberg, muestra que la energía de los fonones existentes en el grafeno (160 meV el más energético) es insuficiente para sostener una transición de fase a tan alta temperatura. La única posibilidad sería que el agua se organice de tal manera que genere fonones de aun mayor energía. La superconductividad en grafeno es uno de los temas candentes de la investigación actual en este campo.

Nanocomposite thin films

S. E. Rodil, S. Muhl

PlasNaMat Research Group, Instituto de Investigaciones en Materiales
Universidad Nacional Autónoma de México.
E-mail: ser42@iim.unam.mx

The development of materials to satisfy the requirements for sophisticated applications in the modern world can no longer be sustained using single materials and alloys. Indeed, the introduction of the nanoscale as a designing element has been shown to be an important factor; as demonstrated by the many examples of improved polymeric and ceramic materials. Similarly, the development of Nanocomposite materials is enabling rapid advancements in structural and functional materials. In particular, thin film nanocomposite technology could revolutionize a wide range of fields; from industrial applications in high-speed machining, tooling, cutting, etc., to optical applications, including electronics (magnetic storage devices or sensors), medicine and intelligent membranes for the water industry. Nanocomposite films and coatings can achieve better properties than those expected from a simple summation of the characteristics of the constituents, with this being, in part, due to the extraordinary size effects. Nanocomposite films comprise at least two phases, a nanocrystalline phase embedded in a continuous amorphous or crystalline matrix, or two nanocrystalline phases. The design of nanocomposite films needs the considerations of many factors, for example, volume fraction, crystallite size, surface and interfacial energy, etc., all of which depend significantly on the materials selection, deposition methods and process parameters.

In this presentation, the use of magnetron sputtering in different configurations to create nanocomposite thin films is presented. As mentioned above, the range of application is diverse and depends on the base materials chosen, therefore the following examples are examined: Aluminum nitride with Ni inclusion to enhanced hardness but also to change the optical response, amorphous carbon-silver nanocomposite as antibacterial coatings, hard metal nitrides with segregated silicon nitride phases for mechanical and corrosion resistance properties and finally, self-lubricating coatings based on the addition of bismuth particles into a hard coating matrix.

The talk gives an overview of the different deposition parameters and their influence in the structure and properties of the films. For each nanocomposite coating, the physical properties of interest are discussed showing that although the general idea of designing nanocomposites is very good, in some specific cases, the materials behave in unexpected ways.

Acknowledgements: DGAPA-PAPIIT, CONACYT, ICTyDF and BisNano (FP7-CONACYT)

Amphidynamic crystals, molecular rotors, and molecular machines

Miguel A. Garcia-Garibay

Department of Chemistry and Biochemistry
University of California, Los Angeles
Los Angeles CA 90095-1569 USA

Amphidynamic crystals are materials designed to display engineered motion and mechanical processes in the solid state. With a combination of order and motion they provide a promising platform for the construction of intelligent materials and artificial molecular machines. Their structures are based on a combination of static components designed to guide crystalline order, and a set of dynamic elements that display controlled conformational motions. One of the most interesting challenges in molecular structure and crystal design is the realization of structures with components that rotate close to their limit of their moment of inertia, as the result of barriers that are below thermal energies. While this is an unchartered territory with interesting implications in solid state physics, research in our group has recently led to the development of promising structural platforms based on extended solids and molecular crystals. This contribution will discuss advances in their syntheses and self-assembly, as well as the strategies used for their structural and dynamic characterization with the help of X-ray diffraction and solid state NMR.

Correlations, quantum entanglement and interference in nanoscopic systems

Karen Hallberg

Centro Atómico de Bariloche, Instituto Carlos Balseiro
Argentina

Nanoscopic systems are an ideal playground to observe quantum effects. For example, the effects of strong correlations between electrons and of quantum interference can be measured in transport experiments through quantum dots, quantum wires, individual molecules and rings formed by large molecules or arrays of quantum dots. In addition, quantum coherence and entanglement can be clearly observed in quantum corrals.

One of the most intriguing features resulting from strong correlations is the separation of charge and spin degrees of freedom in low dimensions. This effect can be directly observed in transport experiments through Aharonov-Bohm rings. On the other hand, coherent electronic transport through individual molecules is crucially sensitive to quantum interference, as shown by our recent calculations of conductance through pi-conjugated annulene molecules. For certain source-drain configurations we obtain a great reduction or even the disappearance of conductance through the molecule, which is fully restored by symmetry-breaking perturbations, leading to the possibility of an interesting switching effect.

Finally, elliptic quantum corrals offer an ideal system to study quantum entanglement due to their focalising properties: two spins located at the foci of the system will strongly interact and will form robust singlet or triplet states depending on the filling of the system. These states can be also analyzed from the quantum information perspective, which shows the change in mutual entanglement when the interaction between the spins and the itinerant electrons of the ellipse is increased. These systems also show interesting quantum dynamical behavior and offer a challenging scenario for quantum information experiments.

Topological surface states: Discovery and recent results

Zahid M. Hasan

Princeton University, USA

Topological Insulators are a new phase of electronic matter which realizes a non-quantum-Hall-like topological state in the bulk matter and unlike the quantum Hall liquids can be turned into superconductors at the bulk and/or at the interface. First part of this talk highlights experimental demonstration of Z2 topological order via bulk-boundary correspondence as it its original definition (Kane-Mele). Experimental results include demonstration of the fundamental properties of topological insulators such as spin-momentum locking, non-trivial Berry's phases, mirror Chern number, absence of backscattering, protection by time-reversal and other discrete symmetries and their persistence up to the room temperature (at the level of M.Z. Hasan and C.L. Kane, Rev. of Mod. Phys., 82, 3045 (2010). I will then present (exciting) recent results demonstrating broken symmetry phases such as superconductivity and magnetism in artificial hetero interfaces as well as outline the emerging experimental research frontiers of the field of topological insulators as a whole. Time permitting; I will also present experimental results on a new class of topological insulators beyond the Kane-Mele Z2 theory.

Studies of the thin film CdS/CdTe solar cells of high efficiency

Juan Luis Peña Chapa

CINVESTAV Mérida, Mexico

Currently, there is a technology to manufacture CdTe panels based in thin film solar cells for a large scale production, where an important step is the chlorination for the cell activation. However, at the industrial level it still using the treatment with $CdCl_2$; that is performed with its aqueous solution sprayed on CdTe film and subsequently heat treated, which has drawbacks because the $CdCl_2$ is dangerous for the health and the liquid wastes. In recent years, Romeo et al. [1] developed a new dry activation method.

The most common chlorination for CdTe solar cells has been performed in air; then oxygen should play an important roll. In the present work, we report about our results using oxygen and other gases mixtures.

Our cell has a superstrate structure and it is fabricated by sequentially depositing several layers onto a commercial Corning glass coated with ITO. The sequence of layers: depositing by rf-sputtering 100 nm of ZnO onto ITO/Glass and 150 nm of CdS onto ZnO/ ITO/Glass, by using CSS 8-10 µm of CdTe onto CdS.; then the activation process at 400 ºC by using: Ar (290 mBar) + $CHClF_2$ (10mBar) , Ar (220 mBar) + O_2 (70mBar) + $CHClF_2$ (10mBar) and another mixtures of gases. After, depositing by rf-sputtering 15 nm of Cu and 500 nm of Mo as the back contact and annealing at 200 ºC for 20 min. in Ar atmosphere [2] At the end, it is performed measuring curve J-V and EQE spectra on dark and under illumination.

Although the solar cell efficiency is improved when it was activated by using Argon-$CHClF_2$, the HR-SEM shows important changes in the CdTe grains such as small holes formed by the $CHClF_2$ presence during the activation process. The images show the compacted and coalesced grains at CdTe surface.

The solar cells were investigated when activated with gases such as argon-$CHClF_2$-oxygen showing that oxygen mainly improves the J_{SC}, V_{OC} and its efficiency. In this case, the small holes between the grains seem have been inhibited by the oxygen, and are observing that coalesces, allowing us to obtain a considerable improvement for series and shunt resistances. Efficiencies higher than 12% have been obtained in the cells with areas of $1cm^2$. Work is underway to understand why there are these improvements.

REFERENCES

[1] N. Romeo, A. Bosio and A. Romeo, "An innovative process suitable to produce high-efficiency CdTe/CdS thin-film modules" *Solar Energy Materials & Solar cells*, vol. 94, pp. 2-7, 2010.

[2] J.L. Peña, O. Arés, V. Rejón, A. Rios-Flores, Juan M. Camacho, N. Romeo, A. Bosio, "A detailed study of the series resistance effect on CdS/CdTe solar cells with Cu/Mo back contact", *Thin Solid Films* vol. 520, pp. 680-683, 2011.

ACKNOWLEDGEMENT: This work has been supported by CONACYT-México under contract FORDECYT-116157 and FOMIX 170098.The Authors acknowledges Dr. José Mendez from UADY for facilities extended for using the solar simulator, O. Gómez, W. Cauich and D. Huerta for technical support, and L. Pinelo for its secretarial assistance.

Coherent diffraction imaging for nanostructure analysis using synchrotron radiation

G van Riessen,[a] M Jones,[a] M Luu,[a] N Philips,[a] A. Tripathi,[a] DJ Vine, [b] B Abbey,[a] and AG Peele[a,c]

[a]ARC Centre of Excellence for Coherent X-Ray Science,
Department of Physics, La Trobe University,
Melbourne, Australia
[b]Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA
[c]The Australian Synchrotron, Melbourne, Australia
E-mail: g.vanriessen@latrobe.edu.au

Methods of lensless imaging that are based on coherent X-ray diffraction represent powerful tools for understanding materials at the nanoscale. In coherent diffraction imaging (CDI), an object is illuminated with a coherent beam of X-rays and an image of the object is reconstructed from the measured intensity of its far-field diffraction pattern. The reconstruction processes users phase retrieval algorithms to retrieve the phases of the (oversampled) coherent diffraction pattern. Free from the limitation of image-forming lenses, CDI can achieve very high spatial resolution, limited only by the numerical aperture of the scattered X-rays that are detected. By combining recent developments in experimental and algorithmic methods it is possible to take full advantage of the high brilliance of modern X-ray sources and to exploit various contrast mechanisms.

In this talk I will provide a brief introduction to coherent methods in the X-ray sciences and an outline of the development of a particular implementation of coherent X-ray diffraction imaging that employs non-planar beams. Recent applications in materials science and cellular biology will be presented to highlight the progress and challenges in quantitative nanoscale imaging in two- and three-dimensions. Finally, the future prospects for coherent X-ray diffraction imaging are given, with particular emphasis on the role it can play in understanding the relationships between structure and function in materials and biological systems

Fulvalene, rotaxane and catenane nanocompounds: Bioremediation and ultraviolet radiation effects on plants

Lightbourn-Rojas L A,[1] **León-Chan R G**,[1] **Heredia J B**[1, 2]

[1] *Instituto de Investigación Lightbourn A.C. Bionanofemtofisiología Vegetal Disruptiva*
[2] *Centro de Investigación en Alimentación y Desarrollo A.C. (CIAD) Unidad Culiacán*

There are several studies on climate change, which focus on different factors: the increase in atmospheric CO2, droughts, variable amount of rainfall, sudden temperature changes and the increase of ultraviolet radiation (UV) due to the deterioration of the ozone layer by atmospheric contaminants. The increase of UV radiation causes adverse responses in plants development, particularly in DNA and in photosynthetic system, especially in photosystem II, therefore the loss of photosynthetic efficiency and a foods reduction. Plants have developed several defense systems which are related to the synthesis of anthocyanins. These compounds can protect plant tissues by absorbing excess of light, UV radiation or by their antioxidant capacity, scavenging UV produced reactive oxygen species. However, sometimes these mechanisms are insufficient due to photosynthetic deficiency; therefore we have developed a new plant nutrition technology, based on fulvalene, rotaxane and catenane nanocompounds. With this approach, an increase in the uptake, storage and availability of monochromatic ray at 563 nm can be achieved. This can induce the photosynthetic optimization and the reduction of metabolic delays in the photosynthetic system. This would help to maintain the plant metabolism and therefore the stability of the food production regardless of the adverse environmental conditions.

Imaging atomic spin to operating nanomachines

Saw Wai Hla
Department of Physics & Astronomy, Ohio University, OH 45701
E-mail: hla@ohio.edu

Scanning tunneling microscopy and spectroscopy combined with atom and molecule manipulation schemes create the most robust experimental setting to date at atomic and molecular scale. In this talk, our recent achievements of atomic and molecular manipulations on surfaces covering spintronics, superconductor, and nanomachines to nanomedicine research areas will be presented. In spintronic area, we will present imaging and manipulation of atomic spin using a spin-polarized STM tip [1]. In nanoscale superconductivity area, donor-acceptor type charge transfer based molecular superconducting systems will be shown [2]. We will discuss proximity effect of nanoscale molecular superconductors and metal boundaries as well as molecule-metal interfaces. In molecular machine area, operations of complex molecular machines on surfaces using STM manipulation will be shown. Finally, we will demonstrate the extension of STM manipulation technique to biology where our recent achievements of manipulation and sequencing of individual proteins will be presented. These innovative experiments are tailored to address several critical issues covering fundamental understanding as well as demonstration of novel atom/molecule based devices on materials surfaces at the nanoscale.

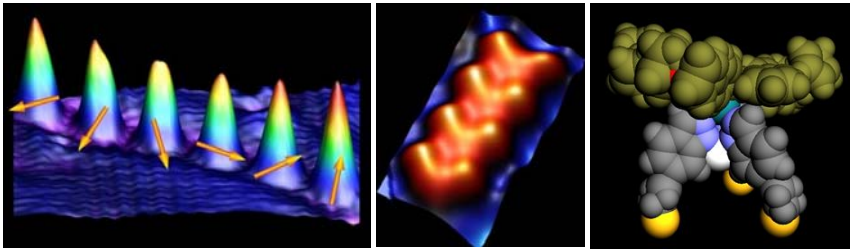


Figure 1: Imaging spin in Co atoms (left). Four-molecule superconducting system (middle). Molecular nanomachine (Right).

[1] D. Serrate, P. Ferriani, Y. Yoshida, S.-W. Hla, M. Menzel, K. von Bergmann, S. Heinze, A. Kubetzka, and R. Wiesendanger. *Imaging and manipulating the spin direction of individual atoms*. ***Nature Nanotechnology*** **5**, 350-354 (2010).

[2] K. Clark, A. Hassanien, S. Khan, K.-F. Braun, H. Tanaka, and S.-W. Hla. *Superconductivity in just four pairs of (BETS)$_2$-GaCl$_4$ molecules*. ***Nature Nanotechnology*** **5**, 261-265 (2010).

[3] U.G.E. Perera. F. Ample, H. Kersell, Y. Zhang, G. Vives, J. Echeverria, M. Grisolia, G. Rapenne, C. Joachim, and S.-W. Hla. *Controlled clockwise and anticlockwise rotational switching of a molecular motor*. ***Nature Nanotechnology*** **8**, 46-51 (2013).

Magnetic anisotropy, exchange bias effect and orthogonal spin configuration in FM/AFM bilayers

Marek Przybylski

Academic Centre of Materials and Nanotechnology
Faculty of Physics and Applied Computer Science,
AGH University of Science and Technology, Kraków, Poland
Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The exchange bias effect has been widely investigated in systems presenting in-plane anisotropy and has been applied, e.g., in spin-valve based devices. However, the mechanism responsible for this effect is still not fully understood due to difficulties in determination of the antiferromagnetic (AFM) spin configuration. The existing models explain the exchange bias effect for uncompensated AFM surfaces assuming a collinear FM (ferromagnetic)/AFM exchange coupling at the interfaces. However, for fully compensated FM/AFM interfaces theory predicts that the AFM and FM spins can be coupled orthogonally [1].

As an example, I will discuss the magnetic properties of Fe/NiO bilayers grown on vicinal (step) surfaces of Ag(001). The easy magnetization axis of the Fe film in the Fe/NiO switches from parallel to perpendicular to the steps at the NiO thickness the AFM order is established, and back to the step direction at the NiO thickness corresponding to its structural relaxation. I will show that the two in-plane spin reorientation transitions (SRTs) in the Fe film are forced by perpendicular coupling between the Fe and NiO spins at the Fe/NiO interface [2].

Even more important candidates for developing new technologies are the systems combining magnetic out-of-plane anisotropy and perpendicular exchange bias. I will discuss the FM/AFM coupling in this case showing the effect of AFM on the anisotropy of FM films. For example, Ni films grown on Pd(001) show perpendicular easy magnetization axis approximately up to a thickness of 17 monolayers (at room temperature). The result confirms the volume character of perpendicular magnetic anisotropy of Ni, which is related to the tetragonal distortion of Ni grown on the strongly mismatching substrates like Pd(001). Co-deposition of fully-compensated AFM (like CoO or NiO) on top of Ni/Pd(001) changes the anisotropy of the system. At temperatures lower than Néel temperature of AFM, the CoO/Ni/Pd(001) bilayers show perpendicular magnetization and perpendicular exchange bias effect up to the thickness of Ni much larger than the thickness up to which Ni films on Pd(001) show perpendicular anisotropy. The effect is explained by perpendicular FM/AFM coupling, which is found to persist also in the case the easy magnetization axis of FM is oriented perpendicular to the sample plane [3].

References:
[1] N. C. Koon, Phys. Rev. Lett. **78**, 4865 (1997).
[2] J. Li, M. Przybylski, F. Yildiz, X.L. Fu, Y.Z. Wu, Phys. Rev. B **83**, 094436 (2011).
[3] P. Kuswik, P.L. Gastelois, M. Soares, H. Tolentino, M. Przybylski, J. Kirschner, will be published.

Cytochome P450, pseudoviral nanoparticles, and chemotherapy

Rafael Vázquez Duhalt

Instituto de Biotecnología UNAM
Centro de Nanociencias y Nanotecnología UNAM

Combined quantum mechanical and molecular mechanical (QM/MM) calculations were used to explore the electron pathway involved in the suicide inactivation of cytochrome CYPBM3 from *Bacillus megaterium*. An extensive mapping of residues involved in electron transfer routes was obtained from density functional calculations on activated heme (i.e. Compound I) and selected amino acid residues. Identification of oxidizable residues (electron donors) was performed by selectively activating/deactivating different quantum regions. This method allowed a rational identification of key oxidizable targets in order to replace them for less oxidizable residues by site-directed mutagenesis. The residues W96 and F405 were consistently predicted by the QM/MM electron pathway to hold high spin density; single and double mutants of P450BM3 on these positions (W96A, F405L, W96A/F405L) resulted in a more stable variants in the presence of hydrogen peroxide, displaying a similar reaction rate than CYPBM3 21B3.

Recently, the encapsulation of enzymes inside VLPs or other protein cages has been a fast growing topic because of its implications in biocatalysis as well as their potential as enzymatic delivery systems. We report for the first time the encapsulation of a CYP450 which belong to a family of enzymes medically and industrially important. The CYPBM3 21B3 from *Bacillus megaterium*, mutant "21B3"which has improved peroxigenase activity, as a model of this family of enzymes since it is stable and soluble in aqueous media, and it can be produced in large quantities, as opposed to human CYP. CYPBM3 21B3 has been encapsulated inside two different VLPs through a charge complementarity strategy. The VLPs used were CCMV and VP1 from murine poliomavirus, these capsids differ in size, porosity and charge of the inside surface. The encapsulation of CYP inside CCMV was favored by the fact that the enzyme (-) and the interior of the capsid (+) have opposite charge at pH 7.2. A range of molar ratio of viral protein to CYP were assayed (1.3-60:1) finding encapsulation at the 1.3:1 ratio. This particular stoichiometry has the characteristic of having a cero net charge. The VLPs formed have an average diameter of 19.9 nm, which is smaller than the reported for the empty capsid (28 nm).
For the VP1-CYP encapsulation three different molar ratio of viral protein to enzyme were assayed (3:1, 5:1, 10:1), only finding nanostructures with CYP activity in the 10:1 stoichiometry. In this case to promote the interaction of the CYP with the negatively charged interior of the VP1 capsid we chemically modified the surface of the enzyme with ethylenediamine to increase the number of positively charged groups at pH 8. The VLPs formed have an average diameter of 23.6 nm.

It is still to be determined the exact number of CYPs encapsulated in each VLP, as well as complete enzymatic characterization of the biocatalytic VLPs. Nevertheless, we have demonstrated that it is possible to encapsulate the CYPBM3 inside CCMV and VP1 VLPs using a charge complementarity approach. The encapsulation of this CYP450 in viral structures will provide a model for the design of bioatallytically nanoparticles with potential medical applications.

Interfacial behavior during bonding of silicon nitride to stainless steel AISI-304

J. Lemus Ruiz

Instituto de Investigaciones Metalúrgicas, Universidad Michoacana de San Nicolás de Hidalgo
Edif. U, C.U., Apdo. Postal 888, Centro, C.P. 58000; Morelia, Mich., México.
E-mail: jlruiz@umich.mx

Silicon nitride (Si_3N_4) is one of the most important ceramics used for structural applications. Brazing is a metal-joining process where a filler metal is heated above its melting point and distributed between two or more closefitting parts. This process is considered to be one of the simplest and by far the most widely methods used to join ceramics to metals based on melting, wetting and solidification of a liquid film between the base materials.
Silicon nitride Si_3N_4 samples prepared by the Spark Plasma Sintering (SPS) technique, which had different amount of oxide additives, were used as disc-preforms. The surfaces of the materials to be bonded during the brazing process (ceramic, metal and filler) were previously coated with thin layer of silver and then stacked together with these preforms. Interface assemblies produced were sandwich-like specimens of Si_3N_4/Cu-Zn/Nb/Cu-Zn/AISI304 combinations joined at 1000°C using 5, 20, and 40 min holding times under an inert atmosphere. Analysis by scanning electron microscopy revealed un-joined zones between the ceramic and metallic parts after 5 min treatment, whereas from 20 min, homogenous and non-porous Si_3N_4/Cu-Zn/Nb interfaces were obtained.

The thickness of resultant ceramic-metal interface increased from ~10 to >25 μm as the holding time was increased. It is found that the amount of additives used during the preparation of Si_3N_4 ceramics has a direct effect on the decomposition rate of Si_3N_4 during the joining process. The largest decomposition of Si_3N_4 was observed at 1000^oC/40min from the less dense ceramic preforms (4wt% of additives in this case), which in turn induced the migration of Si atoms through the interface to promote the formation of Si-based components. In contrast, when using larger amount of additives (8wt%) during sintering of the ceramic preforms it becomes more difficult for nitrogen and silicon to dissociate upon brazing. Therefore, when diffusion rate of Si is low, it migrates towards the metal part, which limits the formation of Si-based components.

Poster Sessions

Wendesday 15

Packing problem approaches for models of nanoporous channel filling

L. Burtseva,[a] B. Valdez Salas,[a] V. Petranovskii[b]

[a]*Instituto de Ingeniería de la Universidad Autónoma de Baja California, Calle de la Normal, S/N, Insurgentes Este, 21280, Mexicali, B.C., México*.
[b]*Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología, Km. 107 Carretera Tijuana-Ensenada, 22860, Ensenada, B.C., México.*
E-mail: burtseva@uabc.edu.mx

The properties of nanostructured porous matrix filled by a substance strongly depend on the density of atoms in nanochannels. The dense filling of the channels by atoms and molecules with diameters comparable with the diameters of pores represents a computational problem of packing and produces a variety of models. Packing problem has attracted much attention in consequence of practical applications and diversity of models, but there is lack of the publications dedicated to the nanotechnologies meanwhile many structural models of nanoporous objects in condensed-matter and materials physics can be described as packing of congruent spheres in a cylinder.
Due to the complexity of the geometry the pure theoretical results are limited and the majority of studies are concerned on determining the packing structure and parameters (density, mean, radial and angular void fractions), through experimentation techniques. Ordered and random packings produce densities from 0.74, which is given by Kepler's conjecture for the compact face centered cubic lattice and is used as the density upper limit, up to 0.64 and 0.56, for the random close and lose packings, respectively. The maximal density can be obtained with ordered packing or random packing with an agitation: vibration, tapping, shaking, etc. Random lose packing represents a bulk of spheres without any agitation. The ratio cylinder-to-sphere diameter has a pronounced effect on the density. When this ratio belongs to the range values from 1/1 till approximately 8/1, the density function drastically depends on the cylinder diameter, meanwhile the effect of this ratio becomes negligible for ratios above 50/1.

Three approaches are employed for NP-hard problem of densest packing solution: i) the numerical simulation, based on the geometrical properties, wall effects, stable position of a sphere under gravity [1]; ii) modeling the 3D channel structure with the Voronoi-Delaunay network [2]; iii) minimal cylinder height search with non-linear mathematical programming methods [3]. These methods can be used for diverse nanoporous structure designs.

[1] G. E. Mueller. Numerically packing spheres in cylinders. Powder Technol., vol. 159, pp. 105–110, 2005.
[2] V. A. Luchnikov, M. Gavrilova, N. N. Medvedev, and V. P. Voloshin, "The Voronoi–Delaunay approach for the free volume analysis of a packing of balls in a cylindrical container", Future Generation Computer Systems, vol. 18, pp. 673–679, 2002.
[3] Yu. G. Stoyan, and G. N. Yaskov, "Packing identical spheres into a cylinder", International Transactions in Operational Research, vol. 17, pp. 51-70, 2010.

Sobre la transición semimetal-aislante en grafeno

S. Hernández, A. Raya

Instituto de Física y Matemáticas de la UMSNH
Edificio C-3, Ciudad Universitaria, 58060, Morelia, Michoacán, México
E-mail: sortiz@ifm.umich.mx, raya@ifm.umich.mx

En este trabajo estudiamos los fenómenos no perturbativos de la Generación Dinámica de Masas (GDM) debido al Rompimiento Dinámico de la Simetría Quiral y el Confinamiento en el Grafeno con el objetivo de estudiar la transición de fase de semimetal-aislante cuando sus portadores de carga adquieren masa, esto mediante el uso de las Ecs. de Schwinger-Dyson. Realizamos nuestro análisis en el caso de Grafeno ideal siguiendo la propuesta de Gusynin et al. [1, 2]. Encontramos que el acoplamiento Coulombiano, o equivalentemente la constante dieléctrica del sustrato donde se crece el Grafeno, debe poseer un valor crítico mínimo para la apertura de una brecha energética entre las bandas de conducción y valencia. Además, en esta fase, los portadores de carga están confinados [2]. Estos resultados están en contraste con los estudios de Grafeno suspendido [3].

Referencias

[1] O. V. Gamayun, E. V. Gorbar, y V. P. Gusynin, *Gap generation and semimetal-insulator phase transition in Graphene*, Phys. Rev. B**81**; 075429 (2010).
[2] S. F. Hernández, *Mapeo a una Mecánica Cuántica SUSY para la ecuación de Dirac en el plano*. Tesis de Maestría, (IFM-UMSNH), (2013).
[3] J-R. Wang y G-Z. Liu, *Absence of dynamical gap generation in suspended graphene*. New J. Phys. **14**; 043036 (2012).

Cálculos puntuales de energía para discernir la trayectoria de crecimiento del decaedro al icosaedro

Esther Elena Hernández-Vázquez,[a] Juan Martín Montejano-Carrizales,[b] José Luis Rodríguez-López[a]

[a]*División de Materiales Avanzados*
Instituto Potosino de Investigación Científica y Tecnológica. A.C.
[b]*Instituto de Física*
Universidad Autónoma de San Luis Potosí
E-mail:esther.hernandez@ipicyt.edu.mx

En este trabajo presentamos resultados de optimización estructural para geometrías con simetría de orden cinco. Como resultado de micrografías de barrido electrónico (SEM) de nanopartículas de Au, además de cálculos previos de nuestro grupo, asumimos una plausible y probable trayectoria de crecimiento de la estructura de simetría decadral hacia el icosaedro. En particular realizamos un análisis de estabilidad energética para diferentes estructuras y tamaños, tales como el decaedro, el decaedro con reconstrucción superficial, el icosaedro truncado y el icosaedro truncado con una muesca en el centro.

El rango de tamaños calculados es aproximadamente hasta 150 mil átomos (entre 30 y 50 nm de tamaño de partícula), obteniendo los mínimos de energía de cada posible estado de transición. Los resultados para las energías de cohesión para cada familia son comparados y discutidos con respecto a la familia del icosaedro. Usando esta referencia, discernimos una probable trayectoria de crecimiento entre estas nanoestructuras. Presentamos también discusiones en base de resultados experimentales para nanopartículas de Au.

Agradecimientos: Al CONACYT por la beca de maestría, el apoyo institucional del IPICYT, y al proyecto SEP-2008-106437.

Quantum efficiency of bi-chromatic rare-earth doped yttrium silicate

D. Cervanes-Vazquez, [a] O.E. Contreras,[b] G.A. Hirata[b]

[a]*Centro de Investigación Científica y de Educación Superior de Ensenada, Carretera Ensenada-Tijuana No. 3918, Zona Playitas, C. P. 22860, Ensenada, B. C., México*
[b]*Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Km. 107 Carretera Tijuana-Ensenada, C. P. 22800, Ensenada, B. C., México*
E-mail: edel@cnyn.unam.mx; ocontrer@yahoo.com, hirata@cnyn.unam.mx

The photoluminescent properties of rare earth-activated Y_2SiO_5:Ce,Tb nanocrystalline phosphor prepared by pressure-assisted combustion synthesis and sol-gel were studied. The synthesized phosphor samples were post-annealed at 1373 K and 1623 K in order to obtain the X1-Y_2SiO_5 and X2-Y_2SiO_5 phases, respectively, which were confirmed by X-ray diffraction measurements. Photoluminescence analysis showed the contribution of two blue-emission bands within the 380 - 450 nm region originating from 5d – 4f transitions in Ce^{3+} ions and a well-defined green emission of Tb^{3+} ions located at 545 nm corresponding to $^5D_4 \rightarrow {}^7F_5$ electronic transitions. Thereafter, Y_2SiO_5:Ce,Tb powders were coated with colloidal silica in order to investigate the effect of coating on their luminescent properties. Absolute fluorescence quantum efficiency measurements were carefully performed, which revealed an increase of 12% of efficiency in coated compared with uncoated Y_2SiO_5:Ce,Tb phosphor.

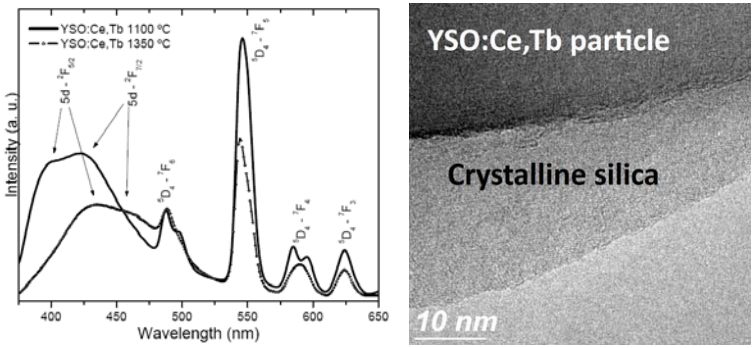


Figure 1: (a) Micrograph of silica-coating/ Y_2SiO_5:Ce,Tb interface and (b) photoluminescence of Y_2SiO_5:Ce,Tb phosphore.

This work was supported by DGAPA-UNAM-PAPIIT (Grants No. IN109913 and IN109612) and CONACYT (Grant No. 100555 and 82984). Technical assistance of E. Aparicio, F. Ruíz, I. Gradilla, E. Flores, Isabel Pérez Montfort and D. Domínguez is gratefully acknowledged

Construcción de una celda solar tipo Grätzel, sensibilizada con colorantes naturales de la región de Baja California, México

A. Perez,[a] O.E. Contreras[b]

[a]*Maestría y Doctorado en Ciencias e Ingeniería, Facultad de Ciencias, UABC, Ensenada B.C.*
[b]*Centro de Nanociencias y nanotecnologia, UNAM, Apdo. Postal 14, C.P. 22800, Ensenada B.C.*
E-mail: anahivaldovinos@hotmail.com, edel@cnyn.unam.mx

Los sistemas alternativos de generación eléctrica, como lo son los sistemas fotovoltaicos, son una alternativa para enfrentar el problema actual de crisis energética. Dentro los sistemas de conversión solar, se continúa la investigación de modelos técnicamente factibles y económicamente viables.

La celda solar tipo Grätzel, consiste de tres materiales diferentes que son responsables para la función de la conversión de la luz solar en energía eléctrica. Una capa de material semiconductor nanocristalino de dióxido de titanio (TiO_2) transparente a la luz visible, una película de moléculas de colorante y un electrolito.

La celda de Gratzel estudiada en este trabajo, está compuesta por una película de semiconductora nanoporosa de TiO_2 depositada sobre ITO (Oxido de Indio dopado con estaño). La película de nanopartículas de TiO_2 es sensibilizada con un colorante natural extraído del fruto Heteromeles Arbutifolia, una planta endémica de la región de Baja California. El colorante natural es un compuesto de moléculas orgánicas que absorben luz en la región visible y esta absorción óptica se lleva a cabo en la región del electrolito que contiene el par redox yodo/yoduro. Las moléculas de colorante liberan la carga eléctrica, promovida por la excitación óptica, al entrar en contacto con el electrodo compuesto de nanopartículas de TiO_2 sobre ITO.

Se agradece el apoyo a los proyectos de DGAPA-PAPIIT IN109612 y Conacyt 82984.

Influence of Bragg reflector in strain-balanced quantum well solar cells

C. I. Cabrera,[a] J. C. Rimada,[b] L. Hernandez,[c,d] A. Enciso,[c] and D. A Contreras-Solorio[c]

[a] *Department of Physics, University of Pinar del Río, Martí 270, 20100 Pinar del Río, Cuba.*
[b] *Solar cell laboratory, Institute of Materials Science and Technology (IMRE), University of Havana, Zapata y G, 10400; La Habana, Cuba.*
[c] *Academic Unit of Physics, Autonomous University of Zacatecas, Czda. Solidaridad y Paseo La Bufa S/N, 98060; Zacatecas, Zac., México.*
[d] *Permanent address: Faculty of Physics, University of Havana, Colina Universitaria. 10400; La Habana, Cuba.*
E-mail: dacs10@yahoo.com.mx

Strain-balanced quantum well solar cells (SB-QWSC) extend the photon absorption edge beyond that of bulk GaAs by incorporation of quantum wells in the i-region of a p–i–n device. The SB-QWSC benefits from a fundamental efficiency enhancement due to anisotropic emission from the quantum wells. This anisotropy arises from a splitting of the valence band due to compressive strain, suppressing a transition which contributes to emission from the edge of the quantum wells. We studied both the emission light polarized in the plane perpendicular (TM) to the quantum well which couples exclusively to the light hole transition and the emission polarized in the plane of the quantum wells (TE) which couples mainly to the heavy hole transition. We found that the spontaneous emission rates TM and TE increase when the quantum wells are deeper. We have also demonstrated that the photo-generated carriers can escape from the quantum wells with near unity efficiency, via a thermally-assisted tunneling process, because gain is several orders greater than radiative recombination. The addition of distributed Bragg reflector (DBR) was investigated in order to increase the photocurrent. Since the dark-current of SB-QWSCs is dominated by recombination in the depletion region of the device, by adding a DBR, thus increasing short-circuit current. Results presented here see reduced dark-currents in DBR cells and improved efficiencies. Provided radiative processes dominate the device dark-current, DBRs may also reveal photon-recycling effects.

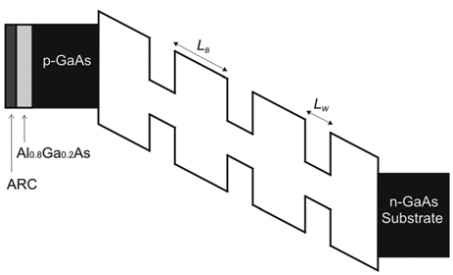


Fig. 1. The schematic band-structure of the SB-QWSC. The QW stack is embedded within the depletion zone of the GaAs cell.

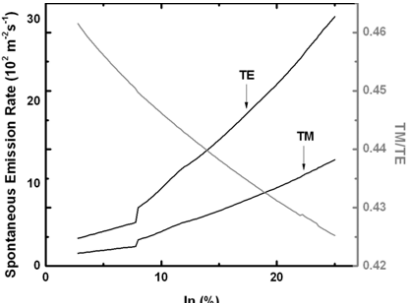


Fig. 2. Modeled spontaneous emission rate for TE and TM modes and TM/TE ratio versus In composition for 10 quantum well.

First principle calculation of the structural and electronic properties of GaN nanowires

R. García-Díaz,[a] G. I. Canto,[b] Gregorio H. Cocoletzi,[a] and N. Takeuchi[c]

[a]*Benemérita Universidad Autónoma de Puebla, Instituto de Física*
[b]*Universidad Autónoma de Campeche, Departamento de Materiales y Corrosión, Centro de Investigación en Corrosión,*
[c]*Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología*
E-mail: reyesgd@ifuap.buap.mx

Gallium nitride (GaN), a wide gap semiconductor (3.47 eV), has been extensively studied because of technological applications [1, 2]. On the other hand, it is well known that low dimensional systems exhibit novel structural and electronic properties suitable for applications in the nano-optoelectronic industry. Particular attention has been paid on semiconductor wires with sizes in the regime of nanometer scale [3, 4] since they may be employed in the fabrication of electronic devices such as field effect transistors. In this work we have performed first principles total energy calculations within the periodic density functional theory (DFT) to investigate structural and electronic properties of GaN nanowires. Calculations have been carried out within the generalized gradient approximation (GGA). We have studied GaN nanowires formation in the wurtzite phase with the growth axis being along the [0 0 0 1] direction. We have investigated different diameters for the nanowires. It is found that the outer Ga atoms move slightly towards the nanowire center while the surface N atoms move in the opposite direction. Band structure and DOS show a band gap with the Fermi energy close to the conduction band. Partial DOS show that the valence bands are formed mainly by N-2p orbitals and conduction bands by Ga-4p orbitals. Formation energy studies reveal that structures with larger diameter are more stable than thinner ones.

We acknowledge the financial supports of CONACyT, Mexico, through the scholarship # 209436. G.H.C. acknowledges the financial support of VIEP-BUAP, grant 31/EXC/06-G, and Cuerpo Académico Física Computacional de la Materia Condensada (BUAP-CA-194). NT thanks DGAPA project IN103512-3 and Conacyt Project 164485 for partial financial support. Calculations were performed at the DGCTIC-UNAM supercomputing center, CNS-IPICYT center and Instituto de Física BUAP.

References:
[1] S. Nakamura, Solid State Commun. **1997**, 102, 237.
[2] Bougrov V., Levinshtein M.E., Rumyantsev S.L., Zubrilov A., Properties of Advanced Semiconductor Materials. Eds. John Wiley & Sons, Inc., New York, **2001**, 1-30.
[3] M. E. Pistol; C. E. Pryor, Phys. Rev. B, **2009**, 80, 035316.
[4] K. Lee; et. al., Phys. Rev. B, **2010**, 82, 245310.

Density functional theory studies of the adsorption of hydrogen sulfide on Al doped silicane

F. Sánchez-Ochoa,[a,*] J. Guerrero-Sánchez,[a] Gabriel I. Canto,[b] Gregorio H. Cocoletzi,[a] Noboru Takeuchi[c]

[a]*Benemérita Universidad Autónoma de Puebla, Instituto de Física "Ing. Luis Rivera Terrazas"*
[b]*Universidad Autónoma de Campeche, Centro de Investigación en Corrosión*
[c]*Universidad Nacional Autónoma de México, Centro de Nanociencia y Nanotecnología*
E-mail: [*]*fsanchez@ifuap.buap.mx*, *querrero@ifuap.buap.mx*, *gcanto@uacam.mx*, *cocoletz@ifuap.buap.mx* , *takeuchi@cnyn.unam.mx*

First principles total energy calculations have been performed to study the hydrogen sulfide (H_2S) adsorption on silicane, an unusual one monolayer of Si(111) surface hydrogenated on both sides. The H_2S adsorption may take place in dissociative or non-dissociative forms. Silicane has been considered as: (A) non-doped with a hydrogen vacancy, and doped in two main configurations; (B) with an aluminum replacing a hydrogen atom and (C-n; n=1, 2, 3) with an aluminum replacing a silicon atom at a lattice site. In addition, three supercells; 4x4, 3x3 and 2x2 have been explored for both non-doped and doped silicane. The non-dissociative adsorption takes place in geometries (A), (C-1), (C-2) and (C-3) while the dissociative in (B). Adsorption energies of the dissociative case are larger than those corresponding to the non-dissociated cases. In the dissociative adsorption, the molecule is fragmented in a HS structure and a H atom which are bonded to the aluminum to form a H-S-Al-H structure. The presence of the doping produces some electronic changes as the periodicity varies. Calculations of the total density of states (DOS) indicate that in most cases the energy gap decreases as the periodicity changes from 4x4 to 2x2. The features of the total DOS are explained in terms of the partial DOS. The reported charge density plots explain quite well the chemisorptions and physisorptions of the molecule on silicane in agreement with adsorption energies.

Initial stages of the adsorption of Sc and ScN thin films on GaN(0001)

J. Guerrero-Sánchez,[a] Gregorio H. Cocoletzi,[a] J. F. Rivas Silva,[a] and Noboru Takeuchi[b]

[a]*Benemérita Universidad Autónoma de Puebla, Instituto de Física "Ing. Luis Rivera Terrazas"*
[b]*Universidad Nacional Autónoma de México, Centro de Nanociencia y Nanotecnología*
E-mail: guerrero@ifuap.buap.mx

We have performed first principles total energy calculations to study structural and electronic properties of the Sc adsorption and ScN thin film formation on the GaN(0001) surface under both N and Ga rich conditions. The scandium adsorption was studied at high symmetry sites: T4 (hcp), H3 (hollow), Top and Br (bridge). Results show that when the Sc is on top of the surface, T4 site is the most favorable structure, while, if the Sc migrates into the first monolayer to replace a Ga atom, the displaced Ga atom occupies a T4 site (only bonded with Ga atoms). Under Ga-rich conditions the same results are obtained, the Sc atom relaxed on top of the surface shows a T4 site as the most favorable structure. Moreover, if the Sc atom is allowed, it will migrate to the third (from top) Ga layer and it will form a ScN bilayer. For high coverage, formation of three different configurations are possible, a ScN bilayer on the bilayer terminated GaN surface is energetically favorable for N-rich conditions, a ScN bilayer under Ga layer for intermediate conditions is formed and there is formation of ScN bilayer underneath of Ga bilayer under Ga-rich conditions. In all of these three configurations wurtzite like ScN is formed. Density of states shows that the three surfaces are metallic.

Acknowledgments; G.H.C. acknowledges the financial support of VIEP-BUAP, grant 31/EXC/06-G. Cuerpo Académico Física Computacional de la Materia Condensada (BUAP-CA-194). NT thanks DGAPA project IN103512-3 and Conacyt Project 164485 for partial financial support. Calculations were performed at the DGCTIC-UNAM supercomputing center, CNS-IPICYT center and Instituto de Física BUAP.

Effect of manganese doping on barium ferrite and its dielectric behavior

D. K. Tiwari,[a] A. K. Thakur[b]

[a]*Instituto de Física y Matemáticas, Universidad Michoacana de San Nicolás de Hidalgo, Cd. Universitaria, C. P. 58040 Morelia, Michoacán, México.*
[b]*Department of Physics & Meteorology, Indian Institute of Technology (IIT) Kharagpur, West Bengal- 721302, India.*
E-mail: dkt@ifm.umich.mx

The growing demands technology and industrial applications catch the interest of researchers for developing new materials [1, 2] in application to different areas like communications, computations, automations, biomedical, space. Considering the physical parameters (conductivity, permittivity, skin depth and permeability) of the developing material we focused to work with ferrites because of its easy design versatility with many types of material compounds and also installation alternatives. The properties of ferrites are also dominated by chemical composition, crystalline structure, grain size and nature of porosity [1-3].

In this study, series of Ba ferrite ($BaFe_{(2-x)}Mn_xO_4$, at x = 0, 0.2, 0.4 , 0.6, 0.8, 1.0) samples with a substitution of Mn with Fe were prepared by solid state reaction method. The crystalline nature and phase formation were confirmed by XRD measurements. The lattice constant and h, k, l values were obtained using powd software analysis and the prepared material showed the cubic spinel structure. The dielectric behavior of the prepared materials was analyzed using impedance analysis techniques and the dielectric constant with doping concentration of Mn was calculated. The doping of Mn (0 to 1) affects the electrical conductivity of the prepared ferrite materials from $6.08*10^{-5}$ to $1.67*10^{-5}$ S/m respectively. The conductivity range of the prepared material showing the prepared material is semiconducting in nature.

Keywords: Ba-Ferrite, Conductivity, Dielectric constant, Semiconducting materials.

References

1. D. K. Tiwari, L. M. Villaseñor-Cendejas, A. K. Thakur, Magnetic Properties of Nanocrystalline Nickel–Cobalt Ferrites ($Ni_{1/2}Co_{1/2}Fe_2O_4$). Int. J. Thermophys, DOI 10.1007/s10765-013-1438-7 (in Press)
2. Jin-Ho Choy et al. Citrate Route to Ultra-fine Barium Polytitanates with Microwave Dielectric Propertie, J. MATER. CHEM., (1995) 5(l), 57-63
3. Yue Liu et al. Preparation and magnetic properties of barium ferrites substituted with manganese, cobalt, and tin, Journal of Magnetism and Magnetic Materials 323 (2011) 945-953

Synthesis and photoluminescence properties of erbium and yttrium nanoparticles supported on carbon nanotubes by microwave and microemulsion methods

M.J. Anguiano Galicia,[a] J. Lara Romero,[a] S. Jiménez Sandoval[b]

[a]*Facultad de Ingeniería Química, Universidad Michoacana de San Nicolás de Hidalgo, Edificio V1, Ciudad Universitaria, 58060, Morelia, Mich., México*
[b]*Centro de Investigación y de Estudios Avanzados del IPN, Unidad Querétaro, Qro., México.*
Email: paradoja2004@hotmail.com

Erbium and yttrium have unique properties which find extensive application in field emission and photoluminescence applications. Efforts to produce nanoparticles of these metals supported have been reported recently. We present a comparative study between microemulsion method and microwave-assisted method on the decoration of carbon nanotubes with erbium and yttrium nanoparticles. Erbium (III) nitrate pentahydrated and yttrium (III) nitrate hexahydrated were used as metal sources. Dioctil sodium sulfosuccinate (AOT) was used as surfactant. $NaBH_4$ was used as a reducing agent. Multiwalled carbon nanotubes were produced by spray pyrolysis of alpha-pinene and purified by a conventional acidic treatment. The microemulsion method was performed by conventional mixing and heating. Microwave method was performed in a Synthos 3000 microwave reactor. The produced composites were characterized by HRTEM, Raman spectrosocopy, TGA and XRD. The photoluminescence were also evaluated. The results indicate that the microwave method produced smaller and more homogeneously dispersed metal nanoparticles on the surface of the carbon nanotubes than the microemulsion method.

Unique self-assembling biomorphic hierarchic properties of SiO_2-nanostructures

O. Martynyuk,[a,b] N. Bogdanchikova,[a] F. Ruiz,[a] R. Luna V. G.,[c] A. Huerta S.,[a] T. Zepeda,[a]
M. A. Pestryakov[b]

[a] *Centro de Nanociencias y Nanotecnología – UNAM, Ensenada, México*
[b] *Tomsk Polytechnic University, Tomsk, Russia*
[c] *Universidad Autónoma de Baja California, Ensenada, México*
E-mail: oxanam@cnyn.unam.mx

Unexpected unique property of mesoporous hexagonal silica with supported $[Au(C_2N_2H_4)_2]Cl_3$ complex of the formation of self-assembling biomorphic hierarchic nanostructures was observed by HRTEM. It was shown that for SiO_2 three revealed phenomena: self-assembly, biomorphism, and hierarchy take place simultaneously. Observed complex SiO_2 nanostructures were formed from hexagonal mesoporous silica without any template.

Phenomenon of self-assembling of SiO_2 nanounits revealed in our work demonstrates that they can form self-organized structures similar to biological systems (for example, DNA) and opens perspective for creation of new type of biomorphic SiO_2 structures such as toroids, chains, spirals, spheres, sphere chains, loops and their combinations. This unique property of mesoporous silica will be compared with self-assembled SiO_2-carbonate biomorphs.

Cálculo de propiedades ópticas lineales y no lineales en un pozo δ- dopado doble asimétrico en GaAs aplicando un campo eléctrico externo

K. A. Rodríguez-Magdaleno,[a] J. C. Martínez-Orozco,[a] I. Rodríguez-Vargas,[a] C. A. Duque[b]

[a] *Académica de Física, Universidad Autónoma de Zacatecas, Calzada Solidaridad esquina con Paseo la Bufa S/N, CP. 98060, Zacatecas, Zacatecas, México.*
[b] *Instituto de Física, Universidad de Antioquia, AA 1226, Medellín, Colombia.*
E-mail: karelyrod@fisica.uaz.edu.mx

Los pozos δ-dopados (DDQW por sus siglas en inglés) son sistemas de confinamiento cuántico que han atraído mucho la atención desde su propuesta en 1980 por Wood *et al.* [1]. Estos sistemas, consisten en la incorporación de una gran cantidad de impurezas, donoras (*tipo n*) o aceptoras (*tipo p*) en una sola capa de algún material semiconductor. Un modelo de potencial analítico autoconsistente propuesto por Ioratti en 1990 [2] es usado para estudiar este tipo de sistemas. El objetivo del presente trabajo es reportar el estudio de las propiedades electrónicas de sistemas *δ*-dopados dobles tipo *n* en *GaAs*, así como el estudio de algunas propiedades ópticas del sistema basado en la matriz densidad, en particular, el coeficiente de absorción óptica y el cambio relativo del índice de refracción relacionados con las transiciones intersubbanda, exclusivamente con la transición fundamental E_{10}. El estudio de estas propiedades se realiza aplicando un campo eléctrico externo al sistema de estudio. Los resultados obtenidos muestran que la asimetría del sistema, así como el campo eléctrico aplicado da lugar a picos de resonancia bien definidos en los espectros de las propiedades estudiadas.

[1] C. E. C. Wood. G. Metze, J. Berry and L. M. Eastman. J. Appl. Phys. **51**(1), 383 (1980).
[2] L. Ioriatti. Phys. Rev. B. **41**, 8340 (1990).

Nanocellulose extraction from garden waste

R. Salazar,[a] M. Medina,[a] A. Franco[a, b]

[a] *División de Tecnología Ambiental y Nanotecnología, Universidad Tecnológica Fidel Velázquez Ex-Hacienda La Encarnación, Emiliano Zapata s/n, Col. El Tráfico, C.P. 54400; Nicolás Romero, Estado de México, México.*
[b] *Departamento de Estado Sólido, Instituto de Física, Universidad Nacional Autónoma de México Circuito de la Investigación Científica s/n, Ciudad Universitaria, Del. Coyoacán, C.P. 04510; México, D.F., México*
E-mail: rodrigoiq@hotmail.com

The interest on the production of nanocellulose and its technological applications is growing constantly due to the high strength and stiffness, low weight and biodegradability exhibited by cellulose nanostructures. In this work we propose the use of garden waste as an abundant nanocellulose resource. Garden waste from urban areas is constantly increasing and it is usually an underutilized resource because it has not a well defined production function. In comparison with the use of forest residues, garden waste is much more suitable for the nanocellulose extraction because its use does not impact on the balance of natural ecosystems.
We extracted nanocellulose from both green and brown garden waste. The nanocellulose extraction was done by a chemical method, using sulfuric acid as hidrolyzing agent. The final product was obtained in the form of powder, after washing it with distilled water and drying it at 78 °C for 5 Hr. The structural and morphological features corresponding to each one of the nanocellulose samples were studied by Fourier Transform Infrared Spectroscopy (FTIR), X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM); the results are compared and discussed, paying special attention at the differences existing between the nanocellulose samples obtained from each one of the two different waste resources.
The method here proposed for nanocellulose extraction is industrial scalable and enviromentally friendly, it facilitates the use of nanocellulose in biomedical applications, polymer composites and in the pulp and paper industries.

Figure 1: Photography of the as-obtained nanocellulose samples. (a) Nanocellulose obtained from brown garden waste. (b) Nanocellulose obtained from green garden waste.

Estudio de la transmisión, transporte y estructura de niveles de barreras magnéticas en grafeno

V. H. Carrera-Escobedo, J. R. Suárez-López, I. Rodríguez-Vargas

Unidad Académica de Física, Universidad Autónoma de Zacatecas, Calzada Solidaridad Esquina Con Paseo La Bufa S/N, 98060 Zacatecas, Zac., México
E-mail: jrsuarez@fisica.uaz.edu.mx

Los sistemas multibarreras en grafeno están siendo ampliamente estudiados teóricamente dada la variedad de efectos o mecanismos que se pueden emplear para generarlos: campo electrostático, campo magnético, interacción con sustratos, esfuerzos, hidrogenación e iluminación, entre otros. Una de las características más reportada en estos sistemas es la conductancia, en particular el carácter oscilante que ésta presenta independientemente del mecanismo empleado para generar las barreras. Sin embargo, son pocos los trabajos en los cuales se explica el por qué de los picos en la conductancia que dan origen al carácter oscilante de la misma. En un trabajo previo, nosotros encontramos que los picos en la conductancia obedecen a la apertura de canales de conducción o subbandas para el caso de barreras electrostáticas, y a la apertura y cierre de subbandas para el caso de barreras generadas a través de sustratos [1]. Así, la estructura de niveles en grafeno, que hasta ahora ha sido muy poco seguida, es la respuesta a las oscilaciones en los sistemas multibarreras en grafeno. En el presente trabajo ampliamos nuestro estudio en sistemas multibarreras incorporando el efecto de campo magnético aplicado perpendicularmente a la sabana de grafeno para el caso de barreras electrostáticas. Específicamente, hemos considerado el caso de un potencial vectorial tipo escalón, el cual da origen a barreras magnéticas deltaicas. Nuestros resultados arrojan un par de picos en la conductancia, para parámetros típicos, en ausencia de campo magnético. Estos picos presentan un corrimiento al rojo y al azul, respectivamente, una vez que el campo magnético es incorporado. Los corrimientos mencionados los hemos podido explicar estudiando las particularidades de la estructura de niveles del presente caso.

References

[1] I. Rodríguez-Vargas, J. Madrigal-Melchor, O. Oubram, J. Appl. Phys. 112, 073711 (2012).

Strontium aluminates ($SrAl_2O_4:Eu^{2+}$, $Dy3^{+}$) nanopowders by combustion synthesis, thermal and optical stimulated luminescence studies

N. J. Zúñiga,[1,2a] M.Barboza-Flores,[2b] R.García,[2c] R.Melendrez,[2d]

[1]*Centro de Investigación en Materiales Avanzados CIMAV. Maestría en Ciencias de Materiales. Chihuahua, Chihuahua, 31109, México.*
[2]*Departamento de Investigación en Física, Universidad de Sonora, Hermosillo, Sonora, 83000, México.*
E-mail: [a]amatizta082@hotmail.com ,[b] mbarboza@cajeme.cifus.uson.mx ,[c] rgarcia@cajeme.cifus.uson.mx ,[d] rodrigo@cifus.uson.mx

Los aluminatos conocidos como fósforos que poseen propiedades físicas y químicas únicas en su clase, comúnmente son obtenidos a altas temperaturas por calcinación de los precursores que rondan entre 1000 °C y 1300°C en un tiempo de 10 a 14 horas en equipos que conservan sistemas controlados. En este trabajo se logró obtener aluminato de estroncio dopado con Europio y Disprosio ($SrAl_2O_4:Eu^{2+},Dy^{3+}$) vía combustión con carbohidrazida. Se obtuvo una serie donde varía la cantidad de combustible la cual va en aumento en un 10% en exceso (1M-6M). DRX muestra la presencia de $SrAl_2O_4$ a partir de la muestra 4M. Aluminatos excitados con 280 y 370 nm muestran FL debida a Eu^{+2} a partir de la muestra 5M y más intensa en la 6M. MEB muestra fisuras, vacios y poros debidos al escape de gases en la reacción, disminución de partícula conforme aumenta la cantidad de combustible y la formación de una semicristalinidad. ATG muestra poca perdida de % peso de la muestra 6M hasta 1400°C dado a un comportamiento cerámico. En Termoluminiscencia (TL), Afterglow (AG), y Luminiscencia Ópticamente Estimulada (OSL), obtenemos una mejor intensidad en señal en las muestra 5M, además de tener un comportamiento lineal con la dosis de irradiación beta en el rango de 0 hasta los 5.64 Gy. En todos los casos, se observa que existen dos bandas anchas de TL, que pueden tener dos o más picos, cada una de estas. La banda de baja temperatura esta en el rango de 50 a 160 °C y la de alta temperatura está en el rango de 160 a 300 °C. Con los resultados preliminares podemos concluir que los materiales de aluminatos de estroncio perteneciente a 5M tienen una mayor intensidad en su señal de TL, AG y OSL, que les posibilita para posibles aplicaciones en señalizaciones aplicaciones en pinturas luminiscentes entre otros. Por otro lado, tienen una buena respuesta con dosis de irradiación beta en el rango de 0 a 5.64 Gy, el cual puede tener aplicaciones en dosimetría ambiental, personal y medicina nuclear.

Propiedades ópticas lineales y no lineales en un pozo δ-dopado doble asimétrico con barrera de Schottky en GaAs

J. G. Rojas-Briseño,[a] J. C. Martínez-Orozco,[a] I. Rodríguez-Vargas,[a] C. A. Duque[b]

[a] *Unidad Académica de Física, Universidad Autónoma de Zacatecas, Calzada Solidaridad esquina con Paseo a la Bufa S/N, CP. 98060, Zacatecas, Zacatecas, México.*
[b] *Instituto de Física, Universidad de Antioquia, AA 1226, Medellín, Colombia.*
E-mail: jgrojas@fisica.uaz.edu.mx

Los dispositivos semiconductores han sido mejorados gracias al uso del dopaje tipo delta de impurezas debido a la gran cantidad de portadores de carga que proveen al sistema. La primera propuesta de un dispositivo consistió de pozo *δ*-dopado con una barrera de Schottky en la terminal puerta en un transistor efecto de campo (FET) [1]. En este trabajo reportamos el espectro de niveles de energía para un pozo *δ*-dopado doble con barrera de Schottky en una matriz de Arseniuro de Galio (GaAs) tomando en cuenta los efectos de canje y correlación. Además de considerar la aproximación óptica lineal, también consideramos la corrección de tercer orden del coeficiente de absorción y el cambio relativo del índice de refracción. Estas propiedades son reportadas como función de la altura de la barrera de Schottky, la distancia de separación entre los pozos *δ*-dopados y además de considerar los efectos de presión hidrostática aplicada al sistema. Los resultados obtenidos muestran que la magnitud de la intensidad de los picos resonantes son controlados por la asimetría del sistema. Dichos resultados son importantes para su aplicación en dispositivos optoelectrónicos tales como dispositivos fotodetectores.

[1] E. F. Schubert and K. Ploog. Jpn. J. Appl. Phys. **24**(8), L608 (1985).

Ruptura de simetría de la perovskita $La_{0.7}Sr_{0.3}Cr_{0.4}Mn_{0.6}O_{3-\delta}$ como material anódico para una SOFC

J. Alvarado-Flores,[a, b] L. Ávalos-Rodríguez,[c] A. Reyes-Rojas[d]

[a]*Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México*
Circuito Exterior, Ciudad Universitaria, Coyoacán, 04510, México, D.F.
[b]*Escuela Nacional de Estudios Superiores*
Antigua carretera a Pátzcuaro No 8701, Col. Ex Hacienda de San José de la Huerta,
CP. 58190, Morelia, Michoacán, México.
[c]*Universidad Michoacana de San Nicolás de Hidalgo, Facultad de Ingeniería Eléctrica,*
Santiago Tapia 403 Morelia, Michoacán, México.
[d]*Centro de Investigación en Materiales Avanzados S.C. (CIMAV)*
Complejo Industrial Chihuahua, Cd. de Chihuahua, Chihuahua, México.
E-mail: cedhryck@hotmail.com

Esta investigación se enfoca en la síntesis y caracterización de ánodos tipo perovskita $La_{0.7}Sr_{0.3}Cr_{0.4}Mn_{0.6}O_{3-\delta}$ con adiciones de níquel para su aplicación en Celdas de Combustible de Óxido Sólido (SOFC). El análisis de la transformación de los óxidos tipo $La_{0.7}Sr_{0.3}Cr_{0.4}Mn_{0.6}O_{3-\delta}$-NiO al compuesto $La_{0.7}Sr_{0.3}Cr_{0.4}Mn_{0.6}O_{3-\delta}$-Ni, se realizó mediante pruebas de reactividad química y composición de fase. Los polvos se obtuvieron a través del método sol-gel, utilizando alcohol polivinílico como precursor orgánico para obtener un electrodo cerámico poroso, después de sinterizarlos a 1365°C y reducirlos en hidrógeno a 800°C y 1050°C por 8 horas en un horno tubular horizontal bajo una atmósfera de 10%H_2-90%N_2. Los cerámicos resultantes conteniendo de 25 a 75% en peso de Ni, se prensaron, obtiéndose discos con un diámetro de 10 mm. Se realizó un análisis estructural a través de SEM, y XRD en alta temperatura. Los resultados identificaron y confirmaron la ruptura de simetría, debido a la transición de fase en alta temperatura, lo cual puede ser producido por la introducción de cationes Ni^{+2} en la estructura de la perovskita en solución sólida. El análisis morfológico mostró que las partículas con estructura perovskita están alrededor de las partículas de NiO. Las observaciones concuerdan con el comportamiento de la cinética del proceso de reducción, debido a que existen partículas que obstruyen la perovskita.

Hydrogen sorption and evolution reaction on Au-Pd core-shell nanoparticles

A.M. Velázquez Orozco,[a] Y.A. Leon Nataret,[a] M. G. Montes de Oca Yemha,[b] M. A. Romero Romo,[b] T. de J. Licona-Sánchez,[b] M. E. Palomar Pardavé [b]

[a]*Universidad Politécnica del Valle de México, Tultitlan, Estado de México, C. P. 54910*
[b]*Universidad Autónoma Metropolitana-Azcapotzalco. Departamento de Materiales. Av. San Pablo 180, Col. Reynosa-Tamaulipas, C.P. 02200, México, D.F., México.*
e-mail: mepp@correo.azc.uam.mx

Au-Pd core-shell (CS) nanoparticles (NPs) have been studied for by their high catalytic activity for hydrogen sorption (adsorption and absorption) and evolution reaction, which are important in the generation of clean energy. In this work, the catalytic activity of Au-Pd CS NPs supported on carbon Vulcan XC-72R is evaluated for hydrogen sorption and evolution reaction by the electrochemical response. The Pd shell thicknesses from 1 to 10 nm (Figure 1A) were obtained on Au nanoparticles with a diameter of 19 nm by the chemical reduction of Pd precursor with ascorbic acid. Glassy carbon is used as the working electrode modified with the Au-Pd CS NPs. The HER is analyzed by the electrochemical responses obtained from cyclic voltammograms at different cathodic limits (Figure 1B) in acid solution. Electrochemical parameters, *i.e.* the exchange current density (j_0) and energy transfer coefficient (α), were obtained to rationalize the catalytic activity of Au-Pd CS NPs. The electrochemical results demonstrated that the parameters of HER are modified by the Pd shell thickness.

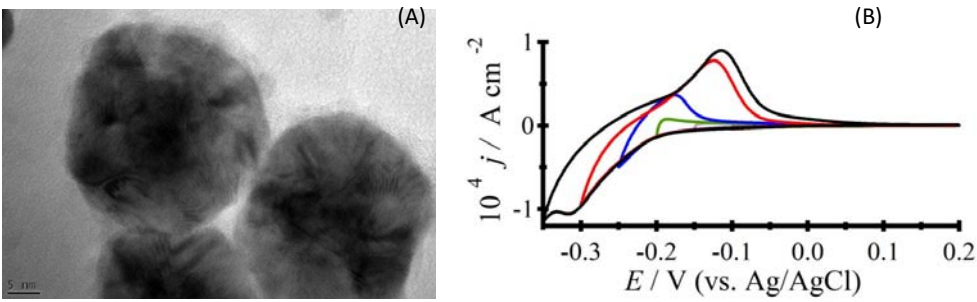


Figure 1: TEM image (A) and cyclic voltammetries (CV) in 0.5 mol dm^{-3} H_2SO_4 at different cathodic limits (B) of 20Au-80Pd core-shell nanoparticles on carbon Vulcan.

Synthetic chemical synthesis of hematite substituted aluminum by sol-gel route

N.N. Zurita-Méndez, M.A. Espinosa-Medina, G. Carbajal-De la Torre, A.B. Martinez-Valencia

Facultad de Ingeniería Mecánica, Universidad Michoacana de San Nicolás de Hidalgo
Santiago Tapia 403, C.P. 58000; Morelia, Michoacán, México
Email: maresmed@gmail.com

The sol gel process is method used to produce coatings, powders with homogeneous nanostructure at low temperatures, with look out properties like resistance, porosity and chemical durability [1]. With nanotechnology advances, functional metal oxides [2] have been of high interest in technological applications, as: microelectronic circuits, sensors, fuel cells, coatings, and catalysts [3]. Also binary oxides M_2O_3 [4,5] as hematite α-Fe_2O_3 which had been of interest in both electro and magnetorheological fluid applications. In this work, synthetic hematite with isomorphically substituted aluminum (Al) contents were obtained by the sol-gel chemical synthesis. Nanomaterials with Fe, Al contains were prepared by the sol gel route by mixing stoichiometric mixtures of ferric chloride ($FeCl_3$) and aluminum isopropoxide ($Al(OC_3H_7)_3$) by sol-gel. The resulting sol was then dried at 60ºC followed by calcinations at 400ºC and 1100ºC. The resulting powders were characterized by X-Ray diffraction analysis and Scanning Electron Microscopy. Results showed a α-Fe_2O_3 powder structure Al_3Fe5O_{12} cubic structure; that is suggested as a promising nanoinductor application.

Keywords: sol gel, X-Ray diffraction (XRD), nanostructures

References

[1] "Proceso Sol-Gel" Laboratorio de Nanotecnología. Universidad Autonoma Metropolitana.
[2] S.S. Shinde et al. "Physical properties of hematite α-Fe_2O_3 thin films: application to photoelectrochemical solar cells". Journal of Semiconductors. Vol. 32. 2011.
[3] M. Fernández-García. "Metal Oxide Nanoparticles" Brookhaven National Laboratory. N.Y. 2007.
[4] V.M. Aroutiounian et al. "Photoelectrochemistry of semiconductor electrodes made of solid solutions in the system Fe_2O_3-Nb_2O_5". Solar Energy, 2006
[5] N. Yahya, R. Al-Habashi et al. "Synthesis of $Al_3Fe_5O_{12}$ Cubic Structure by Extremly Low Sintering Temperature of Sol Gel Technique". American J. of Engineering and Applied Sciences 2 (1): 76-79, 2009.

Modulation of the optical absorption coefficients in δ-MIGFET transistor in GaAs by means of contact voltage and an applied electric field

O. Oubram, L. Cisneros-Villalobos

Facultad de Ciencias Químicas e Ingeniería, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Col. Chamilpa, CP 62209, Cuernavaca, Morelos, México.
E-mail: oubram@uaem.mx

The effects of an applied electrical field and contact voltage on subband structure and optical transitions in GaAs δ-MIGFET (delta- Multiple Independent Gate Field Effect Transistor) are theoretically studied. The electronic structure of delta-MIGFET under an applied electrical field and contact voltage is determined by solving the Schrodinger equation. From calculations, it is found that the subband energies and intersubband optical absorption are quite sensitive to the applied electrical field and contact voltage. These give a new degree of freedom in various device applications based on the intersubband and play an important role in the optical absorption coefficients in a delta-MIGFET.

Oxidación de CO a CO_2 mediante el uso de catalizadores heterogéneos de Ti/TiO_2 impregnados con oro

R. Arreola-Sánchez, J. A. García-Macedo, A. González-Millán, A. Franco

Departamento de Estado Sólido, Instituto de Física, Universidad Nacional Autónoma de México, Circuito Exterior Cd. Universitaria Coyoacán. México, D.F., 04510, México,
Tel. (5255) 56225103; Fax (5255) 56161535
E-mail: arreola@fisica.unam.mx

Se sintetizó, por medio del método sol-gel, un soporte para un catalizador de $Au/Ti/TiO_2$ con 1.5% de Au [1]. La preparación del catalizador de oro se realizó por la técnica depósito-precipitación, utilizando urea como agente precipitante, lo cual permitió obtener una alta homogeneidad en el tamaño de las partículas de oro [2]. La actividad del catalizador se evaluó mediante la reacción de oxidación de CO a CO_2. Se estudiaron las propiedades estructurales y superficiales, mediante las técnicas de microscopia SEM, TEM, área BET, DRX y XPS.

Los resultados correspondientes a la actividad catalítica muestran que estos materiales son capaces de alcanzar un 50% de conversión de CO a CO_2 a una temperatura de 96°C, y una conversión del 100% a una temperatura de 215°C. Adicionalmente, se observó que este tipo de catalizador muestra una actividad estable de CO a CO_2 durante un período de 160 días (Figura 1).

a) b)

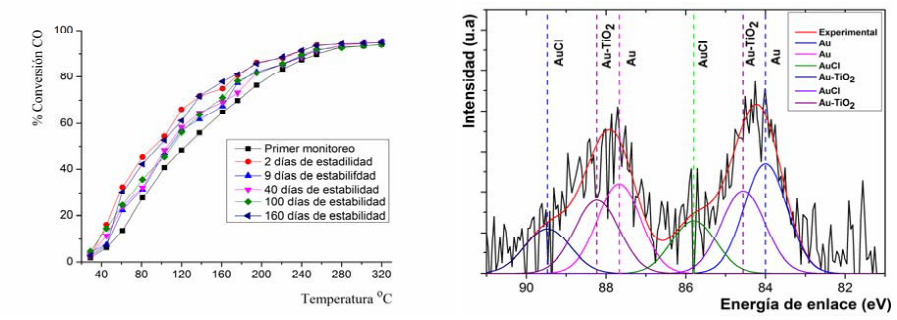


Figura 1:a) Conversión de CO a CO_2, b) Perfiles de XPS para catalizador de Au 4f.

[1] Haruta, M. 2004. Gold as a Novel Catalyst in the 21st Century: Preparation, Working Mechanismand Applications. Gold Bulletin., **37**, 1-2.
[2] Zanella, R. 2005. Mechanism of deposition of gold during the preparation by deposition-precipitation with NaOH and urea. Applied Catalysis A., **291**, 62-72.

Modeling of the surface passivation and size effects on the optical vibrational modes of Ge nanostructures

A. Trejo, M. Ojeda, M. Cruz-Irisson

Instituto Politécnico Nacional-ESIME Culhuacan,
Av. Santa Anna 1000, C. P. 04430 D. F., México
E-mail: atrejob0800@ipn.mx

Recently, semiconductor nanostructures have received great attention in the photovoltaics field because of their potential applications as back side reflectors for light confinement in thin film solar cells. Especially, Germanium (Ge) nanostructures like porous Germanium (pGe) and Germanium nanowires (GeNWs) are attractive for the higher electron mobility of Ge with respect of Silicon which make them suitable for applications such as in biological sensing, optoelectronics, electrochemistry materials, and solar cells. However there have only been a few theoretical works, which try to characterize the vibrational properties of these materials, which are important because many of its properties that can be understood in terms of phonons such as the Raman scattering and infrared response. The vibrational dispersion relations of pGe and GeNWs were calculated using the ab initio density functional perturbation theory with the generalized gradient approximation using norm-conserving pseudopotentials. The germanium nanostructures were modeled using the supercell technique [1-2]. To address the difference in the confinement between the pores and the nanowires, we calculated the vibrational density of states of the two materials. The results indicate that there is a slight shift in the highest optical modes in the frequency interval with mainly Ge contribution to the vibrational spectrum in all of the nanostructures due to the phonon confinement effects. Low diameter GeNWs exhibit a reduced phonon confinement compared with highly porous Ge with a similar confinement distance, due to the mixed Ge-dihydride vibrational modes around the maximum bulk Ge optical mode of approximately 300 cm^{-1}; however, the general effects of such confinements could still be noticed, such as the shift to lower frequencies of the highest optical mode belonging to the Ge vibrations.

References:

[1] A. Trejo, J. L. Cuevas, R. Vázquez, M. Cruz-Irisson, *Microelectron. Eng*. **90**, 141 (2012).
[2] J. L. Cuevas, A. Trejo, M. Calvino, E. Carvajal, *Appl. Surf. Sci*. **258,** 8360 (2013.)

Acknowledgments
This work was supported from Secretaría de Ciencia Tecnología e Innovación del Distrito Federal (SECITIDF) by projects ICyTDF/PICSO12-085, ICyTDF/325/2011 and multidisciplinary project 2012-1439 from SIP-Instituto Politécnico Nacional.

Surface modifications effects on the electronic band gap of porous β-SiC from density functional calculations

M. Calvino,[a] A. Trejo,[a] M.I. Iturríos,[b] M. C. Crisóstomo,[b] M. Cruz-Irisson[a]

[a] *Instituto Politécnico Nacional, ESIME-Culhuacan*
Av. Santa Ana 1000, C.P. 04430; D.F., México.
[b] *Instituto Politécnico Nacional, CECyT-Narciso Bassols García*
Av. de las Granjas 618, C.P. 02530; D.F., México.
E-mail: mcalvino@ipn.mx

Nanostructured materials like porous semiconductors have enormous surface area, which leads to significantly enhanced surface reactivity, compared to bulk crystals. Particularly porous cubic SiC (β-pSiC) has some potential applications as fast response hydrogen sensors. Hence surface passivation is vital for most applications. Motivated by the recent studies and experimental development on the synthesis and characterization on pSiC, the effects of different chemical passivation agent, on the structure and electronic properties of pSiC by means of density functional theory (DFT) and the supercell technique [1,2] were analyzed. In particular, we have used a revised version of Perdew, Burke, and Ernzerhof (RPBE) exchange-correlation functional, based on the pseudopotential plane-wave approach. The effects of the porosity and the surface chemistry composition on the energetic stability of pSiC were also investigated. The porous structures were modeled by removing atoms of an otherwise perfect SiC crystal in the [001] direction producing two different surface chemistries, one fully composed of silicon atoms and one composed of only carbon atoms. The changes in the electronic states of the porous structures as a function of the oxygen (O), hydroxyl (OH), fluorine (F) content at the surface were studied. The results show that the pore surface chemistry greatly influences the behavior of the electronic properties of these structures; for instance, in the hydrogenated case a C-rich configuration creates larger electronic band gaps than the Si-rich case. The changes of the band gap that arise due to surface pore chemistries leads to the possibility of band gap engineering [3].

References

[1] Cuevas J.L., Trejo A., Calvino M., Carvajal E., Cruz-Irisson M., *Appl. Surf. Sci.* **258**, 8360 (2012).
[2] Trejo A., Calvino M., Ramos E., Cruz-Irisson M., *Nanoscale Res. Lett.* **7**, 471 (2012).
[3] M. Calvino, A. Trejo, J.L. Cuevas, E. Carvajal, G.I. Duchén, M. Cruz-Irisson, *Mater. Sci. Eng. B*. **177**, 1482 (2012).

Acknowledgments

This work was supported from Secretaría de Ciencia Tecnología e Innovación del Distrito Federal (SECITIDF) by projects ICyTDF/PICSO12-085, ICyTDF/325/2011 and multidisciplinary project 2012-1439 from SIP-Instituto Politécnico Nacional.

Estudio de propiedades ópticas de nanopartículas de plata mediante el método FDTD

José Antonio Robledo Torres,[a, b] Juan Martín Montejano-Carrizales,[b] José Manuel Nápoles Duarte,[c] José Luis Rodríguez-López[a]

[a]*División de Materiales Avanzados*
Instituto Potosino de Investigación Científica y Tecnológica. A.C.
[b]*Instituto de Física*
Universidad Autónoma de San Luis Potosí
[c]*Facultad de Ciencias Químicas*
Universidad Autónoma de Chihuahua
E-mail: pepetoni.robledo@gmail.com

Todos los fenómenos relacionados con campos electromagnéticos son correctamente descritos por la teoría desarrollada por James Clerk Maxwell en 1873, donde se conectan y formulan matemáticamente las leyes conocidas de Gauss, Faraday y Ampere, confirmando así, la naturaleza ondulatoria de la luz que se propaga tanto en el vacío como en medios materiales.

La teoría de Drude esta basada en un modelo conocido como gas de electrones libres y nos permite estudiar ciertas propiedades físicas de los metales; esta teoria nos proporciona una función dieléctrica la cual podemos introducir en las ecuaciones de Maxwell para estudiar la interacción entre los metales y la luz, esto con el objetivo particular de estudiar el acoplamiento u oscilacion en fase de todos los electrones libres de conducción (Modelo de Drude) con el Campo Eléctrico de la Luz, fenómeno conocido como Plasmón Superficial.

Una herramienta que nos permite resolver las ecuaciones de Maxwell dependientes del tiempo de forma numérica, es el metodo de Diferencias Finitas en el Dominio del Tiempo (FDTD, por sus siglas en Inglés). Este método ha sido ampliamente utilizado en diversos campos de investigación en ingeniería, tales como el eléctrico, el militar, en sistemas de telecomunicaciones, etc.; y más recientemente en el estudio de nanoestructuras metálicas, el cual es nuestro caso de estudio.

Complementamos el método FDTD con la implementación de condiciones de frontera absorbentes, como son las capas perfectamente adaptadas (PML, por sus siglas en Inglés). Se presentan los resultados del algoritmo desarrollado para partículas individuales de plata con diferente morfología (geometrías elementales) y tamaño (nanómetros) en una (1D) y dos (2D) dimensiones.

Agradecimientos: Al CONACYT por la beca de maestría, el apoyo institucional del IPICYT, y al proyecto SEP-2008-106437.

Study of the behavior of the nano γ-alumina powders during microwave sintering

A.Arellano Lara,[a] J.Lemus Ruiz,[a] L.Olmos[b]

[a]*IIM, Universidad Michoacana de San Nicolás de Hidalgo, Edificio "U" Ciudad Universitaria, J. Mujica s/n, Morelia, Michoacán, C.P. 58700, México*
[b]*Coordinación de la investigación científica CIC, Universidad Michoacana de San Nicolás de Hidalgo Edificio "C-2" Ciudad Universitaria J. Mujica s/n, Morelia, Michoacán, CP 58700, México*
E-mail: flychena@gmail.com

Sintering is used to consolidate a mass of powders throughout exchange of matter between particles at temperatures under the melting point by using different diffusion mechanisms. Sintering is a process strongly influenced by the powders characteristics, like size and shape of particles, chemical composition and green packing. Particularly, the behavior of nanoparticles during sintering is different compared to micro-particles because they have higher energy due to its size. Thus, different diffusion mechanisms could appear during nano-sintering enhancing the grain growth in consequence the nanostructure is lost. Additionally the non-thermodynamically stable powders, induces an excessive grain growth because the transition of phases. Therefore is important to control the phase transition conditions in order to assess the optimal parameters to obtain nanostructured bulk materials. The aim of this work is study the evolution of the alumina transition nano-powders during the microwave sintering. To achieve our goal, spherical γ-alumina powders TAEMICRON with an average of 50 nm were used. Powders were isostatically pressed by using an isostatic press with mobile box fabricated by AVURE. The green density obtained by this procedure ranged between 0.48 and 0.5. Then the compacts were sintering in a typical unimodal microwave furnace with a 2.5 GHz frequency. Sintering was carried out under air atmosphere at temperatures between 1100 and 1500°C with a heating rate of 100 y 200°C/min with a sintering plateau of 5 minutes. The relative density of the compacts was estimated by Arquimidez before and after sintering. The evolution of the phase transitions was followed by DSC/TGA experiments between 800 and 1500°C. Right after, the actual existent phases were confirmed by XRD experiments. Finally the samples were cut and polished in order to observe the microstructure with the aid of SEM. We found 4 different transition phases from the gibbsite to the corundum which is the stable phase. We assessed the temperature for each one of those phases which ranged between 750-1100°C. It was found that -alumina can reduce the grain growth. Secondary phases were obtained by microwave sintering when 100°C/min or higher heating rates were used. We found that increasing the heating rate helps to the control of θ-alumina. However the relative density is lower than that obtained with lower heating rates. The final grain size after sintering was 500 nm for samples with density higher than 90%. We conclude that microwave sintering allows enhancing the properties of the bulk nanomaterials.

Microstructural studies of HDS catalytic nanomaterials

E. M. Rivera-Muñoz,[a] R. Huirache-Acuña,[b] R. Nava,[c] C.V. Loricera,[d] B. Pawelec[d]

[a] *Centro de Física Aplicada y Tecnología Avanzada, Universidad Nacional Autónoma de México, A.P. 1-1010 Querétaro, Qro. C.P. 76000, Mexico*
[b] *Facultad de Ingeniería Química, Universidad Michoacana de San Nicolás de Hidalgo, Ciudad Universitaria, Morelia, 58060, México.*
[c] *Facultad de Ingeniería, Universidad Autónoma de Querétaro, Centro Universitario, Cerro de las campanas, 76000, Querétaro, Mexico*
[d] *Instituto de Catálisis y Petroleoquímica, CSIC, c/ Marie Curie, 2, Cantoblanco, 28049 Madrid, Spain*
E-mail: emrivera@fata.unam.mx

Mesoporous materials (SBA-15 and SBA-16) were used as supports of novel ternary Co(Ni)-Mo-W hydrodesulphurization (HDS) catalysts. These materials have shown a high catalytic activity in HDS of dibenzothiophene (DBT) reactions, even much higher compared with commercial catalysts. An exploration was made on the structure of both the supports as well as on tri-metallic sulfide HDS catalysts prepared by simultaneous impregnation via incipient wetness method.

Since it has been found that both the morphology of the supports, as its modification with varying amounts of phosphorus, affect the catalytic activity of the materials in HDS of DBT reactions, the present work shows the microstructural study of these nanostructured materials, obtained from HRTEM images and X-ray diffraction analysis.

Authors acknowledge the support of Dr. Beatríz Millán Malo for XRD analysis as well as the financial support of DGAPA-UNAM PAPIIT IN107311 project, CONACYT, CIC-UMSNH and PROMEP PTC 273 Project.

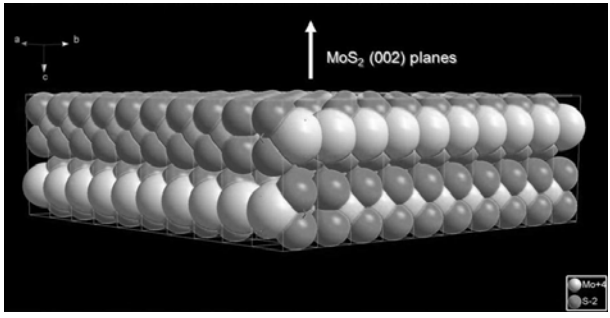


Figure 1: Structural simulation of the growth of nanosized MoS2 in [002] direction.

Functionalization of polyurethane for bone graft substitutes

A. B. Martínez-Valencia, [1]G. Carbajal-De la Torre, [2]H. E. Esparza-Ponce

[1]*Facultad de Ingeniería Mecánica, Universidad Michoacana de San Nicolás de Hidalgo UMSNH, Santiago Tapia 403. Centro C.P. 58000. Morelia, Michoacán, México*
[2]*Centro de Investigación en Materiales Avanzados CIMAV, Ave. Miguel de Cervantes 120 C.P. 31109, Complejo Industrial Chihuahua, Chihuahua, México.*
E-mail: anitvalencia@gmail.com

Recently, a promising issue is the functionalization of polymeric materials either during the step-growth polymerization or afterwards, to generating materials with additional properties that are not characteristic of the starting macromolecules.

Polyurethanes (PUs) are a class of polymer materials with excellent mechanical properties and good biocompatibility, and have found a position in biomedical applications mainly because of their interesting mechanical properties rather than for their biological response. For example many biomedical applications are involved among which coating materials for breast implants, pacemaker leads, catheters, and prosthetic valve leaflets. The PUs are generally prepared from three materials; a diisocyanate, a chain extender and a macrodiol.

In the present study PU/hydroxyapatite composites were produced by a two-step polymerization method using hexamethylenediisocyanate (HDI), Polycaprolactone (PLC) and Butanediol (BD). The hydroxyapatite (HA) was added *in situ* during the polymerization reaction with different contents (0, 10, 20 wt%) to functionalize polyurethane and promote formation of bone-like apatite on its surface, which is essential requirement for an bioactive artificial material. This *in vivo* apatite formation can be reproduced in a simulated body fluid (SBF) with ion concentrations nearly equal to those of human blood plasma. The formation of bone-like apatite microstructure was corroborated by X-Ray Diffraction (XRD), Fourier transformed infrared spectroscopy (FTIR) and Scanning Electron Microscopy (SEM). The obtained materials showed different behavior during the bioactivity test, and the study revealed the fact that composite exhibits advantages compared with pure polyurethane.

[1] P. Vermette, H.J. Griesser, G. Laroche y R. Guidoin, "Biomedical Applications of Polyurethanes", *Landes Bioscience*, 2001.
[2] D. Fournier, B. G. De Geest, F. E. Du Prez, "On-demand click functionalization of polyurethane films and foams", Polymer 50(2009)5362–5367.

Estudio de materiales vitrocerámicos luminiscentes

A. García Murillo, Felipe de J. Carrillo Romo, Angel de J. Morales Ramírez, Luz Carrera Jota, J. Torres Rodríguez

Instituto Politécnico Nacional – CIITEC Azcapotzalco
Cerrada de Cecati S/N Col. Santa Catarina Azcapotzalco, C.P. 02250; D. F., México.
E-mail: jorge62442@gmail.com

Recientemente, existe un gran interés de activar (dopar) óxidos cerámicos con iones de tierras raras para el desarrollo de nuevos dispositivos ópticos. En este ámbito, el desarrollo de nuevos dispositivos ópticos está estrechamente relacionado con el diseño, desarrollo y fabricación de recubrimientos ópticos de alta calidad. Materiales como Lu_2O_3, Y_2O_3 y $BaTiO_3$ dopados con tierras raras como el Europio III, son excelentes candidatos debido a las propiedades luminiscentes que le confiere el ion dopante. Una forma de mejorar dichas propiedades, además de reducir costos, ha sido incorporar una parte vítrea a los sistemas cerámicos para incrementar las propiedades emisivas.

En el presente trabajo, se describe la síntesis de polvos de los sistemas Y_2O_3: Eu^{3+} @SiO_2 y $BaTiO_3$:Eu^{3+}@SiO_2, Lu_2O_3:Eu^{3+}@SiO_2 y $GdPO_4$:Eu^{3+}@SiO_2 sintetizados por los método sol – gel y solvotermal, en donde se ha variado el porciento molar de la sílice. Los materiales así obtenidos son analizados estructural (DRX, IR), química (FT IR), morfológicamente (MEB) y espectroscópicamente (pruebas de absorción y emisión).

Los resultados muestran que los sistemas Y_2O_3: Eu^{3+} @SiO_2 y Lu_2O_3:Eu^{3+}@SiO_2 las partículas obtenidas presentaron fase cúbica, mientras que el $BaTiO_3$:Eu^{3+}@SiO_2 y el $GdPO_4$:Eu^{3+} @SiO_2 presentaron fases tetragonal y monoclínica respectivamente.

Los estudios de fotoluminiscencia mostraron que la formación del vitrocerámico (adición de sílice) tiene por efecto incrementar la emisión luminiscente en todos los sistemas.

A case report of esophagogastric adenocarcinomatreated with Pt-TiO_2 nanoparticles

T. López,[a,b,c] S. León-Carballo,[d] M. Alvarez[b]

[a] Depto. de Atención a la Salud, Universidad Autónoma Metropolitana-Xochimilco, Calz. Del Hueso 1100, Col. Villa Quietud, 04960, Tlalpan, México, D. F.
[b] Nanotechnology Laboratory, National Institute of Neurology and Neurosurgery, "M.V.S" Insurgentes Sur 3877, Col. La Fama, C. P. 14269, Tlalpan, México, D. F
[c] Department of Chemical and Biomolecules Engineering, Tulane. University New Orleans, LA 70118 USA
[d] Universidad Autónoma de Chiapas, Boulevard Belisario Domínguez, kilometro 1081, Sin Número, Terán Tuxtla Gutiérrez, Chiapas, 29050,México,.
[e] ISSTECh, Libramiento Norte Oriente y Blvd. Fidel Velázquez S/n, Col. Infonavit Grijalva Tuxtla Gutiérrez, Chiapas, México
E-mail: tessy3@prodigy.net.mx

Cancer has become one of the main causes of death around the world. Treatment of some types of cancer is difficult because diagnosis techniques are limited. Among all the different cancers, Adenocarcinoma of the esophagogastric junction is not easy to diagnose since commonly, the symptoms are confused with other gastric disorders and the tumor grows obstructing the gastric tube and at this time, the patient is out of treatment. Recently, we report on the in vitro cytotoxicity of Pt-TiO_2nanoparticles and their activity against solid tumors and we developed a clinical trial. $Pt(acac)_2$-TiO_2 nanoparticles were prepared by the sol-gel process. Briefly, acetylacetone was to dissolved $Pt(acac)_2$ in the proper amount to obtain 1% mol of platinum, then was added water (Rw=1:24) and mixed under continuous stirring at 60°C. Later, Titanium butoxide was dropwised to the mixture and kept under reflux and stirring for 24 hr. The sample was dried and milled until an ultrafine powder was obtained. The material was characterized and then tested in different in vivo cancer models where the particles demonstrated significant cytotoxic effect by decreasing the size of treated tumors. A clinical trial is currently undergoing to study bio-safety of these nanoparticles when is administrated in terminal cancer patients. Here we present a clinical case of a 49 years old male, with Adenocarcinoma of the esophagogastric junction diagnosed on March 2011. Endoscopic findings showed esophagus with a cylindrical mass with irregular and friable borders, from 37 cm to 41 cm in the lower third of the esophagus, stomach and retroflexion with tumor mass. The patient was classified as non surgical candidate and ELOXATIN y EPIRUBICINA chemotherapy was prescribed and despite of the treatment, the patient showed no improvement. On April 2012, a first dose of 1 g of nanoparticles was injected directly into the tumor by endoscopic surgery. Three additional applications have been carried out since that date, one dose each two months. After second application, surgery tumor becomes softer and excision of 70% of visible tumor was done. General condition of the patient improves significantly, as he can swallow and is gaining weight. Although to date the tumor has not disappeared, its growth has been slowed allowing the patient a better quality of life.

Clinical case of titanium-based nanoparticles fibrinolytic effect

Tessy López Goërne,[a,b,c] Rubén Argüero Sánchez,[c] Mayra Álvarez Lemus,[b] Francisco Javier González Ruiz[d]

[a] *Depto. de Atención a la Salud, Universidad Autónoma Metropolitana-Xochimilco, Calz. Del Hueso 1100, Col. Villa Quietud, 04960, Tlalpan, México, D. F.*
[b] *Nanotechnology Laboratory, National Institute of Neurology and Neurosurgery, "M.V.S" Insurgentes Sur 3877, Col. La Fama, C. P. 14269, Tlalpan, México, D. F*
[c] *Department of Chemical and Biomolecules Engineering, Tulane. University New Orleans, LA 70118 USA*
[d] *Servicio de Cirugía toráccica y neumología , Hospital General de México O.D.*
[d] *Servicio de Cardiología y Cirugía Cardiotorácica, Jefe de Residentes, H. General de México O.D.*
E-mail: tessy3@prodigy.net.mx

Because of its poor prognosis, Idiopathic Pulmonary Fibrosis (IPF) is one of the most aggressive diseases, even more than some cancers. Characterized by fibroblast proliferation and extracellular matrix accumulation, IPF is a progressive clinical syndrome of unknown etiology and fatal outcome. Nowadays, current therapies are ineffective and are associated with adverse effects. Novel technologies play an important role to develop new strategies for more efficient treatments. In this report, a 75 years old men diagnosed with IPF and out of treatment on January, 2012 was treated with Titanium dioxide nanoparticles. The nanoparticles used in this case, was previously prepared by the sol-gel method, with particle size of 5-10 nm. The particles consist of TiO_2 and Platinum (II) species are dispersed on the surface to be used as an agent to break-down collagen molecules present in fibrosis. Administration was as follow: a homemade nebulizer (Figure 1) was used to deliver the nanoparticles; the air flux was adjusted to 5 L/min, with coordination of the breathing movements of the patient. Previous studies were performed in order to determine that 80% of the nanoparticles are discharged from the device. The patient received 25 discharges one a week, divided in three stages 10-10-5. At the beginning of the treatment the patient referred no changes in O_2 saturation but after 5 applications, the improvement in respiratory performance was substantial, since Six Minute Walk Test (6MWT) significantly improved compared with baseline. Disease was nearly under control during 8 months (more than life expectancy).

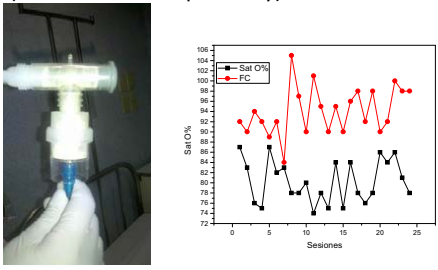


Figure 1: Nebulizer device to deliver nanoparticles and graphic of evolution in heart frequency /O_2 saturation during the treatment

Anticonvulsant effect of clonazepam on the PTZ-induced seizures are improved by solid lipid nanoparticles formulation

Gerardo Leyva-Gómez,[a,c,f] Ma. Eva González-Trujano,[b]* Edith López,[b] Misael González-Ramírez,[d] Pierre-Olivier Couraud,[e] Florence Miller,[f,g] Florence Delie,[f] Eric Allémann,[f] David Quintanar-Guerrero[a]

[a]*Laboratorio de Investigación y Posgrado en Tecnología Farmacéutica, Facultad de Estudios Superiores Cuautitlán, Universidad Nacional Autónoma de México. Av. 1° de Mayo s/n, Campo 1, Cuautitlán Izcalli 54740, Estado de México. México.*
[b]*Dirección de Investigaciones en Neurociencias. Instituto Nacional de Psiquiatría Ramón de la Fuente Muñiz. Calz. México-Xochimilco 101, Col. Sn Lorenzo Huipulco 14370, México, D. F. México.*
[c]*New affiliation: Laboratory of Connective Tissue. Centro Nacional de Investigación y Atención de Quemados, Instituto Nacional de Rehabilitación, México, D.F. México.*
[d]*Unidad de Investigación Médica en Enfermedades Neurológicas, Hospital de Especialidades. CMN S XXI, IMSS. Av. Cuauhtémoc 330, Col. Doctores 06720, México, D.F. México.*
[e]*ICGM, Institut Cochin, 22 rue Méchain, 75014, Paris, France.*
[f]*School of Pharmaceutical Sciences, University of Geneva, University of Lausanne, Quai Ernest Ansermet 30, 1211 Geneva 4, Switzerland.*
[g]*New affiliations: INSERM, unité U1002, Paris, France. Université Paris Descartes, Sorbonne Paris Cité, Faculté de médecine, Paris, France.*
E-mail: gerardoleyva@hotmail.com

The anticonvulsant effect of clonazepam alone (CLZ) and loaded in solid lipid nanoparticles (CLZ-SLN) was compared in the pentylenetetrazole (PTZ)-induced seizures in mice model after oral and/or intraperitoneal (*i.p.*) administration. In order to document the efficiency of CLZ-SLN, the *in vitro* blood - brain barrier (BBB) permeability of the systems has been determined. Furthermore, the behavior and electroencephalograms (EEG) in rats receiving CLZ alone, CLZ-SLN and CLZ in mixed micelles (MM) were studied. The *in vitro* permeability of CLZ was increased when associated with CLZ-SLN, and was decreased in case of MM. The occurrence of myoclonus and generalized seizures, as well as the tonic convulsions induced by PTZ in mice was significantly prevented by CLZ, but also significantly prevented when the same doses of CLZ-SLN were administered via per os (*p.o.*) compared to CLZ in solution. The behavior severity and EEG of the paroxystic activity induced with PTZ in rats were significantly reduced in presence of CLZ alone (0.3 mg/kg) and almost totally prevented in rats receiving the CLZ-SLN (equivalent to 0.3 mg/kg). No difference was observed between CLZ-MM and vehicle on EEG recording. Frequency and duration of the spikes-wave and convulsive behavior was significant reduced with an inhibition on the propagation to the amygdaline central nuclei in rats treated with CLZ-SLN compared to CLZ alone, CLZ-MM or the vehicle. The results of these investigations show an *in vitro* - *in vivo* correlation in enhanced brain permeability of CLZ in CLZ-SLN formulation, and a contribution of CLZ-MM in the carrier effect of drugs to the bloodstream and brain. The results of this study demonstrate that pharmaceutical formulation of CLZ loaded in solid lipid nanoparticles improves the anticonvulsant effect of this benzodiazepine offering further advantage after oral administration.

Antioxidation of human fibroblast by the controlled release of ferulic acid from a hybrid hydrotalcite

Gerardo Leyva Gómez,[a] Edgar Krötzsch,[a] Jorge Flores,[b] Santana Cruz,[b] Enrique Lima[c]*

[a]*Laboratory of Connective Tissue, Centro Nacional de Investigación y Atención de Quemados, Instituto Nacional de Rehabilitación, México D.F., Mexico.*
[b]*Universidad Autónoma Metropolitana, Azcapotzalco, Av. San Pablo 180, Col. Reynosa Tamaulipas, 02200 México D.F., Mexico.*
[c]*Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Circuito exterior s/n, Cd. Universitaria, Del. Coyoacán, CP 04510, México D. F., Mexico.*
E-mail: gerardoleyva@hotmail.com

Oxidative stress has been implicated in several neurodegenerative disorders such as Alzheimer's disease and vitagenes. In this sense, the use of antioxidants has been recognized as an important counter measure against conditions in which oxidative stress is concerned. This work was started with the goal to show the potential use of ferulic acid (FA), a natural antioxidant, intercalated into a biocompatible ZnAl layered double hydroxide (LDH). The materials were characterized structurally, texturally and morphologically, and then tested in two important applications: On the one hand as drug delivery *in vitro* in a system that mimics a biological condition, on the other hand the material was evaluated as an antioxidant of human fibroblasts in the reduction of the reactive oxygen species. By X-ray diffraction patterns, as a consequence of FA intercalation, the interlayer distance goes up from 8.9 Å for the ZnAl-NO_3 to 14.5 Å. As the layer thickness is 4.3Å, the gallery height in ZnAl-FA becomes 10.2Å, within range that previously has been reported for some phenolic anions. A gallery height of 10.2 Å suggested that FA anions were arranged in the interlayer region as a monolayer with the main axis perpendicular to the layer plane of LDH. FT-IR spectrum of ZnAl-FA hybrid showed the antisymmetric and symmetric stretching modes of carboxylate group at 1592 and 1399 cm^{-1}, respectively, confirming that ferulate anion has been intercalated. ^{27}Al MAS NMR results suggest that relaxing behavior of aluminum in LDH is modified by the presence of the high electronic density coming for FA anions. On the other hand, ^{13}C CP MAS NMR spectra showed that with intercalation, all peak resonances of FA became significantly broader which can be explained by a reduction in the motion of the molecule, which is greatly appreciated in a drug delivery material. In the absence of FA the layered sample is roughed, formed by nanoparticles agglomerated to done particles with "like-stone" morphology, whereas with the FA the particles became smoother with a morphology "rose-petale" because of the memory effect used to prepare the FA containing samples. ZnAl-FA is a prolonged release system that provides more than 98% of the drug after 8 hours, compared to FA diffusion that exhibits it at 2.36 hours. The release of the drug from the matrix occurs through a concentration-dependent diffusion mechanism related to time, together with ion exchange. It was demonstrate the potential use of FA into the LDH as an efficient antioxidant of human fibroblasts. Pure FA as well FA protected by LDH reduced significantly intracellular reactive oxygen species; the diminution of the induced superoxide ion deserve special interest. The antioxidant activity was observed for periods as long as 24 h when FA was protected by LDH.

Interferon®-SBA-15 and Copaxone®-SBA-15 release nanoreservoirs to be used in the treatment of demyelization diseases

E. Ortiz-Islas, T. López, M. López, J. Flores, T. Corona

Instituto Nacional de Neurología y Neurocirugía "MVS"
Insurgentes Sur #3877, Col. La Fama-Tlalpan, 14269, México, D. F.
E-mail: emma170@hotmail.com

Interferon® and copaxone®, which are two commercial drugs used to treat demyelinating diseases like to multiple sclerosis, were loaded in ordered mesoporous silica materials (SBA-15) with the aim to obtaining controlled drug release systems. For this purpose, each drug was adsorbed in the material using the impregnation process. The resulted materials were named as SBA 15-CPX and SBA 15-INT, and they were characterized by several physic-chemical techniques such as Infrared spectroscopy, electronic microscopic, N_2 adsorption-desorption and X-ray diffraction, among others. An "*in vitro*" drug release test was made using an aqueous release medium. The drug released amount was determined by ultraviolet spectroscopy monitoring the increment of the maximum intensity of the band at 334 nm. The characterization's results from X ray diffraction patterns, electronic microscopy micrographs and N_2 adsorption-desorption isotherms reveled the characteristic features of an ordered mesoporous silica material of the SBA15 type. The surface area and pore volume values for the silica samples containing the drugs were similar; however, both values were approximately 50 % lower than the value of pure silica. This fact suggest us that drug molecules occupied those spaces when were loaded in the material. The drug release profiles showed two release stages, starting with a fast drug release within first hours, continuing with a slow drug release until the end of the test.

Cambio morfológico en el recubrimiento de ZrO_2 sobre la aleación Ti6Al4V para implantes dentales en saliva artificial

M.M. Machado-Lopez, M.E. Contreras-García, M.I. Espítia-Cabrera, M. Espinosa Medina

Instituto de investigaciones metalúrgicas, Universidad Michoacana de San Nicolás de Hidalgo, Santiago Tapia #403, C.P . 58000; Morelia, Michoacan, México.
E-mail: machadolopez23@gmail.com; eucontre@umich.mx; iesumich@yahoo.com.mx; marespmed@gmail.com

El desarrollo de la investigación y la tecnología de los implantes dentales durante las últimas dos décadas ha hecho que la sustitución de los dientes perdidos con implantes endo-óseo y las prótesis implanto soportadas sean las primeras líneas de tratamiento y rehabilitación duradera (1). La aleación Ti-6Al-4V es la más frecuentemente utilizada para biomedicina e implantes dentales. Sin embargo, todavía hay mucho sin resolver sobre el efecto de los componentes de esta aleación; Aunque la aleación Ti-6Al-4V exhibe excelente resistencia a la corrosión, los iones metálicos liberados por la corrosión o procesos de desgaste pueden inducir el aflojamiento aséptico a largo plazo después de la implantación (2). Por lo tanto para evitar daños al organismo causado por los productos de la degradación de la aleación, es necesario recubrirla con un bioceramico inerte como la ZrO_2. Para obtener el sistema ZrO_2/Ti6Al4V para aplicación en implantes dentales, se partió de una solución coloidal de $ZrOCl_2.8H_2O$ empleando la técnica sol-gel, depositando el hidrogel precursor del óxido de zirconio sobre el sustrato de la aleación Ti6Al4V mediante el método de electroforesis. Los recubrimientos fueron tratados térmicamente a 450, 500, 600, 650 y 700°C para su consolidación. Se observó que el recubrimiento 500°C se encontró distribuido en toda la superficie del sustrato con separaciones de la capa superficial de 0.3 µm. Este recubrimiento al estar expuesto por 24 horas en la solución de saliva artificial a 37°C, mostró en su morfología hendiduras en forma de canales microscópicos y de acuerdo al análisis de los valores obtenidos mediante las técnicas electroquímicas de Tafel, Rp y EIE, mostró una barrera protectora para la aleación Ti6Al4V en condiciones fisiológicas, incrementando su resistencia a la corrosión.

[1] ZAID H.BAQAIN, WAEL YOUSEF MOQBEL, FALEH A.SAWAIR, Early dental implant failure: risk factors, British Journal of Oral and Maxillofacial Surgery, ScienceDirect, 2011, 1.
[2] V.A. Alves, R.Q. Reis, I.C.B. Santos, D.G. Souza, T. de F. Gonçalves, M.A. Pereira-da-Silva, A. Rossi, L.A. da Silva, In situ impedance spectroscopy study of the electrochemical corrosion of Ti and Ti–6Al–4V in simulated body fluid at 25 °C and 37 °C, Corrosion Science 51, 2009, 2473.

Nano-$BaFe_{12}O_{19}$ for drug delivery

S. Torres,[a] M.I. Espítia,[b] M.E. Contreras[a]

[a] *Instituto de Investigaciones Metalúrgicas, UMSNH*
[b] *Facultad de ingeniería Química, UMSNH*
[a,b] *General Francisco J. Mújica s/n Felicitas del Rio, C.P. 58030; Morelia, Michoacán de Ocampo*
E-mail: storres_c@hotmail.com

Nowadays, several processing methods and new chemical strategies allow the engineering of new materials for biomedical purposes. In this regard, magnetic nanoparticles, because of their comparable sizes to biological entities and their unique physicochemical properties [1], are certainly the most suspicious material for applications such as cellular labeling, bioassay, magnetic resonance imaging, hyperthermia, and as drug delivery systems [2].
The present paper reports the synthesis of barium hexagonal ferrites ($BaFe_{12}O_{19}$) by sol-gel method via spray dryer (using a Mini-Spray Dryer ADL31 Yamato). The precursors were iron nitrate $Fe(NO_3)_3.9H_2O$, barium carbonate ($BaCO_3$) and tween-20 as a surfactant. All the former reagents were mixed with distilled water and the pH of the suspension was kept at 9 by adding ammonium hydroxide. The suspension was dried. The Drying temperature was 170 ºC under an absolute pressure of $2Kg/cm^2$. It is also reported the structural characterization. The phases and crystalline structures of $BaFe_{12}O_{19}$ powders were identified with X-ray diffraction (XRD) using a SIEMENS D-500 diffractometer with a Cu Kα radiation (45 kV, 30 mA). It was obtained XRD patterns for $BaFe_{12}O_{19}$ at several temperatures showing two phases: $BaFe_{12}O_{19}$ hexagonal and $BaFe_2O_4$ orthorhombic phase. Scans were made from 10 º to 70 º (2θ) with a constant step width of 0.02 º. The particle size and morphology of synthesized particles were examined with scanning electron microscopy (SEM) (JEOL JSM-6400). It was obtained nanostructured spherical aggregates of $BaFe_{12}O_{19}$ formed by nanoparticles.

[1] Changfa Guo et al, Materials Characterization 62 (2011) 148–151
[2] Caroline de Montferrand *et al*, Acta Biomaterialia 9 (2013) 6150–615

Photocatalytic degradation of trimethoprim by metallic nanoparticles supported on TiO_2 P25

Rodolfo Zanella,[a] Socorro Oros-Ruiz,[a] Blanca Prado[b]

[a] *Centro de Ciencias Aplicadas y Desarrollo Tecnológico, UNAM, Mexico City, Mexico*
[b] *Instituto de Geología, UNAM, Mexico City, Mexico*
E-mail: rodolfo.zanella@ccadet.unam.mx

The presence of pharmaceutical residues in waste waters, as same as their effects on aquatic life and human health have been widely reported for several decades as potentially harmful for living ecosystems. The presence of analgesics, antibiotics, antiepileptics, hormones and many other pharmaceutical products have been reported to cause perturbations to human health and ecosystems. Trimethoprim usually combined with sulfamethoxazole has been widely used for humans and animals since 1968. Its medical use but also the presence of low concentrations in the environment has generated bacterial resistance towards this drug. The advanced oxidation technologies, such as photocatalysis have become an attractive alternative for water decontamination. TiO_2 is one of the most preferred materials for photocatalytic applications since it is stable to photocorrosion, possess strong oxidizing properties of organic pollutants, hidrophilicity, chemical stability, non toxicity and low cost. The photochemical degradation of trimethoprim has been documented in natural conditions in water, under visible and UV light; and also using TiO_2 as a photocatalyst. In this work, it is proposed the photodegradation of trimethoprim by using TiO_2-P25 modified by different metallic noble and non noble nanoparticles supported on this semiconductor, increasing effectively the mineralization extent of the pollutant. It is shown that the use of metallic nanoparticles brings important benefits to the activity of bare TiO_2.

The deposition of gold, copper and nickel on TiO_2-P25 was made by the deposition-precipitation method using urea. The deposition of silver was carried out by deposition-precipitation using NaOH (DPN). The photocatalysts were characterized by TPR, XRD, UV-Vis diffuse reflectance, TEM, ICP and EDS spectroscopy. The evaluation of the photoactivity was followed by UV-Vis spectroscopy and TOC. The photocatalysts were evaluated in the photodegradation of an aqueous solution of trimethoprim (Aldrich 98 %) with a concentration of 40 ppm. The reaction was carried at 25 °C. At the center of the reactor of 250 mL, a lamp UV-Vis UV-PC of primary emission at 254 nm contained in a quartz tube is immersed to perform the photocatalytic reaction. The mass of catalyst was 250 mg.

The photodegradation of trimethoprim was performed in conditions of natural pH=6. All the samples evaluated contained the same metal loadings and practically the same particle sizes. The photolysis presented a degradation of about 20% of trimethoprim after 300 minutes under illumination; the phototocatalyst used as reference (TiO_2-P25) mineralized up to 54% of the organic matter present in the solution. The samples containing Au or Ag nanoparticles increased the activity of TiO_2-P25 and the mineralization to 80%. The kinetic parameters for the degradation of trimethoprim were obtained by following the total organic carbon concentration; the reaction follows a kinetic of order 1. It is observed that all the TiO_2 materials modified by metallic noble and non noble nanoparticles presented a higher activity in the following order $Au/TiO_2 \approx Ag/TiO_2 > Cu/TiO_2 > Ni/TiO_2 > TiO_2$ P25 [1].

[1] S. Oros-Ruiz, R. Zanella, B. Prado **J. Hazard. Mater.** (2013), doi: 10.1016/j.jhazmat.2013.04.010

Simultaneous H_2S removal of biogas by $Ca(OH)_2$ nanoparticles

Martínez M. A. C., [a] Talamantes M. N. J.,[a] Apipilhuasco G. C., [b] Mejía R. N.P., [b] Mojica J., [b] R. Nava, [a] and Villatoro M. W.R. [a]

[a] *Universidad Autónoma de Querétaro. Campus Aeropuerto. Carretera a Chichimequillas Ejido Bolaños, Querétaro, Qro. México, 76140.*
[b] *Sustentabilidad en Energía y Medio Ambiente S.A. de C.V. Río Lerma 196 BIS Primer Piso, Del., Cuauhtemoc, México D.F. 06500.*
E-mail: amartinezmaciel@gmail.com

The main aim in this project is that cellulose acetate membrane (CAM) with $Ca(OH)_2$ nanoparticles, could be improved in an anaerobic digester (AD), in order to obtain pure methane from biogas. It is known that cellulose acetate membrane[1], reacts with H_2S and CO_2 molecules, acting as a hydrophobic nanoporous membrane.
Starting with organic food waste, obtained mainly from restaurant consortia, an AD was developed.
In these preliminary results, a specific process was developed in order to generate enough H_2S. In order to achieve enough H_2S it is used sulfuric acid and sodium sulfide, but in the this case sodium sulfide is incremented for produce por H_2S, so it could be able to be used in the testing of $Ca(OH)_2$ nanoparticles sulfidation. The change of color, reveals the effectiveness of the reaction.
The next step is to evaluate the physical properties of $Ca(OH)_2$ and its stability in other mesoporous materials, in order to use them as functionalized filters.
Now at days the environment is an important topic, many strategies are being investigated in order to innovate with technologies. Nanotechnology is not the exception; catalysis is especially involved in this area.

[1] Ryckebosch, E., Drouillon M., Vervaeren H. Techniques for transformation of biogas to biomethane. Biomass and bioenergy. 2011. 35: 1633-1645

Microwave-assisted synthesis of metal nanoparticles supported on carbon nanotubes

J. Lara-Romero,[a] J. López-Tinoco,[a] M. Anguiano-Valencia,[a] J. Hernández-Vargas,[a]
F. Paraguay Delgado,[b] S. Jiménez Sandoval[c]

[a]*Facultad de Ingeniería Química, Universidad Michoacana de San Nicolás de Hidalgo, Edificio V1, Ciudad Universitaria, 58060, Morelia, Mich., México*
[b]*Centro de Investigación en Materiales Avanzados, Unidad Chihuahua, Chihuahua, México.*
[c]*Centro de Investigación y de Estudios Avanzados del IPN, Unidad Querétaro, Qro., México*
Email: jlara_romero@hotmail.com, lararom@umich.mx

Nanocompsites of carbon nanotube and metal/metal oxides are of great interest in areas such as nanoelectronics, biosensor, catalysis, etc. Due to this diverse set of applications, different methods have been developed to produce these materials (wet-chemical, self-assembly, electrodeposition, physical vapor deposition and microwave methods among others).

In microwave-assisted deposition, the carbon nanotubes are exposed to microwaves and carboxylic groups are generated on the surface of the tubes, followed by the reduction of metal ions on the sidewalls of the carbon nanotubes. This method offers the advantage of uniform heating of the sample resulting in a better particle size control and distribution of the metallic nanoparticles produced. The use of surfactants as stabilizers is an important parameter to achieve uniform distribution and particle size of the metallic particles on the surface of the carbon nanotubes.

In this work, we study the deposition of Ag, Au, Ce, Zr, Er, Yt nanoparticles on multiwalled carbon nanotubes by microwave irradiation. Dioctil sodium sulfosuccinate (AOT) was used as surfactant. $NaBH_4$ was used as a reducing agent. Multiwalled carbon nanotubes were produced by spray pyrolysis of alpha-pinene and purified by a conventional acid treatment. The microwave synthesis was performed in a Synthos 3000 microwave reactor. The produced composites were characterized by HRTEM, Raman spectroscopy, TGA and XRD.

Aplicación de nanopartículas para el control de microorganismos del biodeterioro en monumentos históricos

M.A. Martínez Gómez, M.C. González Chávez, R. Carrillo González

Colegio de Postgraduados Campus Montecillo
km 36.5 Carretera México-Texcoco, C.P. 56230; Texcoco, México.
E-mail: crogelio@colpos.mx

La conservación del patrimonio cultural de edificaciones y bienes inmuebles es transcendental debido a que representa la identidad del pasado; una expresión estética y utilitaria de las diferentes culturas humanas, además son de interés económico y turístico. Sin embargo, hay procesos implicados en el detrimento y desgaste de materiales de construcción. Entre los principales, se considera el biodeterioro debido a que la microflora y organismos en asociación, crecen sobre fachadas, cimientos y monumentos al aire libre, son de difícil control, esto se debe a sus formas de reproducción, colonización, metabolismo con consecuencias destructivas sobre los materiales. Tal es el caso de la solubilización de silicatos, carbonatos, alteraciones por cristalización de sales [1]; presencia de variaciones cromáticas, crecimiento de microorganismos heterótrofos e inclusive plantas [2].

El uso de nanopartículas (NPs) dentro del campo de la conservación [3] es una alternativa novedosa y eficaz. La obtención de NPs mediante biosíntesis con extractos acuosos de vegetales es un proceso amigable con el ambiente y con amplias ventajas químicas. Lo anterior, probablemente a que los extractos funcionan como agentes inductores de la síntesis de NPs, confiriéndoles estabilidad y durabilidad durante periodos más prolongado. Las NPs de biosíntesis presentan características específicas que les permiten interactuar con los microorganismos que colonizan las superficies rocosas. Tal es el caso de las NPs de plata que desencadenan mecanismos de inhibición microbiana importantes en el control biológico.
Existen escasos estudios sobre la aplicación de NPs en el control de microorganismos del biodeterioro. Sin embargo, resulta esencial no sólo evaluar el efecto inhibitorio de las NPs sobre los microorganismos que crecen sobre los materiales, sino también considerar la estabilidad y comportamiento de las NPs sobre diferentes sustratos. La evaluación del efecto inhibitorio de las NPs sobre el crecimiento de algunos organismos que causan el deterioro se discute en este trabajo.

Agradecimientos. Se reconoce el apoyo otorgado por la LPI 16 del CP para este proyecto.

Referencias

1. CANEVA, G.; NUGAR, M.; SALVADORI, O. **La biología en la restauración**. Segunda edición. ed. Sevilla: Nerea, 2000.
2. PÁRAMO, L.; NARVÁEZ, J. Aislamiento e identificación de microorganismos en biopelículas provenientes del Castillo de Chapultepec, Ciudad de México. **Nexo, Revista Científica**, v. 24, n. 02, p. 83-91, 2011.
3. GÓMEZ-VILLALBA, L. Nanopartículas para la conservación del patrimonio. In: GÓMEZ-VILLALBA, L. S. **La conservación de los geomateriales utilizados en el patrimonio**. Madrid: Instituto de Geociencias (CSIC-USM), 2011.

Síntesis y caracterización de recubrimientos de titania-alúmina sobre sustrato de vidrio para aplicaciones en procesos de oxidación avanzada

F. Magaña-Arreola,[a] I. Espítia-Cabrera,[b] M. E. Contreras-García[a]

[a] *Instituto de Investigaciones Metalúrgicas,*
[b] *Facultad de Ingeniería Química, Universidad Michoacana de San Nicolás de Hidalgo, C.U. Edificio "U", C.P. 58000, Morelia, Michoacán, México.*
E-mail: fco.imt@gmail.com

La contaminación del agua, causada por químicos usados por la industria y agricultura es un grave problema. Por lo que es necesario el desarrollo de métodos altamente eficientes para la eliminación de contaminantes [1]. El uso de tecnologías de oxidación avanzada se plantea como solución única para la destrucción de moléculas contaminantes en efluentes de aguas tratadas para poder hacerlas aptas para su descarga en ríos y lagos asegurando que éstas no sean dañinas para los seres vivos y aún para poder considerar el consumo humano. El dióxido de titanio (TiO_2) es uno de los materiales cerámicos semiconductores más usados para varias aplicaciones, ya que posee alto índice de refracción, estabilidad química y costo de producción significativamente bajo. La fotocatálisis es una prometedora tecnología para la purificación de aguas residuales pre-tratadas y no biodegradables, ya que el radical hidroxilo es una de las principales especies responsables de la inactivación de microorganismos [2].

El recubrimiento de dos sistemas: TiO_2-100% y Ti-Al10, fue obtenido mediante, el proceso sol gel siendo este una ruta química que, consiste en la preparación de soles sometidos a hidrólisis y policondensación de derivados metalorgánicos en soluciones alcohólicas, el tamaño de las partículas suspendidas en la suspensión coloidal (sol) son del orden de 1–100 nm. El solvente se le extrae al gel simplemente dejándolo reposar a temperatura ambiente durante un periodo de tiempo llamado envejecimiento, en el cual el gel se encogerá expulsando el solvente y agua residual, dejando una estructura abierta con porosidad nanométrica. Una vez obtenido el gel se continuó con la depositación del mismo, sobre la fibra vidrio usando la técnica de inmersión [3]. Los recubrimientos fueron calcinados a 500°C. Se caracterizaron los sistemas TiO_2-100% y Ti-Al10. Para ello se empleó Difracción de rayos X, Microscopia electrónica de barrido y BET.

1. Castro AL, Nunes MR, Carvalho AP, Costa FM, Flor MH, "Synthesis of anatase TiO2 nanoparticles with high temperature stability and photocatalytic activity," Solid State Sciences, V. 10, No. 5. 2008, pp. 602-6.
2. Byrne JA, Ibañez PAF, Dunlop PSM, Alrousan DMA, Hamilton JWJ, "Photocatalytic Enhancement for Solar Disinfection of Water," Photoenergy, V. 2011.
3. Merino MRP, "*Propiedades ópticas de películas compósitos TiO2:Co2+, TiO2:Er3+ y TiO2:Eu3+ crecidas mediante Sol-Gel*," Book *Propiedades ópticas de películas compósitos TiO2:Co2+, TiO2:Er3+ y TiO2:Eu3+ crecidas mediante Sol-Gel*, Editor, ed.^eds., Universidad Autonoma Metropolitana Iztapalapa, City, 2003, pp.

Theoretical study of electronic and mechanical properties of SiC nanowires grown along [001]

F. Salazar Posadas,[a] L. A. Pérez López[b]

[a] *Instituto Politécnico Nacional, ESIME-Culhuacan*
Av. Santa Ana 1000, 04430 D.F. México
[b] *Instituto de Física, Universidad Nacional Autónoma de México*
Apartado Postal 20-364, C.P. 01000, México D.F., México
E-mail: Fsalazar.Posadas@gmail.com, lperez@fisica.unam.mx

In this work, we present a density functional study of the electronic band gap and the Young's modulus of hydrogen passivated silicon carbide (SiC) nanowires with diamond structure and grown along the [001] crystallographic direction. The study is performed for nanowires with different diameters and with substitutional impurities, where one surface carbon (C) atom is replaced by a boron (B) one. Four diameters were studied (3.57, 5.72, 7.76 and 9.97 Angstroms) with boron concentrations of 4.8%, 2.2%, 1.3% and 0.8 % with respect to the number of atoms in the corresponding unit cell. The results show that the electronic band gap of nanowires with boron atoms diminishes when the diameter increases and it is smaller than the band gap of the pure hydrogen passivated SiC nanowire with the same diameter. On the other hand, the Young's modulus of the boron-doped nanowires show a similar behavior than the pure hydrogen passivated SiC nanowires. This result indicates that the surface boron atoms with the considered concentrations do not affect the Young's modulus of the passivated [001] SiC nanowires. Then, the band gap could be reduced without affecting the mechanical properties of the nanowire.

Acknowledgments:
This work was supported by Secretaría de Ciencia Tecnología e Innovación del Distrito Federal (SECITIDF), projects ICyTDF/PICSO12-085, ICyTDF/325/2011, multidisciplinary project 2012-1439 from SIP-Instituto Politécnico Nacional and DGAPA-UNAM IN102511.

Effects of metal transition substitution on the crystal structure, electric and magnetic properties of $Ru_{0.9}M_{0.1}Sr_2GdCu_2O_8$ (M = Zr, Nb, Mo, Mn, Co and Fe)

M. Abatal,[a] V.García-Vázquez,[b] R. Valenzuela,[c] G. González,[c] I. Alfonso[a]

[a] *Facultad de Ingeniería, UNACAR, C.P. 24180, Ciudad del Carmen, Campeche, México*
[b] *Instituto de Física LRT, Benemérita Universidad Autónoma de Puebla, A. P. J-48, Puebla, Pue. C.P. 72570, México.*
[c] *Instituto de Investigaciones de Materiales, UNAM, AP 70-360, C.P. 04510, México D.F., México*
E-mail: mabatal@pampano.unacar.mx

In this work, we report the synthesis, structural, electrical and magnetic properties of $Ru_{0.9}M_{0.1}Sr_2GdCu_2O_8$ with M = Zr, Nb, Mo, Mn, Co and Fe. The samples were synthesized through the solid-state reaction method at ambient pressure, in air, at temperatures between 980 and 1000 °C. X-ray diffraction data indicate that all samples are single phases. Rietveld-Refinement analysis indicates that all compounds have a $RuSr_2GdCu_2O_8$ type a structure of a tetragonal symmetry (space group P4/mmm, no. 123). The Cu-O(1) and Ru-O(1) bond lengths, as well as Cu-O(2)-Cu and Ru-O(2)-Ru bond angles increase with the atomic radius of Zr, Nb, Mo, Mn, Co and Fe. Magnetization measurements show that the exhibit ferromagnetic behavior above 130 K. The electrical resistance measurements show that the samples with M = Zr, Nb, Mo and Fe exhibit a semiconductor-like behavior. Whereas when M= Mn and Co, the compounds show a superconductor behavior. All samples were annealed in flowing oxygen flux at 1050 °C for 5 day.

Density functional theory study of Au_n (n=1–5) clusters supported on montmorillonite

C. Briones-Jurado,[a] P. de la Mora,[b] E. Agacino-Valdés[a]

[a] *Departamento de Ciencias Químicas, Facultad de Estudios Superiores Cuautitlán, UNAM. Av. 1º de Mayo S/N, C.P. 54740; Col. Sta. María de las Torres, Cuautitlán Izcalli, Estado de México. Blvd. Enrique Reyna Hermosillo #140, C.P. 25250; Saltillo, Coahuila, México.*
[b] *Departamento de Física, Facultad de Ciencias, Universidad Nacional Autónoma de México, Av. Universidad 3000 Circuito Exterior S/N, CP 04510 Ciudad Universitaria, Ciudad de México, México*
E-mail: brionesjurado@comunidad.unam.mx

The adsorption and nucleation of gold clusters Au_n (n=1–5) on montmorillonite (MMT) is studied using the density functional theory. All the calculations were performed using the full-potential linearized augmented-plane-wave method as implemented in the WIEN2k code. We constructed a MMT supercell of formula $Si_{16}Al_6Mg_2O_{40}(OH)_8$ containing four unit cells and the first moments of the nucleation process were studied by adding the gold atoms one by one on the MMT. The results show that the interaction energies between the gold clusters and the MMT are negative indicating that the Au_n–MMT complexes are stable. In the Au_n–MMT systems (n= 3–5), two gold atoms maintain the coordination with basal oxygens and the Au-O distance was about 2.0–2.3 Å. The Au-Au average distance is 2.6 Å in the supported gold clusters. The formation of the second layer of gold atoms occurs upon the arrival of the third gold atom. We are reporting that the transition of 2D→3D gold cluster structures is located from Au_3 to Au_4 on MMT. The total density of states of clusters Au, Au_2, Au_3, Au_4, and Au_5 on MMT allows us to affirm that i) gold atoms are the main contributors to the states closest to the Fermi level and ii) in Au_4–MMT and Au_5–MMT systems, the main contributors to the states closest to the Fermi level are the most external gold atoms, and therefore these atoms are probably the most susceptible to interact with adsorbates and the most active sites. Odd–even oscillations in the values of the energy gap and interaction energy were found: the odd-numbered supported clusters, Au_3 and Au_5, have larger energy gaps and more negative interaction energies.

Gold nanoparticles for biomedical applications: carcinogenic cervix tissue

A. Ceja,[a] E. De La Rosa,[a] T. López-Luke,[a] A. Torres-Castro,[b] A. L. González-Yebra,[c]
B. González-Yebra[c]

[a]*Centro de Investigaciones en Óptica, A. C. León, Gto. 37150. México*
[b]*Universidad Autónoma de Nuevo León. Monterrey, N.L. México*
[c]*Facultad de Ciencias Médicas, Universidad de Guanajuato. León, Gto. 37320. México*
E-mail: andreacf@cio.mx, elder@cio.mx

In recent years, there has been increased interest en Nanotechnology, because it permits great versatility and a wide range of uses. In the case of Nanomaterials, they have been used in different research areas, such is the case of medical and biological purposes, this, because it is becoming more necessary the earliest detections of diseases or pathogens. Nanomaterials have been used as Fluorescent biological labels, Bio detection of pathogens, detection of proteins, tissue engineering, to show some examples, however all of this applications depend on their different and specific properties, in this work we present the use of gold nanoparticles as markers in cervix tissue, and we show how their properties, mainly optical ones, are very important depending on what they want for, and for this, it is therefore necessary to have complete control of the synthesis, resulting in obtaining well- defined size and shape.

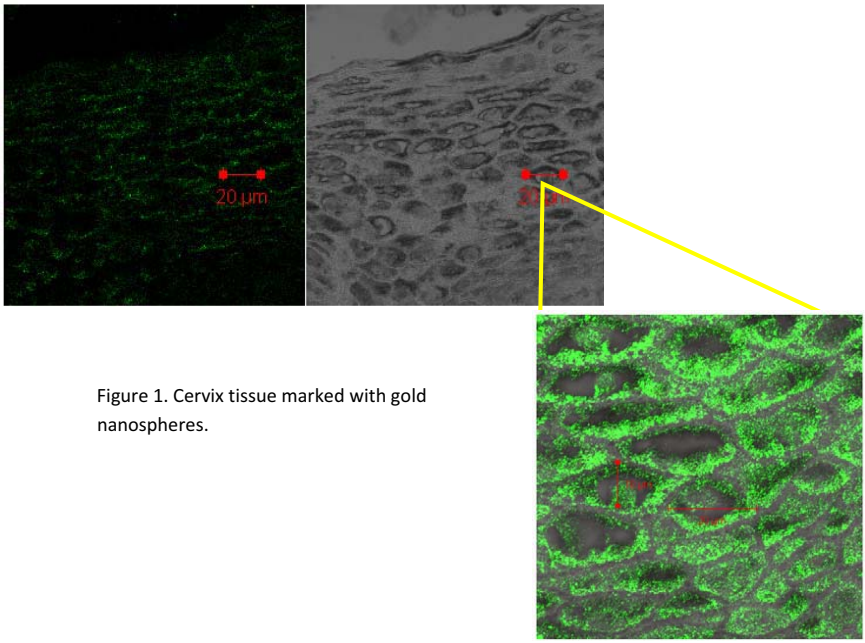


Figure 1. Cervix tissue marked with gold nanospheres.

Preparation of a biocompatible layer on $ZrO_2:Er^{3+}$-Yb^{3+} and $Y_2O_3:Yb^{3+}$-Er^{3+} luminescent nanoparticles for cancer cervix detection

L. A. Martínez,[a, b] T. López-Luke,[a] E. De la Rosa,[a] A. Ceja,[a] R. A. Rodríguez,[b]
A. L. González-Yebra,[c] B. González-Yebra[c]

[a]*Centro de Investigaciones en Óptica, A. P. 1-948, León, Gto., 37150, México*
[b]*Universidad de Guadalajara, Unidad Lagos, Lagos de Moreno Jal. 47460, México*
[c]*Departamento de Ciencias Aplicadas al Trabajo, Universidad de Guanajuato,*
Ave. Eugenio Garza Sada, # 572, Lomas del Campestre, secc II, León, Gto. 37150, México
[d] *Departamento de medicina, Universidad de Guanajuato,*
20 de enero # 929, centro, León, Gto, 37320, México
E-mail: tzarara@cio.mx, luz.andrea.martinez@hotmail.com

Recently, upconversion fluorescence from lanthanide-doped nanocrystals has attracted much attention due to the potential applications as sensitive biolabelings, as improved alternatives to fluorophores and Quantum Dots (QD's). Zirconium and yttrium oxide is an excellent material in photonic applications due to its optical properties and low phonon energy, also can easily be doped with rare earth due to its structure; in this particular case they were doped with ytterbium and erbium. The interest on the rare earth doped nanophosphors is to produce emission in the visible for a width range of application such as solid state lighting, new generation television screen, biomedical diagnostics and photodynamic therapy etc. The main advantage of this approximation is the absence of absorption by tissue avoiding the self-fluorescence. Zirconium oxide nanoparticles doped with lanthanides and functionalized with a thin silica layer will be used with the purpose of allowing the nanoparticles adherence to the tissue though antibodies or proteins added to the shell. The silica shell can prevent possible toxic effects from the nanoparticles and have a surface that facilitates the conjugation with biomolecules.

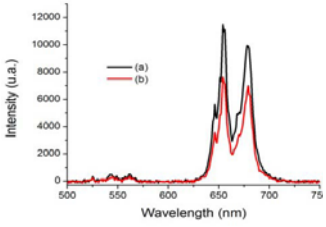


Figure 1: ZrO_2:Yb-Er luminescence nanoparticles a) with biocompatible layer and b) without biocompatible layer.

Non linear dynamics of nanomagnets: Appearance of limit cycles under ferromagnetic resonance conditions

V. L. Villegas Rueda,[a] E. Piña Garza[b] and R. Zamorano Ulloa[a]

[a]*ESFM-IPN, Departamento de Física y Departamento de CM, UPALM-IPN, Av.IPN S/N, S. Pedro Zacatenco, C.P.07738, México D.F.*
[b]*UAM-I, Departamento de Física, Universidad Autónoma Metropolitana – Iztapalapa, P.O. Box 55 534, México, D.F., 09340 México.*
E-mail: veyarle@yahoo.com.mx

The development and the fundamental study of nanomagnetic materials is of great relevance today due to the miniaturizing tendency of the electronics in general and to the potential development of ever larger and larger magnetic memory-capacities. A better understanding of the full dynamics of the magnetization, **m**(t), of a nanomagnet under different excitation schemes is desired in order to develop nanomagnetic devices.

In this work, we focus on the non-linear dynamics of an isotropic, single-domain (nanometric) magnet, **m**(t), under ferromagnetic resonance (FMR) excitation conditions, i.e.; a Zeeman magnetic field, $\mathbf{H}_0$ and a microwave magnetic field, $\mathbf{H}_1$ are applied at 90°. We solve numerically the Landau-Lifshitz [1] equation of motion for **m**(t), while Kittel resonance condition [2] holds. We use standard published FMR parameters for Fe, H_r=2.17KOe and α=0.003. We find that for these kinds of isotropic nanomagnets, obeying simultaneously LL and Kittel equations, there exists a final asymptotic state, **m**(t), which is a limit cycle (θ_{asyn}, ϕ_{asyn}), that is reached in a time, t_{asyn}, shorter than 70ns. In such state, θ_{asyn} is constant and ϕ_{asyn} is linear in time. The dynamics of **m**(t) is pure precession but at an angle, θ_{asyn}, rather large. This dynamics is as described in regular linear treatments of FMR, but we find that θ_{asyn}, can reach values up to θ_{asyn}=21°, far beyond what a perturbation is expected to produce. And quite unexpectedly, the dynamics of **m**(t) in terms of (θ, ϕ) and ($\dot{\theta}$, $\dot{\phi}$) is very complex before reaching the limit cycle.

Under these conditions, the Landau-Lifshitz-damping parameter α, (in our calculations 0.003) strongly affect the onset and radius of these limit cycles. So, the equation of motion for **m**(t) under Kittel´s resonance condition produces limit cycles of pure precesion, and very sensitive to damping. This result agrees with the linear-FMR estimation of pure precession, except that the radius of the limit cycles that are proportional to θ_{asyn} (< = 21°) are far greater than expected from the usual point of view that $\mathbf{H}_1$ plays only a perturbative role.

[1] L. Landau and E. Lifshitz, Physik. Zeits. Sowjetunion **8**, 153, 1935; Reprinted from Phys. Zeitsch. der Sow. 8, pp. 153–169 (1935).
[2] C. Kittel, On the Theory of Ferromagnetic Resonance Absorption, Phys. Rev. **73**, 155, 1948.

Non-reciprocal microwave behavior on magnetic nanowired substrates

J. De la Torre Medina,[a] C. E. Carreón González,[b] G. Hamoir,[c] A. Encinas,[b] L. Piraux,[c] I. Huynen[d]

[a] *Facultad de Ciencias Físico-Matemáticas, Universidad Michoacana de San Nicolás de Hidalgo, Morelia, Mexico*
[b] *Instituto de Física, Universidad Autónoma de San Luis Potosí, Mexico*
[c] *Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium*
[d] *Institute of Information and Communications Technologies, Electronics and Applied Mathematics, Université Catholique de Louvain, Belgium*
E-mail: j.delatorre.medina@gmail.com

Nowadays the growing demand for novel miniaturized and more functional passive non-reciprocal microwave devices has motivated very much research activity around nanotechnology and nanosciences. This has promoted the application of novel structures based on nanocomposite materials, which consist of a very large number of magnetic nano-objects embedded in a porous host matrix with properties that are only characteristic at the nanoscale. For instance, nanocomposites like the so-called magnetic nanowired substrates are self-biased, so the application of an external magnetic field using electromagnets is unnecessary, which in turn lead to a significant miniaturization of potential devices based on these systems [1-3].

In this work we present a study, on one hand, on the realization of magnetic nanowired substrates with specific geometric factors and magnetic properties. This has been achieved by controlling the nanocomposites microstructure by using an electrodeposition technique for obtaining an asymmetrical growth of the nanowires inside a nanoporous template. On the other hand, we present results on the application of magnetic nanowired substrates for obtaining a microwave non-reciprocal behavior, which is observed from the difference between the microwave absorption in the forward and backward directions using a microstrip line geometry. This behavior can be tuned by an adequate choice of the nanowires materials, but also by controlling the nanowire array geometry, which lead to a microwave absorption dependence on the permittivity and permeability of the magnetic nanowired substrate.

References

[1] Catalina E. Carreón-González, et al, *Nanoletters* **11**, 2023 (2011).
[2] Gaël Hamoir, et al, *IEEE Trans. Microw. Theory Tech.* **60**, 2152 (2012).
[3] B. K. Kuanr, et al, *Appl. Phys. Lett.* **94**, 202505 (2009).

Poster Sessions

Thursday 16

Interdisciplinary, inter-institutional and international group "NanoSilver": Application of silver nanoparticles Argovit in biomedicine and veterinary

N. Bogdanchikova,[a] C.A. Almonaci H.,[b] A. Salinas R.,[c] M. Maldonado V.,[d] J. H. Almanza Reyna V.,[e] I. Plascencia L.,[e] A. Pena J.,[f] A. Pestryakov,[g,h] V. Burmistrov,[h] L. García M.,[i] R. Vázquez M.,[j] M. E. Arellano G.,[e] R. L. Vázquez G.,[e] G. Galicia S.,[k] M. Galindo C.,[l] C. Vera H.,[e] B. Ruiz R.,[e] F. Casillas F.,[e] M. I. Montes P.,[e] D. Rodarte V.,[e] O. Martynyuk,[a,g] J. E. Cortés R.,[m] H. Uraga P.,[n] F. A. Rivera A.,[e] E. Castro L.,[e] M Avalos B.,[a] 15, D. A. Camarena P.,[d] G. Aguilar U.,[p] J. R. Chávez M.,[e] J. G. Rodríguez V.,[e] A. Huerta S.,[a] G. Odegova,[k] L. E. Rojas Á.,[q] M. Núñez M.,[r] R. A. Luna V. G.,[s] A. A. Núñez S.[s]

[a]*Centro de Nanociencias y Nanotecnología, UNAM, Ensenada, B.C.*
[b]*Hospital Regional del IMSS, San Quintín, B. C.*
[c]*Comercializadora de Sistemas de Innovación SA de CV (CSI), León, Guanajuato*
[d]*CIATEC, León, Guanajuato*
[e]*Universidad Autónoma de Baja California, campus Tijuana y campus Ensenada, B.C.*
[f]*Hospital Veterinario, Ensenada, B.C.*
[g]*Universidad Politécnico de Tomsk, Tomsk, Rusia*
[h]*Vector-Vita Ltd, Novosibirsk, Rusia*
[i]*Hospital General de las Playas de Rosarito, Rosarito, B.C.*
[j]*Centro de Investigación Científica y Educación Superior de Ensenada, Ensenada, B.C.*
[k]*ISESALUD, de B.C., jurisdicción N 4, San Quintín, B. C.*
[l]*CAAPS, Del. Maniadero Ensenada B.C.*
[m]*Rancho Cortes, Ensenada, B.C.*
[n]*Consejo de Desarrollo e Innovación Tecnológica de Baja California, Ensenada, B.C.*
[o]*Instituto Potosino de Investigación Científica y Tecnológica, San Luis Potosí, S.L.P.*
[p]*Centro Veterinario AGUZVET, Ensenada, B.C.*
[q]*Promoción de la Coordinadora de Fomento al Comercio Exterior, León, Guanajuato*
[r]*Integración y Comercio SA de CV, León, Guanajuato*
[s]*Oficinas Centrales, ISSSTECALI, Mexicali, B.C.*
E-mail: nina@cnyn.unam.mx

A new network "NanoSilver" under the leadership of UNAM, dedicated to application of silver nanoparticles in biomedicine and veterinary has been created in 2012. The network is interdisciplinary, inter-institutional and international. It includes 26 groups, 115 participants from 27 government institutions and 11 private companies of Mexico, Russia, Spain, Puerto Rico and United States. The results obtained by the network are of great impact for public health, especially in the treatment of diabetic foot syndrome, which is a direct consequence of diabetes; the number one cause of death in Mexico. More than 80 amputations have been avoided in patients with legs exhibiting diabetic ulcers, which were recommended for amputation. Amputations were prevented during a clinical study for the treatment of diabetic foot with an innovative product of Argovit silver nanoparticles. Currently, clinical trials in hospitals of ISSTECALI are beginning. Progress in the comprehensive studies of toxicity, geno-toxicity, histological and lethal dose of Argovit in Russia and Mexico shows, that this drug is non-toxic. The development of the new type of footwear with Argovit silver nanoparticles for diabetic foot is one of the main achievements of the group. The use of this innovative product of Argovit silver nanoparticles represents an alternative to the use of antibiotics; whose use and development is currently in a silent crisis. Argovit application in the prevention and treatment of epidemics and pandemics of livestock and poultry is expected to make a great contribution to Mexican economy. Three emerging spin-off companies resulted from the NanoSilver Network and are generating new high level skilled jobs. It is important to mention that number of projects that are developing technologies of high impact grows rapidly, incorporating new universities, institutions and companies.

Vibrational characterization of Si nanowires and the effect of the anisotropy on their radial breathing mode

A. Trejo, L. López, M. Cruz-Irisson

Instituto Politécnico Nacional-ESIME Culhuacan
Av. Santa Anna 1000, C. P. 04430 D. F., México
E-mail: atrejob0800@ipn.mx

Silicon nanowires (SiNWs) are 1-D semiconductor nanostructures that have been extensively studied theoretical and experimentally in the recent years due to their potential applications. For the development of SiNWs technologies is important to have knowledge of the cross section length of the nanowire without altering much its structure. Raman spectroscopy could be a great tool for the characterization of the nanowires through the analysis of one especially interesting phonon mode, which is the so called Radial breathing mode (RBM). This mode has been studied in 1-D nanostructures such as carbon nanotubes which consist on a radial expansion and contraction of the nanotube. The RBM frequency depends on the diameter of the nanotube. SiNWs are also 1-D nanostructures and is expected that a kind of radial breathing could be found in this nanostructures. In this work we study the effect of anisotropy and quantum confinement on the frequency of the optical vibrational modes of Silicon Nanowires, by means of first principles Density Functional Theory approach, using the generalized gradient approximation and the finite displacement algorithm. The nanowires are modeled by removing atoms outside a circumference in the desired growth direction. We compare optical vibrational mode frequencies of SiNWs orientated in three different directions [001], [111] and [110]. The radial breathing mode is identified through the eigenvectors of each vibrational frequency in the Gamma point [1-2] the rest of the vibrational modes is analyzed through partial phonon density of states to identify the main contributors to the phonon vibration at determined frequencies. Results show an inverse power relation between the nanowire diameter and its RBM frequency and a shift to lower frequencies of the highest frequency optical modes probably due to phonon confinement effects. These results could be useful for characterization of the nanowires through Raman spectroscopy techniques.

References:

[1] A. Trejo, R. Vázquez-Medina, G. I. Duchén and M. Cruz-Irisson, *Physica E*, i**n press** (2013), DOI: 10.1016/j.physe.2013.02.006i
[2] A. Trejo, M. Cruz-Irisson, *Molecules* **18**, 4776 (2013)

Acknowledgments

This work was supported from Secretaría de Ciencia Tecnología e Innovación del Distrito Federal (SECITIDF) by projects ICyTDF/PICSO12-085, ICyTDF/325/2011 and multidisciplinary project 2012-1439 from SIP-Instituto Politécnico Nacional.

Magnetic moments in the double perovskites $Sr_2Fe_{1+x}Mo_{1-x}O_6$

J. Pilo,[a] E. Carvajal,[a] R. Oviedo-Roa,[b] M. Cruz-Irisson,[a] O. Navarro[c]

[a] *Escuela Superior de Ingeniería Mecánica y Eléctrica-Culhuacán, Instituto Politécnico Nacional*
Av. Santa Ana 1000, México, D. F., C. P. 04430, México
[b] *Programa de Investigación en Ingeniería Molecular, Instituto Mexicano del Petróleo*
Eje Central Lázaro Cárdenas Norte 152, México, D. F., C. P. 07730, México
[c] *Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México*
A.P. 70-360, México, D. F., C. P. 04510, México
E-mail: jorge.pilo.ipn@gmail.com

It is well known that every double perovskite shows a characteristic magnetic behavior, as a consequence of interactions among the magnetic moments associated with the atoms in their cells; at the same time, the electric and magnetic properties of the bulk double perovskite Sr_2FeMoO_6 are well characterized. In this work we studied the iron rich compounds $Sr_2Fe_{1+x}Mo_{1-x}O_6$, using a supercell to model such concentrations that made Fe richer perovskites by 6.25, 12.5 and 25%. Starting from the stoichiometric double perovskite, and modifying the Fe/Mo ratio in the compound, the study of these materials were based on the calculation of the magnetic moment at each atom, as well as the partial density of states.

Acknowledgements
This work was partially supported by the multidisciplinary project 2012-1439 from SIP-IPN, PIFI-IPN, PICSO12-085 from Instituto de Ciencia y Tecnología del Distrito Federal (ICyTDF) and IN108710 from PAPIIT-UNAM.

Phase transformation of $FeAl_2$ intermetallic induced by ball milling

J. R. Romero-Romero, [a] J. Luis López-Miranda,[b] M. A. Espinosa-Medina,[a] G. Rosas

[a]*Instituto de Investigaciones Metalúrgicas, UMSNH, edificio U., Ciudad Universitaria, Morelia, Mich. 58000, México*
[b]*Facultad de Ingeniería Mecánica, UMSNH, edificio W., Ciudad Universitaria, Morelia, Mich. 58000, México.*
E-mail: ing_roman_romero@hotmail.com

In this study, $FeAl_2$ and Fe_2Al_5 intermetallic alloys were synthesized by conventional cast. In order to study the structural stability during ball milling, these alloys were worked in the mechanical process for 1, 2.5, 5 and 10 h. The mechanical milling processing was carried out using hardened steel vials and balls with a weight to balls ratio of 5.6. The structural and chemical characterizations were conducted by X-ray diffraction, scanning electron microscopy, transmission electron microscopy. After 5h of milling, the experimental results indicated a phase transformation from $FeAl_2$-triclinic phase to Fe_2Al_5-ortorrombic structure [1, 2]. However, after 10h of ball-milling of Fe_2Al_5-ortorrombic phase neither phase transformation was observed. Thus, the milling processes demonstrate that $FeAl_2$ intermetallic had poor thermodynamic stability [3, 4].

References:
1. Luke Luke S.J. Peng and Gary S. Collins. Point defects and the B2 to FCC transformation in milled FeRh. Phase transformations and systems driven far from equilibrium, eds. E. Ma, P. Bellon, M. Atzmon, R. Trivedi, Mat. Res. Soc. Symp. Proc. 481, 631 (1998).
2. S. Shukla a, A. Banas b, R.V. Ramanujan. Atomistic mechanism of cyclic phase transitions in NdeFeeB based intermetallics. Intermetallics 19 (2011) 1265e1273.
3. Gary S. Collins and Praveen Sinha. Atomic defects and disorder in mechanically-milled intermetallic compounds. International Symposium on Mechanically-Alloyed and Nanocrystalline Materials, Quebec, July 1995 (ISMANAM'95), Materials Science Forum 225-227, 275 (1996).
4. Luke S.J. Peng and Gary S. Collins. Disordering of FeAl by mechanical milling. International Symposium on Mechanically-Alloyed and Nanocrystalline Materials, Rome, May 1996. Materials Science Forum 2 35-23 8, 537 (1997).

Sol-gel derived Y_2O_3:Eu^{3+} F127 modified thin films

A. Morales,[a] F. Sarabia,[b] A. García,[a] F. Carrillo,[a] J. Torres,[a] L.Olmos,[b] C. Marin[b]

[a] *CIITEC-IPN. Cerrada CECATI s/n CP 02250. México, DF.*
[b] *ESIQIE-IPN. UPALM s/n CP 07738, México, DF.*
E-mail: amoralesra@ipn.mx

For luminescent applications of thin films, is important to ensure that at least a thickness 1 µm and transparency in order to avoid the light scattering and to obtain a better quality of the formed image. However, despite the sol-gel and the dip-coating technique has been widely used to obtain optical quality thin films due to its high capacity to obtain transparent ceramics deposits, as well as high chemical and physical homogeneity, it is difficult to obtain high value thickness, and therefore it´s not sufficient to fulfill the technical requirements. A possible alternative is to increment the viscosity of the sol in order to minimize the number of coatings and increment the thickness. In this work, a high melting point polymer, pluronic acid F127 has been used. Eu^{3+} doped Y_2O_3 films has been synthetized starting with 2,4 yttrium pentanedionate and europium nitrate as precursors, methanol as solvent and acetic acid as pH modifier. Several Y/F127 relationships have been investigated (0-10). It has been possible to obtain transparent and high optical quality films with the addition of F127 to the sol. The thickness has been increased 3 times with a 2.0 relationship compared with the sample without F127. The XRD shows a perfect C2-type cubic structure, meanwhile m-lines spectroscopy has been used in order to evaluate the optogeometrical parameters. Finally, excitation (λ_{em}=612 nm) and emission (λ_{ex}=254 nm) measurements has been carried out.

Estudio preliminar para la síntesis verde de nanopartículas de plata mediante extracto de A*rbutus cf. bicolor*

J. A. Luna Sánchez, L. García Hernández, D. Arenas Islas, P. A. Ramírez Ortega

Área de Electromecánica Industrial, Universidad Tecnológica de Tulancingo,
Camino a Ahuehuetitla #301 Col. Las Presas, Tulancingo, Hidalgo, México. CP 4364
E-mail: laura.garcía@utec-tgo.edu.mx

En el presente trabajo se analizó la viabilidad de procesos para la síntesis de nanopartículas de plata mediante el empleo de extractos de origen natural, cuyo fin es el reducir el uso de solventes, lo cual conlleve a disminuir el impacto al medio ambiente que estos originan. En trabajos recientes, se ha reportado la síntesis a través de la especie *Arbutus unedo* [1], lo cual da pauta al presente trabajo, en el que se reporta la síntesis de nanopartículas de Ag mediante el uso de la especie *Arbutus cf bicolor* [2], la cual se presenta en la figura 1, dicha especie es típica del estado de Hidalgo, México. La obtención de las partículas se realizó mediante el extracto de la planta, mezclado con una solución 1mM de $AgNO_3$. Es importante mencionar, que la mezcla presentó una aglomeración de partículas de color oscuro, las cuales precipitaron de forma inmediata a la incorporación del $AgNO_3$, las cuales son atribuidas a la reducción de la especie iónica de plata. Con la finalidad de verificar la naturaleza de los precipitados así como determinar la morfología y tamaño de partícula, se efectuó la caracterizaron del extracto mediante IR, la naturaleza, morfología y tamaños se determinó mediante SEM y EDS. Los resultados obtenidos, confirman que en efecto las partículas precipitadas son Ag, y que la morfología tiende a ser esférica y el tamaño de las partículas es nanométrico.

Figura 1.A*rbutus cf bicolor*

Referencias:

[1] *P. Kouvaris, A. Delimitis, V. Zaspalis, D. Papadopoulos, S.A. Tsipas, N. Michailidis, Materials Letters Vol. 76* ***(2012)*** *18–20*

[2] *M. S. González-Elizondo, M. González-Elizondo, P. D. Sørensen, Arbutus Bicolor (Ericaceae, Arbuteae), A New Species From Mexico, Acta Botanica Mexicana, 99:* ***(2012)*** *55-72*

Chemical band gap engineering of H-terminated SiC nanowires: surface dangling bonds and oxygen effects

J. L. Cuevas, A. Trejo, M. Cruz-Irisson

Instituto Politécnico Nacional, ESIME-Culhuacan
Av. Santa Ana 1000, 04430, D.F., México.
E-mail: jcuevasf0600@ipn.mx

In this work, the effects of surface oxygen and dangling bonds in the chemical band gap of cubic silicon nanowires (3C-SiCNWs) are studied. The nanowires are modeled in the [110], [111] direction using the supercell scheme [1-3], where, at a first instance, all surface dangling bonds are passivated with H atoms. In order to study the effect of surface dangling bonds some hydrogen atoms are removed in specific positions along the nanowire surface. To analyze the oxygen effect in the surface of the NWs, two hydrogen atoms are replaced by one oxygen atom creating two types of bridge bonds Si-O-Si and C-O-C for the [110] oriented nanowires while double bonds (Si=O, C=O) are modeled for the [111] direction. Electronic band structure and density of states of the fully and partially saturated 3C-SiCNWs were calculated based on spin polarized density functional theory scheme using the Generalized Gradient Approximation. The exchange correlation functional used was a revised version of the Perdew–Burke–Ernzerhof (RPBE) with ultrasoft Vanderbilt pseudopotentials to describe the core electrons. The results show that for the dangling bond configuration in the [110] nanowire, a different band structure behavior for the two spin channels can be observed when the dangling bond is located in atoms which create a dihydride in the surface. Meanwhile, a similar behavior can be observed when the dangling bonds in the 3C-SiCNWs grown in [111] are created along layers that contain C atoms in the surface. The half metallic nature of these nanowires is still to be addressed, however the results are encouraging towards the magnetic properties engineering of this nanostructure, opening the possibility of implement such nanowires in the spintronics field. Additionally it was observed that the surface O increases the energetic stability in all 3C-SiCNWs compared with the only H-terminated ones.

References:

[1] A. Trejo, J.L. Cuevas, F. Salazar, E. Carvajal, and M. Cruz-Irisson, *J. Mol. Model.*, **19**, 2043 (2013).
[2] A. Trejo, A. Miranda, L. Niño de Rivera, A. Díaz-Méndez, M. Cruz-Irisson, *Microelectron. Eng.* **90,** 92 (2012).
[3] A. Miranda, A. Trejo, E. Canadell, R. Rural, M. Cruz-Irisson, *Physica E* **44**, 1230 (2012).

Acknowledgements

This work was supported from Secretaría de Ciencia Tecnología e Innovación del Distrito Federal (SECITIDF) by projects ICyTDF/PICSO12-085, ICyTDF/325/2011 and multidisciplinary project 2012-1439 from SIP-Instituto Politécnico Nacional.

Evaluación de la reacción de hidrólisis de aluminio para la generación de hidrógeno empleando el intermetálico Fe_2Al_5

J. Luis López-Miranda, G. Rosas

Instituto de Investigaciones Metalúrgicas, Universidad Michoacana de San Nicolás de Hidalgo Edificio U, Ciudad Universitaria, Morelia Michoacán. México. C.P. 58060
E-mail: lopezfim@gmail.com

En este trabajo se reportan los resultados obtenidos de la generación de hidrógeno empleando el compuesto intermetálico Fe_2Al_5 activado mecánicamente. El intermetálico se fabricó por medio de colada convencional a partir de metales con alta pureza, Fe (99.97%) y Al (99.92%). Subsecuentemente, la aleación fue sometida a activación mecánica en un molino de alta energía variando los tiempos en 1, 5 y 10 horas y posteriormente, someterlos a la reacción de generación de hidrógeno. Por otra parte, se emplearon diferentes sustancias (NaOH y CaO) en soluciones acuosas, para incrementar el PH y de esta forma incrementar tanto la velocidad como la cantidad de hidrógeno liberado [1-2]. La reacción de generación de hidrógeno se llevó a cabo colocando los polvos activados en agua desionizada o en la solución correspondiente, evaluando la cantidad de hidrógeno por medio de un sistema de desplazamiento [1-4]. Los resultados indicaron que en la medida que el tiempo de molienda se incrementa una menor liberación de hidrógeno se obtiene; lo anterior debido a la pasivación por la rápida oxidación de los polvos activados [4]. Finalmente, la caracterización de los subproductos sólidos de la reacción se realizó mediante DR-X, MEB y MET y en todos los casos se observó que la fase bayerita es el principal subproducto de la reacción de generación de hidrógeno.

REFERENCIAS

[1] J. Skrovan, A. Alfantazi and T. Troczynski. Enhancing aluminum corrosion in wáter. J Appl Electrochem (2009) 39:1695–1702.

[2] Jorge Macanás, et al. Hydrogen generation by aluminum corrosion in aqueous alkaline solutions of inorganic promoters: The AlHidrox process. Energy, 2011. 36(5): p. 2493-2501.

[3] Manoj Pudukudy, et al., Hydrogen production from sea water using waste aluminium and calcium oxide. International Journal of Hydrogen Energy, 2012. 37(9): p. 7451-7456.

[4] Fan, et al. Study of the controllable reactivity of aluminum alloys and their promising application for hydrogen generation. Energy Conversion and Management, 2010. 51(3): p. 594-599.

Nano hydroxyapatite synthesis by co-precipitation method assisted with microwave

M. Juárez-Raya, A.B. Martínez-Valencia, C. Mendoza-Covarrubias, G. Carbajal de la Torre

Facultad de Ingeniería Mecánica de la Universidad Michoacana de San Nicolás de Hidalgo Santiago Tapia 403. Colonia, Centro. Morelia, Michoacán.
E-mail: ginnadelatorre@gmail.com

Hydroxyapatite is the essential component constituting the mineral matrix of the teeth and bones in the human body by providing rigidity. The stoichiometric formula of synthetic hydroxyapatite is $Ca_{10}(PO_4)_6(OH)_2$ being synthesized and used in various forms (solid and porous) to make various implants and has also been tested as artificial bone because of its similarity with the natural bone [1]. It is important to find new options in conventional synthesis methods for reducing the time of synthesis, obtaining a better structure, crystallinity and smaller particle size, and one of the options was the microwave [2]. In the present study a synthesized hydroxyapatite by a conventional wet method (co-precipitation) and microwave, in order to obtain nanometer particle size, was realized and to show the comparison with the simple and co-precipitation method. The hydroxyapatite was synthesized from calcium hydroxide and phosphoric acid solutions, adjusting the pH between 8.5 and 9. The techniques of X-Ray diffraction and Infrared Spectroscopy were used for the chemical and structural characterization, the morphology was characterized by scanning electron microscopy. This results shown a remarkable difference with co precipitation method in the crystal morphology and size in comparison with the use of microwaves.

References

[1] Farzadi, A., Solati-Hashjin, M., Bakhshi, F., Aminian, A. Synthesis and Characterization of hydroxyapatite/β-tricalcium phosphate nanocomposites using microwave irradiation. Biomaterial group, Faculty of Biomedical Engineering, Amirkabir University of Technology (Tehran Polytechnic), Tehran, 15875-4413 Iran. Available online 22 August 2010

[2] Martinez-Perez, C., Garcia-Casillas, P., Martinez-Villafañe, A., Romero-Garcia, J. Preparación y caracterización de un material compuesto poli(uretano)/hidroxiapatita mediante separación de fases. Departamento de Biomateriales, División de Deterioro de Materiales, Centro de Investigación en Materiales Avanzados S.C. Miguel de Cervantes # 120, Chihuahua, Chih. , México C.P. 31109. Biomecánica, 9 (1), 2001, pp. 39-44

Evaluación mecánica de un compósito con nanotubos de carbono

L. Domratcheva Lvova,[a] A. Gómez Sánchez,[a] F.G. Granados Martínez,[a] N. Flores Ramírez,[a] L. García González,[b] P. González García[b]

[a] *Universidad Michoacana de San Nicolás de Hidalgo, Av. Francisco J. Mujica s/n, Ciudad Universitaria, C.P. 58030, Morelia, Michoacán, México*
[b] *Centro de Investigaciones en Micro y Nanotecnología, Universidad Veracruzana, Calzada Ruiz Cortínes No. 455 Col. Costa Verde C.P. 94294, Boca del Rio, Veracruz, México*
E-mail: lvova@umich.mx

El descubrimiento de nanotubos de carbono por Iijima[1] en 1991 abrió nuevos horizontes para desarrollo de diferentes materiales novedosos con propiedades y posibles aplicaciones extraordinarias gracias a que los nanotubos de carbono tienen propiedades mecánicas, eléctricas, químicas y etc. únicas. Las áreas de su aplicación van desde electrónica, mecánica, química, hasta medicina. En este trabajo se presentan resultados de obtención y de evaluación de propiedades mecánicas de un material compuesto hecho en base a nanotubos de carbono y resina epóxica.

Los nanotubos de carbono fueron obtenidos por deposición química de vapor en un reactor experimental [2] a base de benceno como fuente de carbono y ferroceno como precursor de catalizador, así como también fuente complementario de carbono. Se uso argón como gas transportador y para evitar la combustión. La temperatura de síntesis fue de 850^{o}C, y el tiempo una hora. Como resultado se obtuvieron nanotubos de carbono multicapa con diámetros entre 20 a 100 nm. Fueron caracterizadas con FESEM, XRD y FTIR. El material compuesto fue formado con 3% de nanotubos de carbono en relación con resina epóxica. Las muestras obtenidas fueron curadas y secadas en horno. Después se sometieron a pruebas de dureza Vickers con cargas de 0.1 y 0.05 Kgf. Se observaron valores que fueron mas de 8 veces mayores que la dureza de resina y incluso mayores de dureza de acero 1018.

Se agradece apoyo financiero a la CIC de la UMSNH y a la Red de Colaboración de Cuerpos Académicos “Materiales Nanoestructurados” de PROMEP (SEP).

Referencias:

1. Iijima, S. *Nature*. **1991**, 354, 56.
2. Gómez Sánchez A., Domratcheva Lvova L., López Garza V., Román Doval R., Mondragón Sánchez Ma. de L., *Mater. Res. Soc. Symp. Proc.* 2012, 1479

Estudio de nanomateriales por microscopía electrónica con aberración esférica corregida

R. Esparza,[a] R. Pérez,[a] M. José-Yacamán[b]

[a] *Centro de Física Aplicada y Tecnología Avanzada,*
Universidad Nacional Autónoma de México,
Boulevard Juriquilla 3001, Santiago de Querétaro, Qro., 76230, México.
[b] *Department of Physics and Astronomy, The University of Texas at San Antonio,*
One UTSA Circle, San Antonio, TX 78249, USA.
E-mail: resparza@fata.unam.mx

El estudio de las propiedades de los materiales a escala atómica es un tema clave para la nanotecnología y otros campos de la ciencia de materiales. La microscopía electrónica de transmisión (TEM) y más aún de transmisión/barrido (STEM) son las técnicas más usadas para la caracterización estructural a escala atómica. La principal ventaja de STEM, es que es posible obtener una imagen de contraste por número atómico (contraste Z ó HAADF) que se relaciona a la estructura de la muestra, además de su versatilidad: imágenes y espectroscopía a una escala atómica que pueden ser obtenidas simultáneamente de una región específica del espécimen. Las imágenes de alta resolución de STEM obtenidas con microscopios con aberración esférica (Cs) corregida, permiten a los investigadores de materiales analizar átomo por átomo la estructura de los materiales [1]. En este trabajo se presentan los resultados obtenidos en el estudio de nanomateriales por STEM con Cs-corregida de diferentes tipos de nanomateriales. La figura 1 muestra las imágenes de HAADF-STEM de diferentes muestras. Monocapas de MoS_2, nanopartículas bimetálicas Pt_{core}-Pd_{shell} y finalmente, nanopartículas bimetálicas PtPd del tipo aleación, note el contraste y la resolución alcanzada por el uso de correctores de Cs.

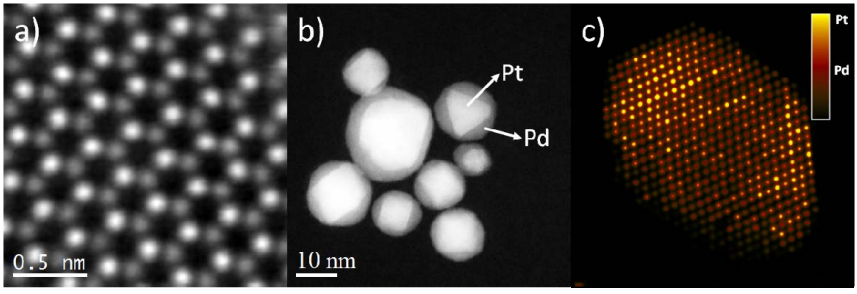


Figura 1:a) Monocapas de MoS2, b) Nanopartículas bimetálicas Pt_{core}-Pd_{shell} y c) Nanopartícula bimetálica PtPd.

Referencias

[1] R. Esparza, Amado F. García-Ruiz, J. J. Velázquez Salazar, R. Pérez and M. Jose-Yacaman, *Journal of Nanoparticle Research* **15**, 1342 (2013).

Linear and nonlinear refractive index changes in δ-MIGFET transistor modulated by contact voltage and Hydrostatic pressure

L. Cisneros-Villalobos, O. Oubram

[a]*Facultad de Ciencias Químicas e Ingeniería, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Col. Chamilpa, CP 62209, Cuernavaca, Morelos, México.*
E-mail: luis.cisneros@uaem.mx

The effect of hydrostatic pressure and contact voltage on the refractive index changes (RIC) are studied in delta-Multiple Independent Gate Field Effect Transistor (delta-MIGFET) in GaAs. We use a theoretical model of low pressure to calculate the electronic structure and RIC. Our results show that the position and the magnitude of the linear, nonlinear and total RIC are sensitive to hydrostatic pressure, voltage contact and bidimensional density. The incident optical intensity has a great effect on these optical quantities.

Fluorescent labeling of amine-functionalized titanium dioxide nanoparticles. Synthesis and characterization

M. Alvarez,[a] R. López,[b] H. Monroy,[c] A. Hernández,[d] T. López[e,a,f]

[a] *Laboratorio de Nanotecnología, Instituto Nacional de Neurología y Neurocirugía, Manuel Velasco Suárez, Insurgentes Sur 3877, Col. La Fama, Tlalpan, CP 14269, México, D.F.*
[b] *Department of Chemistry, Metropolitan Autonomous University Iztapalapa, Av. San Rafael Atlixco 186, Col. Vicentina, Iztapalapa, 09340, México*
[c] *Department of Cell Biology, CINVESTAV-Zacatenco Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco,07360, México D.F.*
[d] *Depto. de Atención a la Salud, Universidad Autónoma Metropolitana-Xochimilco, Calz. Del Hueso 1100, Col. Villa Quietud, 04960, Tlalpan, México, D. F.*
[d] *Lab. de Microscopía Electrónica , Instituto Nacional de Rehabilitacion, Calz. México-Xochimilco 289, Col. Arenal de Guadalupe, Tlalpan, C.P. 14389, México D.F.*
[e] *Department of Chemical and Biomolecular Engineering, Tulane. University New Orleans, LA 70118 USA*
E-mail: myalemus@yahoo.com

Nowadays, Titanium dioxide (TiO_2) nanoparticles are used in a wide variety of products. Because of their unregulated use, scientist are concern about the safety and biosecurity of these nanomaterials. In order to follow up where nanoparticles are located in vivo, fluorescence seems to be a relatively easy and rapid technique. However, binding fluorophores to a specific material requires surface modification of the nanomaterial. Some reports about fluorescent labeling of TiO_2 nanoparticles have been made and the most commonly used molecules are acridine orange or Fluorescein Isothiocyanate (FITC). The last one, is an amine-reactive molecule and is used after modifying TiO_2 with Dopamine [1] or 3-aminopropyl trimethoxysilane [2]. In this research, TiO_2 nanoparticles were functionalized with γ-aminobutyric acid and glutamic acid. The nanoparticles were labeled with FITC and then characterized by FTIR and UV-Visible spectroscopies. In spectroscopic characterization, we observed how the inclusion of FITC molecules modified characteristic spectra of TiO_2, since new bands associated to FITC appeared around 500 nm, while IR middle region showed some bands corresponding to vibrations of the N-C=S bonds. Transmission electron microscopy showed that nanoparticles are conforming clumps of about 20-50 nm. In order to asses labeling, optical fluorescence images were taken. The results prove that two different molecules used, exhibited similar behavior and ability for binding FITC. This fact represents an alternative to effective fluorescent labeling in order to track nanoparticles by optical microscopy.

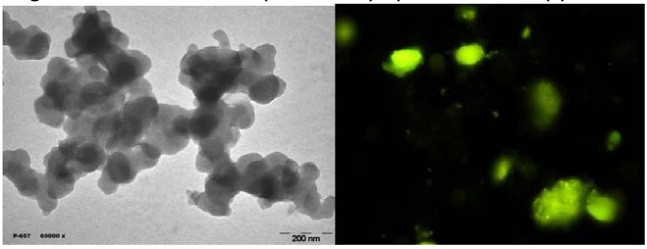


Figure 1: TEM and fluorescence micrographies of TiO_2-GABA nanomaterial

Theoretical approach of the surface effects on the vibrational spectrum of porous SiC

J.S. Sánchez, A. Trejo and M. Cruz-Irisson

Instituto Politécnico Nacional, ESIME-Culhuacan,
Av. Santa Ana 1000, 04430 D.F., México
E-mail: jsanchezh1010@alumno.ipn.mx

In the last years semiconductor nanostructures have attracted great attention because of the enhanced electronic and optical properties. Nanoporous cubic Silicon carbide (pSiC) is of special interest due to its potential applications in optoelectronics, communications and as fast response gas sensors, which can operate on harsh environments of high frequencies and temperatures. On the other hand vibrational properties are of great interest in the characterization of these materials since physical phenomena such as the Raman, IR response and heat conductivity of the material can be understood in terms of phonons. In this work we study the vibrational band structure and density of states of pSiC by means of the ab-initio Density Functional Theory using the generalized gradient approximation with a revised version of Perdew Burke Ernzerhof (RPBE) exchange correlation functional using norm-conserving pseudopotentials. The porous structures were modeled using the supercell scheme [1-3] by removing atoms along the [001] direction of an otherwise perfect SiC crystal, producing different surface chemistries one only with Silicon (Si-rich) and other with Carbon (C-rich) atoms. All surface dangling bonds are saturated with H atoms. The phonon dispersion and density of states were calculated through the finite displacement algorithm. Results show that low porosity structures are unstable since their phonon spectrum has imaginary frequencies that point to a mechanical instability. In the high porosity case only the C-rich structures are structurally stable due to the absence of imaginary frequencies.

References

[1] Cuevas J.L., Trejo A., Calvino M., Carvajal E., Cruz-Irisson M., *Appl. Surf. Sci.* **258**, 8360 (2012).
[2] A. Trejo, A. Miranda, A. Díaz-Méndez, M. Cruz-Irisson, *Microelectron. Eng*. **90**, 92 (2012).
[3] A. Trejo, J.L. Cuevas R. Vázquez-Medina, M. Cruz-Irisson, *Microelectron. Eng.* **90**, 141 (2012).

Acknowledgments

This work was supported from Secretaría de Ciencia Tecnología e Innovación del Distrito Federal (SECITIDF) by projects ICyTDF/PICSO12-085, ICyTDF/325/2011 and multidisciplinary project 2012-1439 from SIP-Instituto Politécnico Nacional.

Surface functionalization with maleic anhydride of titanium dioxide nanoparticles

P.C. Hernández-Del Castillo, [a] S. Robles, [b] F. Ruiz [b,c]

[a] *Doctorado Institucional en Ingeniería y Ciencia de Materiales, UASLP, Av. Salvador Nava S/N, Zona Universitaria, C.P. 78290 San Luis Potosí, S. L. P., Mexico*
[b] *Facultad de Ciencias, UASLP, Álvaro Obregón No. 64, Col. Centro, C.P. 78000 San Luis Potosí, S. L. P., Mexico*
[c] *Centro de Investigación en Materiales Avanzados, S.C. (CIMAV), Miguel de Cervantes 120 Complejo Industrial Chihuahua, México*
E-mail: paveldelcastillo@gmail.com, saulroblesmanuel@aim.com, facundo@fciencias.uaslp.mx

In this work, titanium dioxide (TiO_2) nanoparticles were functionalized with maleic anhydride (MA), the reaction was carried out in toluene as dispersion medium and maintained at constant volume by refluxing. Samples were prepared with different weigth percentages of MA. In the characterization, Infrared Spectroscopy (FT-IR), Differential Scanning Calorimetry (DSC), Differential Thermal Analysis (DTA), X-Rays Photoelectron Spectroscopy (XPS) and BET (Surface Area) were used. Residual reaction products were analyzed by spectroscopy UV-Vis and TOC to determine the amount of unreacted MA. Through the results obtained chemical interaction between the two compounds as well as the adsorption form MA molecule on the surface of TiO_2 were identified. Also, the percentage of functionalization and the reaction efficiency was calculated. MA molecules chemically anchored to TiO_2 by covalent bonds providing the ability to interact chemically with organic materials to be applied in the fabrication of photovoltaic cells and polymeric composites.

Keywords:
functionalization, maleic anhydride, titanium dioxide, nanoparticles

Nanocomposites reinforced with functionalized multi-walled carbon nanotubes (MWNT's) in biopolymers

Y. Estévez-Martínez,[a,c,d] M.E. Mendoza-Duarte,[b] E. Cuevas-Yañez,[c] S. Duron-Torres,[a]
D. Alaníz-Lumbreras,[a] V.M. Castaño-Meneses[d]

[a] *Facultad de Ingeniería Eléctrica, Universidad Autónoma de Zacatecas*
Av. Ramón López Velarde #801, C.P. 98000, Zacatecas, Zacatecas, Mexico.
[b] *Centro de Investigación en Materiales Avanzados, S.C. (CIMAV)*
Miguel de Cervantes 120, Complejo Industrial Chihuahua, Chihuahua, Chihuahua, Mexico.
[c] *Centro Conjunto de Investigaciõn en Química Sustentable, UAEM-UNAM*
Carretera Toluca-Atlacomulco Km.14.5 C.P. 52000, Toluca, Estado de México, México.
[d] *Centro de Fisica Aplicada y Tecnologia Avanzada, Universidad Nacional Autónoma de México*
Boulevard Juriquilla 3001C.P. 76230, Querétaro, Querétaro, Mexico.
E-mail: yoxkin@fata.unam.mx

The viscoelastic properties of chitosan-starch composites [1, 2], reinforced with functionalized multi-walled carbon nanotubes was characterized by Dynamic Mechanical Analysis (DMA), canning Electron Microscopy (TEM), Raman and Infrared spectroscopy, are presented. The MWNT's was oxidized and functionalized with keratin, by grafting (covalent bond) to different conditions, to obtain a good dispersion in the polymer matrix specific conditions.

References

[1] Abdou, E.S., El-Hennawi, H.M., Ahmed, K.A., Preparation of novel chitosan-starch blends as thickening agent and their application in textile printing., Journal of Chemistry, 2013 art. no. 595810
[2] Liu, H., Adhikari, R., Guo, Q., Adhikari, B., Preparation and characterization of glycerol plasticized (highamylose) starch-chitosan films., Journal of Food Engineering, 2013

Bond order in perovskite type octahedral clusters

O. Cruz,[a] E. Carvajal,[a] R. Oviedo-Roa,[b] M. Cruz-Irisson,[a] O. Navarro[c]

[a] *Escuela Superior de Ingeniería Mecánica y Eléctrica-Culhuacán, Instituto Politécnico Nacional*
Av. Santa Ana 1000, México, D. F., C. P. 04430, México
[b] *Programa de Investigación en Ingeniería Molecular, Instituto Mexicano del Petróleo*
Eje Central Lázaro Cárdenas Norte 152, México, D. F., C. P. 07730, México
[c] *Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México*
A.P. 70-360, México, D. F., C. P. 04510, México
E-mail: osalcruz@yahoo.com

The characteristic half-metallic behavior shown by the double perovskite Sr_2FeMoO_6 (SFMO) is searched at different octahedral clusters excised from the bulk material. The structural stability, density of states, character of molecular orbital and bond order were studied in order to relate the SFMO electronic properties with the corresponding to diverse clusters which have as starting point the FeO_6 and MoO_6. The obtained results for charged octahedral clusters were compared with the corresponding to clusters surrounded by Sr atoms. Also, planar clusters with a squared oxygen coordination were analyzed, as well as one in which both metals were included, with an oxygen atom shared by the octahedra and considering or not the surrounding Sr atoms.

Acknowledgements
This work was partially supported by the multidisciplinary project 2012-1439 from SIP-IPN, PIFI-IPN, PICSO12-085 from Instituto de Ciencia y Tecnología del Distrito Federal (ICyTDF) and IN108710 from PAPIIT-UNAM.

Correlación de los estabilizadores dodecanethiol y PVP sobre el tamaño y estructura de nanopartículas de Au

G. Rodriguez-Ortiz,[a] O. Tellez-Vázquez,[a] F. Tovar-Cárdenas,[a] A. Angeles-Pascual,[b] R. Esparza,[a] R. Pérez[a]

[a] *Centro de Física Aplicada y Tecnología Avanzada, Universidad Nacional Autónoma de México, Boulevard Juriquilla 3001, Santiago de Querétaro, Qro., 76230, México.*
[b] *Departamento de Ingeniería Eléctrica-SEES, CINVESTAV-IPN, Zacatenco, México D.F., 07360, México.*
E-mail: gabriel_ro@ymail.com

Nanopartículas de oro fueron sintetizadas por el método reportado por Brust-Schiffrin [1], el cual permite aislar y redisolver en compuestos orgánicos comunes sin agregación o descomposición. Las partículas sintetizadas por esta técnica pueden ser fácilmente manejadas. La técnica de síntesis está inspirada en el sistema de dos fases de Faraday [2] y usa principalmente tioles como ligantes debido al carácter suave del Au y del terminal de S. En la síntesis el $AuCl_4^-$ es reducido por $NaBH_4$ y transferido por la acetona hacía el hexano en la presencia de los estabilizadores. En éste caso se implementó la técnica para utilizar como estabilizador 1-dodecanethiol y polivinilpirrolidona (PVP); por lo que se pretende estudiar el efecto por separado de ambos estabilizadores sobre el tamaño y estructura de las partículas obtenidas. La imagen de HAADF-STEM (Fig.1) muestra que los diámetros de las nanopartículas estuvieron en el rango de 4-8 nm con un tamaño promedio de 5.58 nm. Los estudios de microscopía electrónica muestran que las nanopartículas utilizando 1-dodecanethiol como estabilizador presentan estructuras del tipo cúbica. Por otra parte, las nanopartículas sintetizadas con PVP como agente estabilizador disminuye el tamaño con un tamaño promedio de 3.73 nm. Además de la disminución en el tamaño promedio de partícula, las nanopartículas presentan también un cambio en estructura ya que la mayor parte de las estructuras son del tipo icosaedral y decaedral.

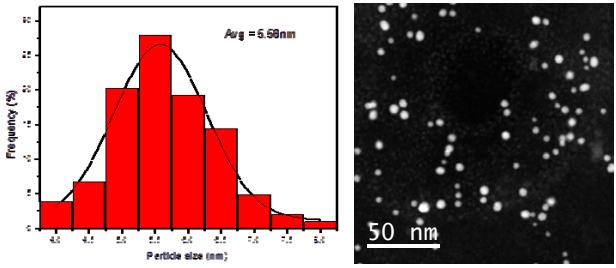


Figura 1: Distribución de tamaño de las nanopartículas de Au estabilizadas con 1-dodecanethiol.

Referencias

[1] M. Brust, M.W., D. Bethel, D. J. Schiffrin, R. Whyman, J. Chem. Soc., 1994: p. 801-802.
[2] Faraday, Philos. Trans. 1857, 147: p.145-181.

High surface area of anatase nanoparticles prepared by low temperature aqueous acidic sol-gel process

O. Muñiz-Serrato, J. Serrato-Rodríguez

Instituto de Investigaciones Metalúrgicas, Universidad Michoacana de San Nicolas de Hidalgo.
Avenida Francisco J. Mujica S/N Ciudad Universitaria, C.P. 58030, Morelia, Michoacán, México.
E-mail: olivermuse@gmail.com

The unique physical and chemical properties derived from nano-size titania are leading to a vast amount of research for a broad range of applications. Tailoring titania nanostructures can have a profound impact on photocatalysis, environmental purification, as well as energy renewal and storage [1]. In the literature are reported many methods to produce TiO_2 nanoparticles including sol – gel, hydrothermal and solvothermal synthesis [2].
In this research, titania nanoparticles were synthesized by Aqueous Acidic Sol-Gel process. Initially, Titanium (IV) butoxide was added into distilled water and a white precipitate was formed immediately. After that, this precipitate was redispersed in water containing nitric and acetic acid. The suspension was then heated at 80°C and vigorously stirred under reflux condition during 12 h. The resulting powders were characterized by X ray diffraction (XRD), transmission electron microscopy (TEM) and BET specific surface area.
This one step low temperature process allowed the formation of anatase with crystallite size around 4 nm, specific surface area of 291m^2/g and a high degree of crystallinity.

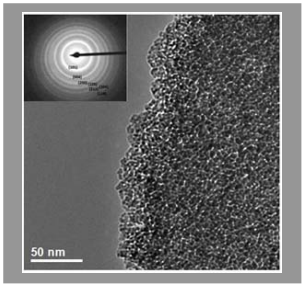


Figure 1: Low magnification TEM image and corresponding electron diffraction pattern, where is observed the high cristallinity degree of anatase.

References

1. X. Chen and S. S. Mao, Chem. Rev. 2007, Vol. 107, No. 7
2. B. L. Cushing, V. L. Kolesnichenko, and C. J. O'Connor, Chem. Rev. 2004, 104, 3893-3946

Synthesis and characterización of polymer nanofibers with pvp nanoparticles $SrFe_{12}O_{19}$ obtained by the electrospinning technique

R. Murillo Ortiz,[a] M. Mirabal García,[a] S.A palomares Sánchez,[a] J. de Jesús Cruz Rivera[b], G. G. López Rocha[c]

[a] *Instituto de Física, Universidad Autónoma de San Luis Potosí, Av. Manuel Nava 6, Zona Universitaria, 78290 San Luis Potosí, SLP, México. C.P. 78000, Teléfono: (01 444) 826 23 62 al 65, Ext. 122.*
[b] *Facultad de Ciencias, Universidad Autónoma de San Luis Potosí, Av. Salvador Nava Martínez S/N Zona Universitaria, San Luis Potosí, SLP, CP 78294, México.*
[c] *Instituto de Metalurgia, Universidad Autónoma de San Luis Potosí, Av. Sierra Leona No. 550, Col. Lomas 2a. Sección, C. P. 78210. San Luis Potosí, S.L.P., México.*
E-mail: raquel_slp@hotmail.com

The $SrFe_{12}O_{19}$/poly (vinyl pyrrolidone) (PVP) composite fiber precursors were prepared by the method Pechini and technique electrospinning. with ferric nitrate, strontium nitrate and PVP as starting reagents. Subsequently, the M-type strontium ferrite ($SrFe_{12}O_{19}$) consists of the thermal decomposition, were derived from calcination of these precursors at 750–800 ºC.The composite precursors and strontium ferrite nanofibers were characterized by X-ray diffraction, scanning electron microscopy and vibrating sample magnetometer.The nanofiber morphology, diameter, crystallite size and grain morphology are mainly influenced by the calcination temperature and holding time. The $SrFe_{12}O_{19}$ nanofibers characterized with diameters of around 90-100 nm which is fabricated by nanosized particles about 60 nm with the plate-like morphology elongated in the preferred direction perpendicular to the c-axis, show the optimized magnetic property with remanent magnetization 61 emu/g and coercivity 58 kA m-1.

Funcionalización de absorbentes potenciales de dióxido de carbono sobre sílice para la reducción de gases de efecto invernadero

V. Morales-Mercado,[a] E. Cuevas-Yáñez,[b] V. Varela-Guerrero,[b] N. M. González-Rivas[b]

[a] *Facultad de Química, Universidad Autónoma del Estado de México, Paseo colon y Tollocan S/N, Toluca Estado de México. C.P 50000, México*.
[b] *Centro Conjunto de Investigación en Química Sustentable UAEM-UNAM, Carretera Toluca-Atlacomulco Km 14.5, Toluca Estado de México. C.P. 50200, México.*
E-mail: ecuevasy@uaemex.mx

El incremento en las emisiones de dióxido de carbono en los últimos años representa un problema asociado al efecto invernadero y al aumento de las temperaturas sobre el planeta; la captura y fijación del dióxido de carbono se ha constituido en un área de investigación creciente y estratégicamente importante. Uno de los procesos que se ha implementado para capturar dióxido de carbono se basa en la interacción de este gas con aminas primarias en fase liquida para generar carbamatos; sin embargo, los procesos tienden a ser ineficientes y costosos debido a los grandes volúmenes de liquido y energía que se requieren en su operación. En este proyecto se pretende generar nuevos absorbentes de dióxido de carbono, soportadas en materiales sólidos como la sílice (SiO_2), los cuales presentan grandes áreas superficiales, de tal manera que esto pueda constituir una opción viable para ser utilizados como empaques sólidos para una columna de absorción, en donde se espera una mayor eficiencia y una menor cantidad de subproductos. [1] Adicionalmente, este proyecto tendría una contribución importante pues representaría una aplicación interesante de la cicloadición alquino-azida catalizada por cobre (reacción "Click") [2] para inmovilizar las diversas aminas propuestas en un soporte sólido a través de un método sencillo y ambientalmente amigable.[3]

Bibliografía

[1] Gheorghe, A.; Cuevas-Yanez, E.; Horn, J.; Bannwarth, W.; Narsaiah, B.; Reiser, O., A facile strategy to a new fluorous-tagged, immobilized TEMPO catalyst using a click reaction, and its catalytic activity. *Synlett* **2006,** (17), 2767-2770.

[2] Lummerstorfer, T.; Hoffmann, H., Click chemistry on surfaces: 1,3-dipolar cycloaddition reactions of azide-terminated monolayers on silica. *Journal of Physical Chemistry B* **2004,** *108* (13), 3963-3966.

[3] a) Guerrero, V. V.; Shantz, D. F., Amine-Functionalized Ordered Mesoporous Silica Transesterification Catalysts. *Industrial & Engineering Chemistry Research* **2009,** *48* (23), 10375-10380; (b) Wang, Q. Q.; Guerrero, V. V.; Ghosh, A.; Yeu, S.; Lunn, J. D.; Shantz, D. F., Catalytic properties of dendron-OMS hybrids. *Journal of Catalysis* **2010,** *269* (1), 15-25.

Au/Y-TiO_2 catalyst. High activity and long-term stability in CO oxidation

Rodolfo Zanella*[a], Vicente Rodríguez-González[b], Yamin Arzola[a], Albino Moreno-Rodriguez[b]

[a] *Centro de Ciencias Aplicadas y Desarrollo Tecnológico, UNAM, Mexico City, Mexico*
[b] *IPICYT, Instituto Potosino de Investigación Científica y Tecnológica, S.L.P., Mexico*
[c] *Departamento de Química General Facultad de Ciencias Químicas, BUAP, Puebla, Mexico*
E-mail: rodolfo.zanella@ccadet.unam.mx

Since the discovery in the late eighties that gold is catalytically active when it is dispersed as small particles on an oxide support, the preparation of gold-based catalysts has been widely studied. They are active in many reactions of both industrial and environmental importance. The most remarkable catalytic properties of supported gold have been obtained for the reaction of CO oxidation at ambient temperature. However catalytic activity decreases during the catalytic run. Deactivation has been proposed to be due to nanoparticles sintering or to formation of carbonates adsorbed on the reactive sites of the catalysts. A way to overcome the deactivation process is to produce oxygen vacancies on the surface of the support particles. These oxygen vacancies generate crystalline defects that work as pinning centers for the gold particles. The steps on the surface of the support particles are also crystalline defects that could work as pinning centers for the gold particles. Theoretical calculations have demonstrated that the gold particles bind stronger to a defect-rich surface than to a defect-deficient surface and that a significant charge transfer occurs from the titania support to the Au particles.

Gold catalysts supported on TiO_2 doped with Y (1, 3 and 6 wt % of Y) were prepared by deposition-precipitation with urea method [1]. The Y-TiO_2 supports were prepared by the sol-gel method. The catalysts were characterized by X-ray diffraction, nitrogen physical adsorption (BET method), Photoluminescence, UV-visible, FTIR and Raman spectroscopy, H_2-TPR, High Resolution Transmission Electron Microscopy (HRTEM) and high-angle annular dark-field scanning transmission electron microscopy (HAADF). The catalytic activity and stability of the catalysts in the CO oxidation was performed using a reactor coupled to a GC analytical apparatus.

The Y-TiO_2 supports prepared by the sol-gel method allowed the formation of solids with high specific surface area. The BET surface area of Y-TiO_2 prepared by the sol-gel method increased with the Y content because the increase of the Y content on the support prevented the growth of the crystallite size of the anatase crystals. Because of the big difference in the atomic radius of Y^{3+} and Ti^{4+}, the substitution of Ti^{4+} by Y^{3+} cations in the titania framework was limited to low Y loadings. High contents of Y produced the segregation of yttrium as Y_2O_3 on the surface of TiO_2. The incorporation of yttrium in TiO_2 lattice favored the formation of oxygen vacancies, which are the preferred adsorption sites for Au nanoparticles, acting as nucleation centers for Au atoms [1]. Gold particles with average particle size of 3 nm were deposited on Y-TiO_2 and TiO_2 (P25) supports. Au/Y-TiO_2 catalysts presented higher activity and stability at room temperature than Au/TiO_2 [1]. The highest activities and stabilities as a function of time on stream were observed for Au/Y-TiO_2 (1-99), in which it is proposed that all Y was doping TiO_2. This behavior is related to the strong anchoring of the gold particles on the structural defects of the support caused by the doping of anatase with yttrium, which naturally gives rise to structures with oxygen vacancies. HRTEM results show that at high content of Y, Y_2O_3 is segregated on the surface of TiO_2. As Y_2O_3 is a not reducible oxide, when it was on the TiO_2 surface, the catalytic activity of the Au/Y-TiO_2 catalyst decreased; however, it was always higher than that obtained from Au/TiO_2 at room temperature and higher temperatures. The higher stability of the Au/Y-TiO_2 catalysts compared with that of the Au/TiO_2 catalyst is due to lower carbonate formation and to lower gold particle sintering during the reaction [1].

[1] R. Zanella, V. Rodríguez-González, Y. Arzola, A. Moreno-Rodríguez, ACS Catal. *2* (2012) 1-11.

Estudio de la estabilidad de nanopartículas AuPt, AuPd y PtPd bajo tratamiento térmico por dinámica molecular

J.O. Téllez-Vázquez, G. Rodríguez-Ortiz, J. García, R. Esparza and R. Pérez

Centro de Física Aplicada y Tecnología Avanzada
Universidad Nacional Autónoma de México, Boulevard Juriquilla #3001, C.P. 76230; Santiago de Querétaro, Qro., México.
E-mail: oswald.tellez@gmail.com

En la actualidad, son de gran interés e importancia nanopartículas metálicas con dimensiones de unos cuantos nanómetros y formas especificas por su potencial aplicación en distintos campos de la tecnología [1-3]. En años recientes, el interés por el estudio de nanopartículas bimetálicas se ha incrementado en relación al interés que hay por las monometálicas. Esto se debe a que las propiedades eléctricas, químicas, catalíticas y ópticas que presentan las nanopartículas bimetálicas tienen mayor potencial de aplicación [4], existiendo la posibilidad de modificarlas al variar la composición y morfología de las mismas. En este sentido, es posible la obtención de NPs con estructuras fcc y bcc, distintas morfologías como cuboctaedros, octaedros, icosaedros, decaedros entre otras. En este trabajo se presentan resultados preliminares del estudio, por dinámica molecular (DM), de la estabilidad de nanoparticulas de AuPt, AuPd y PtPd sometidas a tratamientos térmicos simulados. En los tres casos se utilizaron modelos de composición $A_{25}B_{75}$, $A_{50}B_{50}$ y $A_{75}B_{25}$, con estructura fcc y forma cuboctaedral. Los modelos se sometieron a una simulación en la que se eleva la temperatura desde 300 hasta 1700 K, y posteriormente se realizó el enfriamiento hasta los 300 K. Los resultados obtenidos, indican que la energía de los sistemas al final de los ciclos, es menor, por lo que se obtienen una estructuras de mayor estabilidad bajo las condiciones composicionales y de forma en cada caso. En todos los casos se observo histéresis en las curvas de energía. Durante el calentamiento, a excepción de las composiciones $Pt_{50}Pd_{50}$ y $Pt_{75}Pd_{25}$, todos los modelos modifican su morfología de cuboctaedro a icosaedro, lo que se identifica por un cambio abrupto en la energía, y finalmente llegan a un estado amorfo al llegar al punto de fusión. Sin embargo, a lo largo de las curvas de enfriamiento, las estructuras pasan directamente a la forma de cuboctaedro, lo que podría explicarse mediante las curvas de histéresis de la energía obtenidas.

Referencias

[1] N. Tian, Z.Y. Zhou and S.G. Sun: J. Phys. Chem. C Vol. 112 (2008), p. 19801.
[2] S.P. Mulvaney, M.D. Musick, C.D. Keating and M.J. Natan: Langmuir Vol. 19 (2003), p. 4784.
[3] R. Skomski: J. Phys.: Condens. Matter. Vol. 15 (2003), p. R841.
[4] C. Burda, X. Chen, R. Narayanan and M.A. El-Sayed: Chem. Rev. Vol. 105 (2005), p. 1025.

Síntesis y caracterización de un complejo de triazol-cobalto para su posible uso como catalizador en reacciones de descarboxilación

M. T. Ramírez-Palma,[a] V. M. Apolonio,[b] J. González-Arratia, [a] D. Corona-Becerril,[c] G. Martínez-Barrera,[b] E. Cuevas-Yáñez[c]

[a]*Posgrado en Ciencias Químicas, Facultad de Química, UAEM*
[b]*Facultad de Química, UAEM, Paseo Tollocan esquina Paseo Colón, Toluca, Estado de México, C.P.50120*
[c]*Centro Conjunto de Investigación en Química Sustentable UAEM-UNAM, Carretera Toluca- Atlacomulco, Km. 14.5, Toluca, Estado de México. CP 50200*
E-mail: ecuevasy@uaemex.mx

El estudio de catalizadores de cobalto ha tenido poco desarrollo en relación a metales de transición como Paladio, Níquel y Rodio, entre otros; sin embargo se ha demostrado que el uso de catalizadores de este tipo han funcionado exitosamente en reacciones de descarboxilación de -hidroxiácidos [1], oxidación aeróbica de alcoholes [2] y reacciones de acoplamientos arilo-arilo[3], por lo cual en este proyecto, se planteó el desarrollo de un nuevo catalizador a partir de triazol y una sal de cobalto, cuya caracterización se llevó a cabo mediante Resonancia Magnética Nuclear (RMN), Infrarrojo (IR), Espectroscopía Fotoelectrónica de Rayos X (XPS), Difracción de Rayos X y Análisis por Combustión.

Bibliografía

[1] Gonzalo B., I. Fernández, P. Formentin, J. R. Pedro, A. L. Roselló, R. Ruiz y Y. Joumaux (1998). Catalytic aerobic oxidative decarboxylation of α-hydroxyacids.Methyl mandelate as a benzoyl anion equivalent. *Tetrahedron Letters* 39, 3327-3330.

[2] Suman Jain y Oliver Reiser (2008). Immobilization of Cobalt (II) Schiff Base Complexes on Polystyrene Resin and a Study of Their Catalytic Activit for the Aerobic Oxidation of Alcohols. *ChemSusChem* 1, 534 – 541.

[3] Gérard Cahiez y Alban Moyeux (2010). Cobalt-Catalyzed Cross-Coupling Reactions. *Chem. Rev.* 110, 1435–1462

Efectos de interfase sobre la conductividad iónica en películas delgadas y superredes YSZ /STO para aplicaciones en celdas de combustible de óxido sólido

M. R. Díaz-Guillén,[a] J. A. Díaz-Guillén,[b] A. Rivera-Calzada,[a] O. J. Durá,[a] J. Santamaría,[a] C. León[a]

[a] *GFMC, Departamento de Física Aplicada III, Facultad de Física, Universidad Complutense de Madrid, Campus Moncloa, 28040 Madrid, España.*
[b] *División de Estudios de Posgrado e Investigación, Instituto Tecnológico de Saltillo, V. Carranza 2400, 25280 Saltillo, Coahuila, México*
E-mail: marioroman.diaz@fis.ucm.es

Una de las más prometedoras tecnologías para generar energía eléctrica con elevada eficiencia y sin emisión de contaminantes son las llamadas celdas de combustible de óxido sólido (SOFC). Sin embargo, la mayor limitación encontrada para una implementación definitiva se debe a la baja conductividad iónica que a temperatura ambiente presenta el material empleado como electrolito sólido, la circonia estabilizada con itria (ZrO_2:Y_2O_3 *o* YSZ). Una alternativa para abordar este problema, es la fabricación y estudio de materiales en forma de películas delgadas donde al menos una de las dimensiones espaciales sea de tamaño nanométrico, y donde por tanto se puedan producir efectos de tamaño o de tensión en la estructura cristalina que den lugar a modificaciones de las propiedades físicas respecto del mismo material en volumen. En el presente trabajo de investigación se crecieron películas delgadas y superredes de materiales con diferentes parámetros de red basados en YSZ, con características estructurales realmente interesantes, mediante la técnica de pulverización catódica de alta presión de oxígeno. Esta técnica permite la obtención de capas ultradelgadas y un control del proceso de crecimiento con tal precisión, que es posible llegar a obtener películas de espesor tan pequeño como una celda unidad y de excelente calidad estructural. La caracterización estructural se llevó a cabo mediante las técnicas de difracción de rayos X de ángulo bajo y alto (XRD), microscopía de fuerza atómica (AFM), microscopía electrónica de transmisión-barrido (STEM) y espectroscopia de pérdidas de energía de electrones (EELS). La caracterización eléctrica se realizó mediante la técnica de espectroscopia de impedancias (IS) en un amplio rango de temperaturas. Los resultados obtenidos de la caracterización estructural y eléctrica mostraron que una disminución en el espesor de las películas delgadas y superredes hasta 1nm favorece la aparición de efectos de tensión epitaxial y cambios estructurales debido a la reconstrucción atómica en la interfase entre la YSZ y el STO proporcionando un número considerable de vacancias disponibles para el movimiento paralelo de los iones en dicha interfase y consecuentemente se produce un incremento significativo en la conductividad iónica de oxígeno en la YSZ, permitiendo eventualmente una importante disminución en la temperatura de operación requerida actualmente por las SOFC.

Characterization of copolymer collagen-polyvinylpyrrolidone modified by a heat treatment

Gerardo Leyva-Gomez,[a] Islas Ayala M. Guadalupe,[a] David Quintanar Guerrero,[b] Edgar Krötzsch[a]

[a]Laboratorio de Tejido Conjuntivo del Centro Nacional de Investigación y Atención a Quemados del Instituto Nacional de Rehabilitación de la Secretaria de Salud.
Calz. México Xochimilco No. 289 Col. Arenal de Guadalupe, C.P.14389.
[b]Laboratorio de Investigación y Posgrado en Tecnología Farmacéutica, Facultad de Estudios Superiores Cuautitlán, Universidad Nacional Autónoma de México.
Av. 1° de Mayo s/n, Campo 1, Cuautitlán Izcalli 54740, Estado de México. México.
E-mail: gerardoleyva@hotmail.com

The collagen-polyvinylpyrrolidone (collagen-PVP) copolymer is a compound derived from the gamma irradiation of soluble fibers of collagen type I of porcine origin and polyvinylpyrrolidone (PVP) of low molecular weight. Currently, it has been discovered that hydrolyzed collagen has better biological properties compared to the normal collagen, this finding suggests that Clg-PVP copolymer can improve its currently known properties. The purpose of this study was to investigate whether the physical and chemical properties of copolymer Clg-PVP after being subjected to a process of hydrolysis are modified through the use of analytical techniques such as: capillary electrophoresis, rheology, particle size, calorimetry, SEM and AFM, and its comparison with the copolymer without treatment. For this purpose 6 samples were characterized: collagen, hydrolyzed collagen, Clg-PVP, hydrolyzed Clg-PVP, Clg-PVP/-PVP and hydrolyzed Clg-PVP/-PVP with different analytical techniques mentioned above. The quantification method of residual PVP was optimized and a preliminary percentage of the 18.39% was determined on hydrolyzed copolymer. Also, by rheological analyses were determined non-Newtonian and pseudoplastic fluids for all the samples, after to remove the excess of PVP a rheopectic fluid was determined. The particle size of the hydrolyzed Clg-PVP is lower than Clg-PVP and thermal stability tests showed that the hydrolyzed Clg-PVP has a lower thermal stability than Clg-PVP. SEM and AFM micrographs showed that the hydrolysis process results in the formation of colloidal particles. As conclusion, the process of hydrolysis of the Clg-PVP has an important effect on their physical and chemical characteristics so it is possible that their biological properties will be modified.

Deposition and characterization of bismuth containing hard coatings

R. Mirabal,[a] S.E. Rodil,[a] P. Silva-Bermudez,[a] S. Muhl,[a] G. Ramirez,[a] J. Oliveira,[b] A. Cavaleiro[b]

[a]*Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México. México*
[b]*Faculdade Ciencias E Tecnologia Da Universidade De Coimbra, Portugal*
Email: mirabalroberto@yahoo.com

Bismuth is a soft semimetal with a rhombohedral graphite-like quasi-layered structure and a low melting point of 271oC. These characteristics point to the use of Bi or Bi-compounds for self lubrication applications where low friction and low wear rates are required. However, pure Bi and its compounds are very soft. Therefore our proposal is the inclusion of Bismuth into a hard coating using the methodologies developed for nanocomposite thin films; either as nano-sized particles into a hard matrix or as a lamellar structure, alternating a bismuth layer with a hard-coating layer. Then, the excellent frictional properties of Bismuth could be exploited in combination with materials that provide mechanical resistance. Bismuth sputtered films for mechano-tribological applications and its addition into metal nitride coatings have been poorly studied, therefore there is a strong need to define the deposition conditions adequate to achieve a stable and adhered coating. In this work, we report the deposition of Bismuth containing niobium nitride coatings using a confocal dual sputtering system. Both targets (2") were ignited simultaneously, but using different powers; 400 W direct current for the Nb target (99.95 %) and 6,10 and 20 W radio frequency for the Bi target (99.999%). The coatings were deposited on Silicon at 200 oC using a mixture a fixed Ar/N2 (14/6) flow ratio. The deposition pressure was 3 mTorr starting from a backing pressure below 5x10-6 Torr. The composition of the coatings was obtained by both X-ray photoelectron, to clearly detect the presence of oxidized phases, and energy dispersive spectroscopy, in order to detect the presence of segregated bismuth. The Bi segregation and NbN structure were also studied by X-ray diffraction. The coefficient of friction of the coatings was measured by pin-on-disk tests using a load of 5 N and a sliding distance of 500 m.

Acknowledgement: The research leading to these results has received funding from the European Community Seven Framework Program (FP7-NMP-2010-EU-MEXICO) and CONACYT under grant agreements Nº 263878 and 125141, respectively.

Propiedades ópticas de nanopartículas de cobre: Síntesis, caracterización y estudio teórico

Elda Liliana Arevalo Lara,[a] Noemi Ochoa Mejía,[a] A. L. González,[b] Marco Antonio Camacho López,[c] E. Vigueras-Santiago,[c] Miguel Ángel Camacho López,[d] L. E. Díaz-Sánchez[a]

[a] *LCBMyN, Facultad de Ciencias, Universidad Autónoma del Estado de México, 50000, Toluca, México*
[b] *Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apartado Postal J48, 72570, Puebla, México*
[c] *Laboratorio de Investigación y Desarrollo de Materiales Avanzados, Facultad de Química-UAEMex. Km 14.5 carretera Toluca-Atlacomulco*
[d] *Laboratorio de Fotomedicina, Biofotónica y Espectroscopía Láser de Pulsos Ultracortos, Facultad de Medicina, Universidad Autónoma del Estado de México, Jesús Carranza y Paseo Tollocan s/n. Toluca, México.*

En el presente trabajo sintetizamos nanopartículas de Cobre (NPs-Cu) usando el método de ablación láser de sólidos en líquidos (ALSL) el cual proporciona una forma sencilla y flexible para la síntesis de NPs [1, 2]. El interés por el estudio de NPs-Cu se debe a que a escala nanométrica exhiben atractivas y novedosas propiedades magnéticas, eléctricas y ópticas las cuales son diferentes a las que normalmente ocurren en bulto. Nos interesan las propiedades ópticas de NPs-Cu debido a que, dependiendo del tamaño y morfología, éstas pueden tener aplicaciones potenciales en medicina y en el campo de las energías sostenibles [3,4]. Para los experimentos de ALSL se utilizaron discos de cobre con una pureza del 99.9%, un diámetro de 2.5 cm, y 1 cm de espesor. Como medios líquidos se usó metanol y acetona. Para irradiar el disco de cobre y llevar a cabo el proceso de síntesis se utilizó un láser pulsado de Nd-YAG con emisión en 1064 nm, duración de pulso de 7 ns y una frecuencia de repetición de 15 Hz. Se realizaron experimentos variando el tiempo de ablación de 5 a 35 min a una energía por pulso de 47 mJ. Para la caracterización óptica de las soluciones de NPs-Cu-metanol y NPs-Cu-acetona, se utilizó la técnica de espectroscopía de absorción en el intervalo UV-Vis. Los resultados muestran que las propiedades de absorción de las soluciones de NPs-Cu dependen del medio líquido utilizado. Para entender los resultados experimentales observados nos apoyamos en la teoría de Aproximación de Dipolo Discreto y el código numérico DDSCAT (*Discrete Dipole Scattering*). Estudiamos la respuesta óptica de NPs-Cu a diferentes tamaños y morfologías embebidas en diferentes medios, observando una dependencia de estos factores con la respuesta óptica.

Referencias:
[1] F. Bozon-Verduraz, et al., "Production of nanoparticles by laser-induced ablation of metals in liquids", *Quantum Electronics* ***33***, 714 (2003). [2] R.M. Tilaki, et al., "Size, composition and optical properties of copper nanoparticles prepared by laser ablation in liquids", Appl. Phys. A **88**, 415 (2007). [3] M. A. Yurkin and A. G. Hoekstra, "The discrete dipole approximation: An overview and recent developments", Journal of Quantitative Spectroscopy & Radiative Transfer **106,** 558 (2007). [4] L. Suljo, C. Phillip and B. I. David, "*Plasmonic-metal nanostructures for efficient conversión of solar to chemical energy"*, Nature material **10**, 911 (2011).

Synthesis of bimetallic sulphide nanoparticles M*Mo (M* = Fe, Ni, Co) supported on multiwalled carbon nanotubes and catalytic test for sulfur remotion

L. Zavala S.,[a] R. Huirache-Acuña,[a] J. Lara Romero,[a] E. M. Rivera-Muñoz,[b] G. Alonso-Núñez[c]

[a]*Facultad de Ingeniería Química, Universidad Michoacana de San Nicolás de Hidalgo, Ciudad Universitaria C.P. 58060, Morelia, Michoacán México.*
[b]*Centro de Física Aplicada y Tecnología Avanzada, Universidad Nacional Autónoma de México, A.P. 1-1010, 76000 Querétaro, México.*
[c]*Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, KM. 107, Carretera Tijuana-Ensenada, C.P. 22860, Ensenada, B. C. México.*
E-mail: rose_noir18@hotmail.com

Multiwalled Carbon Nanotubes (MWCNT) were synthesized using an organic precursor (α-pinene) by spray pyrolysis method. Subsequently, bimetallic nanoparticles were impregnated directly on the MWCNT by using a microwave assisted hydrothermal method. After, samples were dried and calcined at 450 °C. Then, catalysts were activated through a reductive atmosphere treatment (H_2S/H_2). Samples were characterized by different techniques: nitrogen adsorption-desorption (BET), X-ray diffraction (XRD), scanning electron microscopy (SEM), temperature-programmed thermogravimetric analysis (TGA). Additionally, their catalytic properties were evaluated in the hydrodesulfurization reaction of dibenzothiophene (DBT). The reactions were carried out in a batch reactor at T = 320 °C, pressure of 800 psi and stirring of 700 rpm.

The evaluated catalysts showed catalytic activity in the HDS of DBT (FeMo > CoMo). It was concluded that the decrease in the catalytic activity for the CoMo catalyst was caused by the formation of agglomerates of bimetallic nanoparticles that possibly were formed by the addition of a higher percentage of metal oxides in the impregnation step. For FeMo catalyst, it was observed a better dispersion of active phase which led to a better catalytic activity in the HDS reaction.

Authors acknowledge the support of CONACYT Project 182191 and CIC-UMSNH 2012-2013.

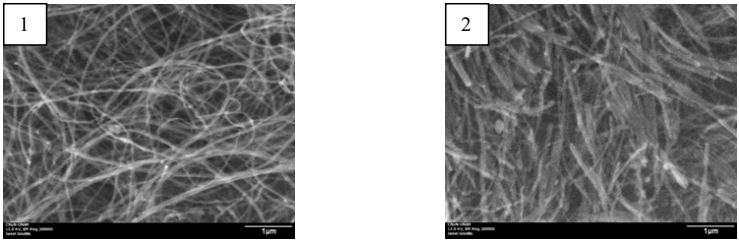


Figure: SEM micrographs of CoMo[1] and FeMo [2] sulphide catalysts supported on MWCNT

Effect of the Al_4C_3 formation on the Young's Modulus of CNT reinforced aluminum matrix composites

I. Alfonso,[a] I.A. Figueroa,[a] V. Rodríguez-Iglesias,[b] C. Maldonado[c]

[a] *Instituto de Investigaciones en Materiales. Universidad Nacional Autónoma de México. Circuito Exterior SN. Ciudad Universitaria. CP. 04510. Del. Coyoacán, México, DF. México.*
[b] *Facultad de Ingeniería. Universidad Autónoma del Carmen. Campus III. Avenida Central S/N, Esq. con Fracc. Mundo Maya, C.P. 24115, Ciudad del Carmen, Campeche, México.*
[c] *Instituto de Investigaciones Metalúrgicas, Universidad Michoacana de San Nicolás de Hidalgo, Edificio U. Ciudad Universitaria, C.P. 58000, Morelia, Michoacán, México.*
E-mail: ialfonso@iim.unam.mx, isme2000@hotmail.com

The use of Carbon nanotubes (CNTs) as reinforcing material may originate a new class of composites due to their exceptionally high mechanical properties. The strength of the interfacial bonding between reinforcement and matrix in CNTs reinforced composites has an important effect on the mechanical behavior of these materials. Specifically for aluminum matrix composites the formation of Al_4C_3 in the CNT-Al interface has an important effect on the interfacial bonding. This effect was analyzed using a Finite Elements Analysis (FEA) model that incorporates different thickness of the Al_4C_3, using commercially available FEA package ANSYS for determining the effective Young's modulus of a Representative Volume Element (RVE). The CNTs were modeled as solid fibers. CNT volume fraction was modified from 0.5 to 5.0 %.
The results showed that the thickness of the Al_4C_3 interface has a significant effect on the elastic properties of the composites. The Young's modulus estimations obtained using this model presented values that disagree with the Rule of Mixtures and the Halping-Tsai model's predictions. Assuming different conditions, it was possible to obtain approximations much closer to the real elastic behavior of the composite.

Graphene / graphite frictional forces

G. Ibarra-Reyes,[a] J. L. Rivera,[a,b] C. McCabe[c]

[a] *Facultad de Ingeniería Química, UMSNH, Morelia, Michoacán, México.*
[b] *Instituto de Investigaciones en Materiales, UNAM, Morelia, Michoacán, México.*
[c] *Chemical & Biomolecular Engineering, Vanderbilt University, Nashville, Tennessee, USA*
E-mail: guillermoibarra@gmail.com

Friction and wear are crucial properties in nanoelectromechanical systems due to the high surface-volume ratio. As a consequence in the last decade, there has been much scientific interest in superlubricity. Superlubricity is the phenomena in which friction ceases to exist or diminishes substantially between two solid surfaces. To date all structural superlubricity experimental evidence has been obtained under vacuum conditions. Zheng et al. displaced graphite islands with a height of 200 nm with varying longitudes from 0.5 to 5 µm and observed the islands spontaneously returned to its original position. The previous behavior was observed and constantly repeated for islands with longitudes of 0.5 and 1 µm. This phenomenon is similar to the auto retraction movement in carbon nanotube walls due to the van der Waals interactions simulated by Rivera et al.

Molecular dynamics simulations were preformed to reproduce experimental results obtained by Zheng et al. The system studied consisted of a block of graphite, represented by six (6) layers of graphene of equal size and a smaller graphene "flake". Molecular dynamic simulations consisted of displacing the "flake" and observing its behavior. The force field potential used consisted of a Lennard Jones potential and flexible interactions. The flake dimensions were varied to observe the size effect.

Next goal was to reduce flake rotations. It's important to note that the flake movement mechanism consisted in oscillations from one end of the graphite block to the other end after a period of time; the flake would rotate around the equilibrium center of mass. When rotating, we suspect that the flake loses all useful movement. A possible solution to reduce rotations was to modify the upper layer of the graphite block. A line of carbon atoms was removed in such a way to provide a "path" or trajectory that the flake could follow and not deviate to the sides and thus reducing rotations. Finally, a system of graphite blocks was put in parallel to provide transport from one extreme to another.

In order to develop an application for this phenomenon, blocks were set up in a series of blocks in a straight line separated by a minimum difference. This arrangement provided insightful information with respect to friction forces involved in the flake displacement from graphite block to block.

References:

Q. S. Zheng et al., Phys. Rev. Lett. 100, 067205 (2008)
J. L. Rivera et al., Nanotechnology 16, 186 (2005)
M. Hirano, K. Shinjo, Phys. Rev. B 41 11837 (1990)

Preparation and characterization of kynurenic acid hosted in sol-gel silica and ordered mesoporous silica release reservoirs

E. Ortiz-Islas,[a] T. López,[a] E. Gómez,[a] V. Pérez,[a] P. Carrillo[b]

[a] *Instituto de Neurología y Cirugía "MVS"*
Insurgentes Sur #3877, Col. La Fama-Tlalpan, 14269, México, D. F.
[b] *Instituto Nacional de Reabilitación*
Calzada México-Xoxhimilco #289, Col. Arenal de Guadalupe, 14389, México, D. F.
E-mail: emma170@hotmail.com

Kynurenic Acid (KYNA) has important therapeutic effects in neurological disorders; however, its use as a neuro-protective agent is restricted due to its very limited ability to cross the blood brain barrier (BBB). For this reason we are looking for new alternative ways to make KYNA reaches the brain; one of them is using drug delivery systems. In reported works we have proposed using an implantable release inorganic reservoir to treat several neurological diseases [1, 2]. To following the same idea, in the present work we propose using silica based materials as reservoirs of KYNA molecules. For this purpose, first, KYNA was hosted in the silica's network when was added during the synthesis of silica via the sol-gel process. Second, KYNA was adsorbed on silica of the SBA-15 type, which was previously prepared. Once the KYNA-silica materials were obtained these were characterized with several physical techniques. The ultraviolet and infrared spectroscopy techniques reveal that KYNA did not undergo any structural change after this was hosted in the silica materials. The N_2 adsorption-desorption measures revel that the surface area values of KYNA-silica materials, which were compared with the pure silica materials values, substantially decreased by the addition of the drug. The electronic micrographs show that the sol-gel KYNA-Silica material is conformed for aggregates of nanoparticles, which have sizes around of 50 nm. In the other hand, the typical hexagonal arrange for SBA-15 has been observed ever after that KYNA was hosted in it. The KYNA release profiles carried out approximately during 300 hours show a first fast stage drug release with a subsequent slowly drug release.

References

[1] T. Lopez, E. Ortiz, P. Quintana, R.D. Gonzalez, A nanostructured titania bioceramic implantable device capable of drug delivery to the temporal lobe of the brain. *Colloids and Surfaces A: Physicochem*. Eng. Aspects 300 (2007) 3–10.

[2] T. López, J. L. Bata-García, D. Esquivel, E. Ortiz-Islas, R. Gonzalez, J. Ascencio, P. Quintana, G. Oskam, F. J Álvarez-Cervera, F. J. Heredia-López, J. L. Góngora-Alfaro. Treatment of Parkinson's disease: nanostructured sol–gel silica–dopamine reservoirs for controlled drug release in the central nervous system. *International Journal of Nanomedicine.* 6(2011)19–31.

Caracterización de una vesicular polimérica para el transporte de oxígeno

N.A.Noguez,[a,c] E.B. Naranjo,[b] R. Herrera,[a] A.E. Chávez[a]

[a] *Dpto.de Ingeniería Química, Facultad de Química*
[b] *Dpto. de Farmacia, Facultad de Química*
Universidad Nacional Autónoma de México, Mexíco DF,04510,México
[c] *Dpto. de Sistemas Biológicos, Laboratorio de Farmacia Molecular y Liberación Controlada*
Universidad Autónoma Metropolitana Unidad Xochimilco,Calz.del Hueso 1100 Col. Villa Quietud,México DF, 04960, México
E-mail: nanoguez@correo.xoc.uam.mx

Los polimerosomas son vesículas sintéticas que imitan el comportamiento de las membranas biológicas [1]. Con base en esto, se realizó la síntesis al azar de un copolímero de poliácido acrílico - poliacrilato de butilo (PAA-PBA) con características anfifílicas, de flexibilidad y con capacidad de encapsular hemoglobina para desarrollar experimentalmente un prototipo de célula artificial tipo eritrocito [1]. Se seleccionaron tres copolímero para el desarrollo de los polimerosomas con PM de 2000-5000 g/mol. La síntesis del polimerosoma se realizó en un dispositivo en forma de T caracterizado con un No. de Reynolds (Re<1) siendo este un flujo de transición y el Número de Capilaridad entre 10^{-3}-10^{-5} coincidente en que la tensión superficial es la dominante para la elaboración de las vesículas. Las vesículas totales para cada copolímero fueron: Cp1con 334, Cp6 con 244 y Cp 40 con 585. Se observaron las vesículas bajo el microscopio de luz, empleando el objetivo de 100X, se tomaron fotografías y se procesaron las imágenes con el paquete ScopePhoto 3.0, se determinó el tamaño por la medida del diámetro (D_L) siendo estos; para Cp1 27.91 µm, Cp6 27.82 µm y Cp 40 29.13 µm, observándose que el copolímero Cp1 y Cp40 formaron vesículas con bicapa y el Cp6 formó micelas. En relación a la encapsulación de la hemoglobina para el copolímero Cp1 fue de 56.9%, y para el Cp40 de 59.76%, estos resultados muestran cierta elasticidad que permitió encapsular a la hemoglobina más allá del valor estimado, en el caso del copolímero Cp6 no mostró este comportamiento. La captación de oxígeno por parte de las vesículas en el tiempo estudiado, el copolímero Cp1 muestra un comportamiento Fickiano, en el caso del copolímero Cp40 observamos un comportamiento anómalo que tiende a la linealidad después de los 600 seg. Los coeficientes de difusión fueron D_{Cp1}= 7.92x10^{-3} cm^2/s y D_{Cp40}= 4.24 x10^{-3} cm^2/s y con los datos de transición vítrea (Tg) para cada uno: TgCp1 = -2.90ºC y el TgCp40 = -10.74 ºC, se ratifica que para los polímeros con una temperatura de Tg baja, como es el caso de los copolímeros estudiados, poseen un segmento de alta movilidad y por lo tanto tendrán alta difusividad. En base a los resultados obtenidos los copolímeros candidatos para el desarrollo de una célula artificial equiparable a un glóbulo rojo son Cp1 y el Cp40.

Referencias

1. Hamidi, M., Shahbazi, M.A., Rostamizadeh, K. Drug Targeting and Gene Therapy. Macromolecular Bioscience. Vol. 12 (2) 144-164 (2012).

Electronic transport in one-dimensional periodic and non-periodic sequences of N delta-function potentials

E.J. Guzmán,[a,b] O. Oubram,[c] O. Navarro[a]

[a] *Instituto de Investigaciones en Materiales*
Universidad Nacional Autónoma de México, Apdo. Postal 70-360, 04510, México D.F.
[b] *Facultad de Cs. Físico Matemáticas*
Universidad Michoacana de San Nicolás de Hidalgo, Morelia, Michoacán, México
[c]*Facultad de Ciencias Químicas e Ingeniería, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Col. Chamilpa, CP 62209, Cuernavaca, Morelos, México.*
E-mail: eric-gio@hotmail.com

Recently, there has been a growing interest in electronic transport at the nano-scale conductors. The electron transport phenomena in a crystal have been modeled assuming an incident particle from the left on one-dimensional sequences of N delta-function potentials. We studied the transport properties using the transfer matrix method to calculate the transmission coefficient in a disorder sequence. The results show that the transport depends of the strength, the geometrical separation, the local disorder and the number of delta function potentials. The Kronig-Penney model explained very well the band-gap structure observed in one-dimensional periodic sequences.

Influence of sintering additives on the oxidation behavior of Si_3N_4-ceramics at 1200°C

L. Ceja-Cárdenas, [a,b] J. Lemus-Ruiz, [a] M. Nanko [b]

[a] *Instituto de Investigaciones Metalúrgicas,UMSNH, Ed. U, C.P. 58000; Morelia, Michoacan, México.*
[b] *Nagaoka University of Technology. 1603-1 Kamitomioka Nagaoka, Niigata 980-2188, Japan.*
E-mail: leocc4@yahoo.com.mx

Silicon nitride (Si_3N_4) has generated considerable interest as a potential material for high-temperature engineering applications. However, the high-temperature properties such as oxidation resistance have been not understood. Although, the excess of oxide additives has been widely used to make densification easy for sintering process, nevertheless the formation of intergranular glassy film upon cooling to believe has a profound influence on the high-temperature oxidation behavior of Si_3N_4-ceramics [1, 2].

The spark plasma sintering SPS technique has been used to densify commercial pure α-Si_3N_4 powder, having Y_2O_3 and Al_2O_3 as additives; two compositions were prepared (Si_3N_4-4 and Si_3N_4-12 series specimens). The high-temperature oxidation test has been applied to Si_3N_4-ceramics. Oxidation treatment was carried out at 1200°C using holding times of 1, 4 and 24 d under an air atmosphere. The evolution of the oxidation layer on the surfaces and microstructural examination in the cross-sections of the Si_3N_4 samples were studied using X-ray diffraction, XRD and scanning electron microscope, SEM analyses. The results obtained showed an insignificant oxidation in Si_3N_4-4 series specimens while the initial composition accelerates oxidation in Si_3N_4-12 series specimens. SiO_2 and $Y_2Si_2O_7$ phases were identified as main products of the oxidation layer, also SEM image revealed the presence of dendrite on the surface and cross-section of the Si_3N_4–ceramics. Data obtained from XRD indicate that crystallization of the glassy phase in the cross-section occurred.

References:

[1] Houjou, K.; Ando, K.; Chu, M. C.; Liu, S. P.; Sato S. *J. Eur. Ceram. Soc.* 2005, *25,* 559-567.
[2] Vetrano, J. S.; Kleebe, H. J.; Hampp, E.; Hoffmann, M. J.; Cannon, R. M. *J.Mater. Sci. Lett.* 1992, *11,* 1249-1252.

Tween-20 and oleic acid effect on TiO_2 nanoparticles morphology obtained by spray drying

M. Lorena García-Benjume,[a] Rigoberto López-Juárez,[b] E. Ortiz-Islas,[c] M. Eugenia Contreras-García,[d] Elder De la Rosa[a]

[a]*Centro de Investigaciones en Óptica, A. P. 1-948, León, Gto. 37150 México*
[b]*Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Circuito Exterior Ciudad Universitaria, Coyoacán 04510 México D.F.*
[c]*Instituto Nacional de Neurología y Neurocirugía, Insurgentes Sur 3877, Col. La Fama, Tlalpan, D.F. 14269 México.*
[d]*Instituto de Investigaciones Metalúrgicas, Universidad Michoacana de San Nicolás de Hidalgo, edificio "U" C.U. Morelia, Mich. 58060 México.*
E-mail: lbenjume@yahoo.com, elder@cio.mx

The interest to develop TiO_2 mesoporous materials in the nanosize regime have increased because the potential applications in solar cells, drug delivery and photocatalysis. In photocatalytic applications the band gap and the efficiency in rate of electron-hole recombination are important properties to study and improve. In this work spherical mesoporous aggregates of TiO_2 nanoparticles by self-assemble of TiO_2 nanoparticles was obtained using Tween-20 and Oleic acid as directing agents in non hydrolytic medium, in order to obtain spherical aggregates the spray drier method was employed. The X-ray diffraction patterns confirm that in all cases the anatase phase was obtained from 150°C. The morphology characterization by SEM suggests that spray dryer method generates aggregates with average sizes of *200-360nm* for Tween-20 and *780-970 nm* for Oleic acid. The surface area and mean pore diameter obtained by absorption-desorption Nitrogen isotherms present the characteristic behavior of mesoporous materials for TiO_2 synthesized with Oleic acid. The optical band gap was determined with the diffuse reflectance measurements and was estimated from 3-3.2 eV.

Photocatalytic activity of bismuth oxide thin films

J.C. Medina, M. Bizarro-Sordo, P. Silva-Bermudez, S.E. Rodil

Instituto de Investigaciones en Materiales-Universidad Nacional Autónoma de México
Circuito Exterior, Ciudad Universitaria, Coyoacán, C.P. 04510, México, D. F., Mexico.
E-mail: juan_mabermon@yahoo.com.mx

The magnetron sputtering technique was used to obtain Bismuth Oxide (Bi_2O_3) thin films having different crystalline phases. The results indicated that it was possible to obtain oxide films in the alpha, beta and delta phase, depending on the deposition conditions; substrate temperature and RF power. X-ray diffraction, X-Ray photoelectron spectroscopy (XPS), profilometry, scanning electron microscopy (SEM), and optical transmission were used to characterize the films. The photocatalytic activity for each one of the Bi_2O_3 phases was evaluated testing the degradation of methyl orange dye ($C_{14}H_4N_3SO_3Na$) under UV, white and solar irradiation. The rate of reaction of the delta-phase samples was nearly double that obtained for the other phases, probably due to the lower optical gap. The delta-phase films were the best to make the degradation of organic dye in an acid solution. However XPS tests showed that after a degradation cycle; bismuth oxide transforms to Bismuth Oxychloride (BiOCl) decreasing the photocatalytic effect of thin films.

Acknowledgement: The research leading to these results has received funding from the European Community Seven Framework Programme (FP7-NMP-2010-EU-MEXICO) and CONACYT under grant agreements nº 263878 and 125141, respectively.

Structural properties and stability of bismuth oxide thin films

O. Depablos-Rivera, [a] C. L. Gomez, [a] S. E. Rodil, [a] P. Silva-Bermudez, [a] E. Camps [b]

[a] *Instituto de Investigaciones en Materiales; Universidad Nacional Autónoma de México*
Circuito Exterior, Ciudad Universitaria,Coyoacán,C.P. 04510; México, D.F.
[b] *Instituto Nacional de Investigaciones Nucleares*
Carretera México-Toluca. La Marquesa, Ocoyoacac. C.P. 52750; Edo. México
E-mail: osmarydep@yahoo.com; zethli83@hotmail.com

Bismuth oxide thin films were deposited by reactive magnetron sputtering from a Bi_2O_3 target (99.95 at%) using RF and an Ar/O_2 atmosphere (80/20). The films were deposited on silicon substrates at 120 W and 150 °C. The films structure was obtained by X-ray diffraction and confirmed by Raman spectroscopy. Under the deposition conditions, the films showed the cubic delta-Bi_2O_3 phase, which is usually the stable phase of bulk bismuth oxide at high temperatures (725 – 850 °C). However, as a thin film, it has been shown that the delta-phase can be obtained even at room temperature conditions. The delta Bi_2O_3 has the highest ionic conductivity, which is searched for solid oxide fuel cell applications. In this work it was studied the structural stability of the delta-phase films as a function of the both thermal treatments in air and the storage-time. The films were storage under environmental conditions (25 °C, 760 Torr). The characterization results showed that the films crystalline structure remained unchanged (delta-Bi_2O_3) up to 225 °C. Higher temperatures lead to phase transitions into the beta-phase up to 360 °C; above this temperature, some regions started to show a mixture of phases and metallic bismuth. The films kept at ambient conditions were analyzed periodically, after a year no changes in the structure have been observed, which is a good indication.

Acknowledgement: The research leading to these results has received funding from the European Community Seven Framework Programme (FP7-NMP-2010-EU-MEXICO) and CONACyT under grant agreements nº 263878 and 125141, respectively.

Preparation and characterization of polymeric membranes mixed MCM-41 and MCM-48

A. Ramírez-Jaime, B.A. Puente-Urbina, Y. A. Perera-Mercado, L.A. García-Cerda

Centro de Investigación en Química Aplicada
Blvd. Enrique Reyna # 140. C.P. 25295. Saltillo, Coahuila. México
E-mail: jaraim1004@gmail.com

Ordered mesoporous particles MCM-41 and MCM-48 were obtained by hydrothermal method. The obtained particles were characterized by infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), differential scanning calorimetry (DSC) and adsorption-desorption nitrogen studies. The mesoporous silicas were modified with aminopropyltrimetoxisilane (APTMS) and then incorporated in two polymeric matrices: polycarbonate and polysulfone. Permeability and selectivity of the polymeric membranes were tested against pure CO_2 and CH_4. The CH4 permeability decreases when MCM48 particles are used, while the CO_2/CH_4 selectivity increased by adding both modified silica particles MCM-41 and MCM-48.

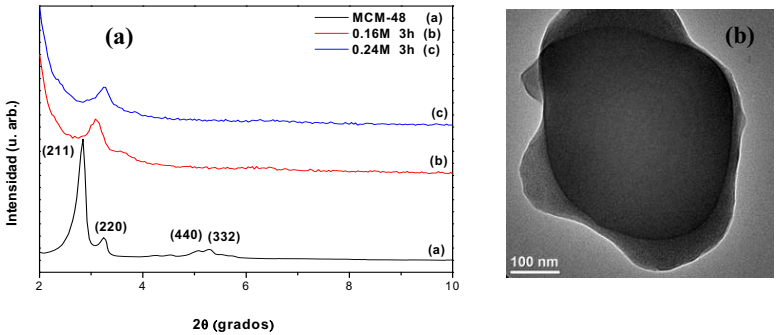


Figure 1: XRD patterns (a) and typical TEM image for funcionalized silica (b).

Producción y evaluación de nanopartículas de sílice sobre las propiedades mecánicas del cemento Portland compuesto 30R

Jaime Amador Schott Martínez, Yibran A. Perera-Mercado, Verónica Corral Flores, Sandra P. García-Rodríguez, José Luis Saucedo Morales

Centro de Investigación en Química Aplicada Blvd. Enrique Reyna Hermosillo #140, C.P. 25294; Saltillo, Coahuila, México.
E-mail: jaimeschott01@hotmail.com

El presente estudio se desarrolló con el propósito de sintetizar y evaluar la influencia de partículas de nanosilice (NS) sobre las propiedades mecánicas (resistencia a la compresión y a la flexión) en el cemento Portland compuesto 30 R (CPC-30R). Para ello, primero se sintetizaron nanopartículas de dióxido de silicio por el método sol-gel modificado con un agente surfactante no-iónico [1]. Se obtuvieron partículas de NS dispersas en medios acuosos a concentraciones entre 0.001 – 0.025% en peso de cemento, para sistemas de pastas que se rigen por las Normas ASTM-C109M-11b, ASTM-C348. Las NS fueron caracterizadas por microscopia electrónica de transmisión de alta resolución (MET-AR) y por espectroscopia de infrarrojo con transformada de Fourier (FTIR). Para evaluar la resistencia a la compresión de las pastas aditivadas con NS, se produjeron cubos de 125 cm3. De igual forma, se realizaron barras rectangulares de 2.54 x 2.54 x 12.7 cm para medir la resistencia a la flexión de estos nuevos sistemas. Todos los sistemas producidos cumplieron con las medidas de consistencia para pastas de cemento. Los ensayos de resistencia a la compresión y a la flexión se llevaron a cabo a 1, 14 y 28 días de envejecimiento de las probetas inmersas en una solución de agua con cal. En general, se observó que el sistema de CPC-30R + NS presenta un incremento de sus propiedades de resistencia a la compresión y de flexión respecto del blanco de cemento.

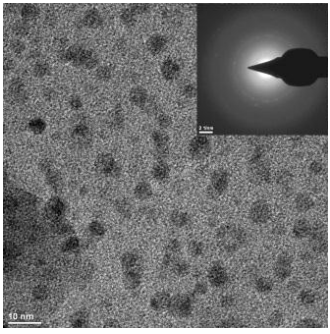


Figura 1: Imagen de MET-AR, Nanopartículas de Sílice sintetizadas.

Referencias:
[1] Y. Perera: “Preparation of nano-ceramics via aqueous sol-gel method modified with surfactans: an overview”; Materials Science Forum Vol. 644; (2010); pp. 79-84

Combustion synthesis and characterization of bimetallic nickel-copper nanoparticles

L.A. García-Cerda, E.L de León-Quiroz, B.A. Puente-Urbina, E.M. Saucedo-Salazar, E. Díaz-Barriga

Centro de Investigación en Química Aplicada
Blvd. Enrique Reyna # 140. C.P. 25295. Saltillo, Coahuila. México
E-mail: luis.garcia@ciqa.edu.mx

In this paper work, nanoparticles of nickel-copper have been synthesized by combustion route. Gel precursors were prepared using citric acid, ethylene glycol and nickel and copper salts and then the nanoparticles were obtained by calcination of the precursor in N2/H2 atmosphere. The influences of parameters, such as amounts of copper and nickel salts, the temperature and time of calcination time, were studied. The obtained nanoparticles were characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM). The studies carried out using XRD and TEM showed the alloy formation with spherical or rod morphology with an average size of about 40 nm and diameters between 120 and 250 nm while the length is of the order between 20 and 70 nm. Magnetic measurements reveal that the nanoparticles and nanorods are typical soft magnetic materials.

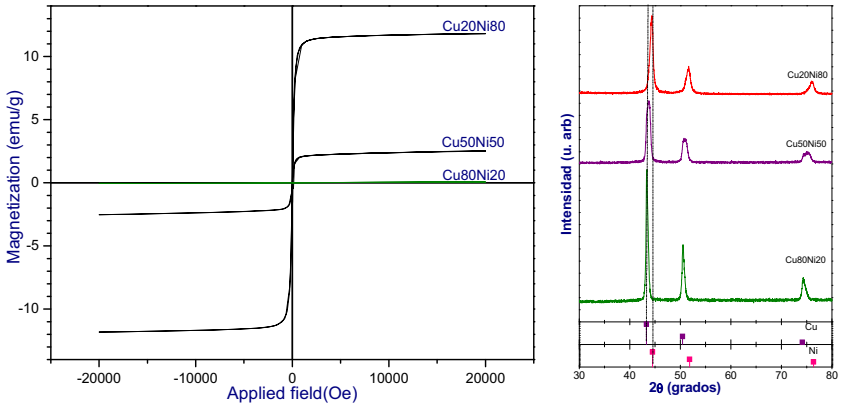


Figure 1. Hysteresis loops and XRD patterns for nickel-copper nanoparticles.

Monoclinic perovskite – orthorhombic perovskite $La_2Ti_2O_7$ to pseudo-cubic $LaTiO_3$ phase transition and their microstructure characterization

G. Herrera,[a,b] J. Jiménez -Mier[c]

[a] *Departamento de Química Inorgánica Universidad de Valencia, 46100 Burjassot Valencia, España*
[b] *Colegio de Física, ENP-P7, Universidad Nacional Autónoma de México, 04510 México D. F. México*
[c] *Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, 04510 México D. F. México*
E-mail: guillermo.m.herrera@uv.es

The layered-structural ceramics, such as lanthanum titanate ($La_2Ti_2O_7$), have been known for their good temperature and low dielectric loss at microwave frequencies that make them good candidate materials for high frequency applications. However, few studies have been conducted on the synthesis optimization by sol gel reaction, in particular by acrylamide polymerization route. The interest in $La_2Ti_2O_7$ ceramic has been greatly increased recently due to the effect of oriented grains. This anisotropy of the microstructure leads to anisotropy in dielectric, electrical and mechanical properties. In this study, grain oriented lanthanum titanate was produced by the sol-gel acrylamide polymerization route [1]. The characterizations of the samples were achieved by thermal analysis, X-ray diffraction (XRD), scanning electron microscopy (SEM), atomic force microscopy (AFM), and transmission electron microscopy (TEM). X-Ray diffraction indicates that the formation of monoclinic perovskite $La_2Ti_2O_7$ nanocrystals (with space group $P2_1$) is a necessary first step to obtain pseudo-cubic $LaTiO_3$ nanocomposites. The microstructure associated consisted of flaky monoclinic $La_2Ti_2O_7$ nanocomposites in comparison with round-shaped $LaTiO_3$ nanocomposites.

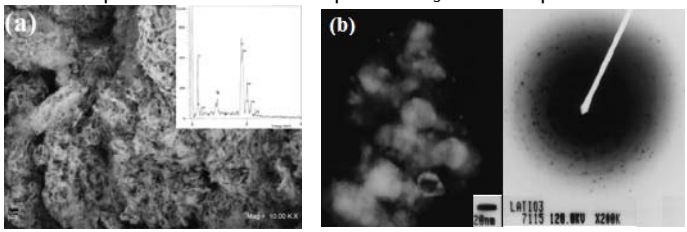


Figure 1: (a) SEM/EDX results for La-Ti powders obtained at 600 °C during 12h. (b) TEM micrograph of LaTiO3.

G. Herrera thanks Mexico-CONACyT for the student fellowships: Grant No. 170588; postdoctoral fellowship: Grant No. 129569 and No. 172529.

References

[1] **G. Herrera Pérez**, E. Chavira, J. Jiménez-Mier, A. Ordoñez, E. Bucio, L. Baños, J. Guzmán, E. Fregoso. *Micros. Micro.* 2007, 13, (2) 676-677

Vibrational spectrum and heat capacity of Au FCC nanoclusters

H. E. Sauceda,[a] F. Salazar,[b] L. A. Pérez,[a] I. L. Garzón[a]

[a] *Instituto de Física, Universidad Nacional Autónoma de México*
Apartado Postal 20-364, C.P. 01000, México D.F., México
[b] *Instituto Politécnico Nacional, ESIME-Culhuacan*
Av. Santa Ana 1000, 04430 D.F. México
E-mail: huziel8507@gmail.com, Fsalazar.Posadas@gmail.com, lperez@fisica.unam.mx, garzon@fisica.unam.mx

In this work, we report a theoretical study of the vibrational spectrum, vibrational density of states (VDOS) and caloric properties of Au nanoclusters with fcc structure as a function of their size. Our study is performed by using Gupta potential to determine the vibrational spectrum and focuses on the behavior of the specific heat in the low-temperature regime. The results show that the VDOS of small clusters is very different from the Au bulk one. The main difference is the existence of an acoustic gap in the vibrational spectrum which diminishes when the cluster size increases. The results also show that the effect of the acoustic gap is reflected directly in the behavior of the specific heat at the very low temperature region where we found that the specific heat path diminishes faster than the Debye T^3 law for the bulk. On the other hand, there is a temperature regime where the nanocluster specific heat is enhanced in comparison to the Au bulk one in concordance with experimental results recently reported in Fe nanoparticles [1].

Acknowledgments:
This work was supported by Secretaría de Ciencia Tecnología e Innovación del Distrito Federal (SECITIDF), projects ICyTDF/PICSO12-085, ICyTDF/325/2011, multidisciplinary project 2012-1439 from SIP-Instituto Politécnico Nacional and DGAPA-UNAM IN102511.

References:

[1] B. Roldan Cuenya, et. al., Phys. Rev. B 86, 165406 (2012).

Hybrid heterojunction solar cell based on Bi_2S_3 and P3HT

D. Esparza,[a] T. Lopez-Luke,[a] D. Villalobos,[b] E. de la Rosa[a]

[a] *Centro de Investigación en Óptica A.C*
[b] *Division de Ciencias Naturales y Exactas, Universidad de Guanajuato (UG)*
Loma del Bosque #115 Col. Lomas del Campestre, C.P. 37150 ; Leon, Guanajuato, México.
E-mail: desparza@cio.mx, elder@cio.mx

The effect of percolation concerns the movement of electrons in materials, higher carrier mobilities mean that charges are transported to the electrodes more quickly; which reduces current losses via recombination. Therefore, polymer photovoltaic devices rely on the introduction of another material for electron transport, which also provides the interface for charge transfer, producing the percolation effect. In this work, we present hybrid heterojunction devices based on polymer poly-3(hexalthiophene) (P3HT) and bismuth sulfide nanorods. Bismuth sulfide (Bi_2S_3) is used as the electron transport material and P3HT is an effective hole transport material. Bi_2S_3 is a metal chalcogenide semiconductor, the optical absorption spectrum is in the visible and near-infrared part of the solar spectrum, and these make it interesting for solar cell application. And the other hands, dispersing the inorganic nanorods at high density within P3HT to facilitate charge transfer. We obtain photovoltaic conversion efficiency enhancement whit different concentration of Bi_2S_3; analyze the fill factor and the incident photon to current conversion efficiency (IPCE).

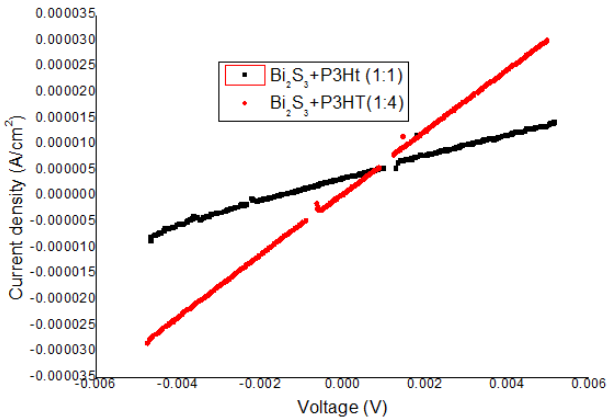


Figure. Characteristic current-voltage curve for different concentration of Bi_2S_3+P3HT

Estados quasi-estables de m_z de nanomagnetos bajo excitación de un campo magnético constante H_0 y un campo de microondas variable $H_1(t)$

V. L. Villegas Rueda,[a] E. Piña Garza,[b] A. E. Torres Zamudio[a] and R. Zamorano Ulloa[a]

[a]ESFM-IPN, Departamento de Física y Departamento de CM, UPALM-IPN, Av.IPN S/N, S. Pedro Zacatenco, C.P.07738, México D.F.
[b]UAM-I, Departamento de Física, Universidad Autónoma Metropolitana – Iztapalapa, P.O. Box 55 534, México, D.F., 09340 México.
E-mail: veyarle@yahoo.com.mx

El estudio de la dinámica de la magnetización de un material ferromagnético es, desde el punto de vista de ciencia básica, fundamental y necesario para entender las respuestas y posibles aplicaciones de los materiales ferromagéticos [1]. En particular esta el interés por los nanomagnetos que podrían ser aplicados en dispositivos micro y nanométricos si es posible inducir y controlar una respuesta magnética [2]. Nosotros estudiamos con dinámica no lineal el efecto de campo magnético constante H_0 y el efecto de campo variable de microondas $H_1(t)$ aplicados a un nanomagneto con monodominio, en un rango de parámetros experimentalmente posibles. Encontramos que a determinado valor de (H_0, H_1) la trayectoria de la magnetización **m** (t) tiene un patrón de estados cuasiestáticos-anillos de corta duración (<0.5ns) observados con mejor claridad a lo largo de la componente m_z. El número de anillos -N- en la trayectoria es independiente de las condiciones iniciales. La dinámica de **m** (t) se rompe (break down) naturalmente en al menos cuatro regiones de comportamiento: a) desde las condiciones iniciales, el inicio del movimiento, b) la parte media de la dinámica donde están incluidos los N estados cuasiestáticos de corta duración, c) la parte final de la trayectoria que incluye el acercamiento no monótono (justo previo a alcanzar el ciclo límite) de **m**(t) a una región acotada y estrecha de ángulos polares $\Delta\theta \leq 3°$) y d) la aproximación final al ciclo límite cercano a alinearse totalmente con el eje **z** . Este comportamiento de "cuantización" de la trayectoria en la dinámica de la magnetización es sorprendente y complejo, además de ser independiente de las condiciones iniciales. Lo más sorprendente es que se dé en un nanomagneto de dominio simple sin anisotropías magnéticas.

[1] R. Kikuchi, On the Minimum of Magnetization Reversal Time, J. Appl. Phys. 27, 11, 1352, 1956.
[2] M. Buer, et. al., Swiching behavior of a Stoner particle beyond the relaxation time limit, Phys. Rev. **61**, 5, 3410, 2000; Z. Z. Sun, et. al., Magnetization reversal through synchronization with a microwave, Phys. Rev. B **74**, 132401, 2006.

Shear and compression rheology of Langmuir monolayers of natural ceramides: Solid character and plasticity

Iván López-Montero,[a] Elisa R. Catapano,[a] Gabriel Espinosa,[b,c] Laura R. Arriaga,[b] Dominique Langevin[b] and Francisco Monroy.P[a,b]

[a] *Departamento de Química Física I, Universidad Complutense, 28040 Madrid, Spain*
[b] *Laboratoire de Physique des Solides, Université Paris Sud XI, 91405 Orsay, France*
[c] *Instituto de Física y Matemáticas, Universidad Michoacana de San Nicolás de Hidalgo, 58060 Morelia, Michoacán, Mexico*
E-mail: gespinosa@ifm.umich.mx

The present work addresses the fundamental question of membrane elasticity of ceramide layers with a special focus on the plastic regime. The compression and shear viscoelasticity of egg-ceramide Langmuir monolayers were investigated using oscillatory surface rheology in the linear regime and beyond. High compression and shear moduli were measured at room temperature, a clear signature for a solid behavior. At deformations larger than one per mill, egg-ceramide monolayers display plastic features characterized by a decrease of the storage modulus followed by a viscous regime typical of fluid lipids. This behavior is accompanied by a marked decrease of the loss modulus with increasing stress above a yield point. The results permit to univocally classify ceramide monolayers as 2D-solids able to undergo plastic deformations, at the difference of typical fluid lipid monolayers. These unusual features are likely to have consequences in the mechanical behavior of ceramide-rich emplacements in biological membranes.

Dipolar interaction in arrays of magnetic nanotubes

Y. Velázquez-Galván,[a] J. M. Martínez-Huerta,[a] J. De La Torre Medina,[b]
Y. Danlée,[c] L. Piraux,[c] A. Encinas[a]

[a] *Instituto de Física, Universidad Autónoma de San Luis Potosí, Mexico*
[b] *Facultad de Ciencias Físico-Matemáticas, Universidad Michoacana de San Nicolás de Hidalgo, Morelia, Mexico*
[c] *Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium*
E-mail: armando.encinas@gmail.com

Arrays of nanotubes (NTs) either continuous or in multilayer have recently gained a lot of interest since they are promising for future applications and devices [1-3]. Cylindrical nanotubes are expected to show a behavior close to that of NWs, however differences between them are known and they relate to the demagnetizing factor and their volume, in particular the volume difference changes the effective packing fraction and thus the value of the dipolar interaction field [4,5].

In this work, the dipolar interaction field in arrays of tall nickel nanotubes has been investigated by means of expressions derived from the effective demagnetizing field of the assembly as well as magnetometry measurements and comparison with the corresponding solid nanowires. The results show that the interaction field in nanotubes is smaller than the one in solid nanowires and these differences have been related to the lowering of the packing fraction in nanotubes with respect to nanowires due to their inner cavity. Furthermore, the dependence of the interaction field as a function of the nanotube wall thickness is determined from the model and shows good agreement with the experimental values. Finally, a simple expression is derived to calculate the nanotube wall thickness using the measured values of the interaction field, whose results show a good agreement with those measured by scanning electron microscopy.

References

[1] S. J. Son, et al, *J. Am. Chem. Soc.* **127**, 7316 (2005).
[2] K. Nielsch, et al, *Adv. Eng. Mater.* **7**, 217 (2005).
[3] K. Pitzschel, et al, *Nanotechnol*ogy **23**, 495718 (2012).
[4] M. Beleggia, et al, *J. Magn. Magn. Mater.* **321**, 1306 (2009).
[5] B. Nam, et al, *J. Appl. Phys.* **111**, 07E347 (2012).




Chairman

Oracio Navarro (IIM-UNAM, SMF)

Local Organizing Committee

Yesenia Arredondo León (IIM-UNAM)
Milton Muñoz Navia (INAT-UCM)
Alan Dierick Ortega Gutiérrez (IIM- UNAM)

Organizing Committee

Elder de la Rosa (CIO, SMF)
Takeuchi Noboru (CNyN-UNAM)
Gian Carlo Delgado Ramos (CEIICH-UNAM)
Rodolfo Zanella (CCADET-UNAM)
Claudia Gutiérrez Wing (ININ)
José Luis Rodríguez López (IPICyT)