6th Mexican Workshop on Nanostructured Materials

October 12–14, 2016

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Abstract Book

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FOREWORDS

The 6th Mexican Workshop on Nanostructured Materials, like its preceding versions is aimed to provide a common forum for the scientists and students involved in the design, synthesis, and application of nanomaterials in Mexico for presenting their research results and exchange scientific views and informations.

The Workshop is focused on all aspects of nanomaterials; from design and synthesis, physical and chemical phenomena associated to nanometric materials for their practical applications. Among the emerging fields of research, fabrication, characterization and application of nanomaterials became some common areas of interest for the physicists, chemists, materials scientists, and technologists.

We, the organizers, tried to bring together some eminent scientists, experts in the fields of nanomaterial and nanotechnology as invited speakers to provide an opportunity for the young researchers to update their knowledge on the recent progress in this highly emerging research filed. Although the first version of this event was a small gathering, the number of participants increased substantially in its following versions.

With the persisting constrains and small budget, keeping in mind the demand and necessity of young researchers of Mexico, the organizers arranged two courses on the *electron microscopic characterization of materials* and *fabrication of porous materiales through electrochemical techniques,* delivered by two experts in these fields, 12 invited talks by eminent scientists and nanomaterial specialists of Mexico, United States, Spain, Brazil and Argentina, 9 oral presentations and 73 presentations in the form of poster.

The proceedings of the workshop containing full-length papers submitted by the participants will be published in a special issue of the journal Advances in Nano Research (Techno Press, KIST, Korea) after rigorous screening and reviewing by experts. Therefore, all the participants are advised to prepare their full-length articles according to the guidelines of the journal and submit before November 15, 2016.

We wish to express our sincere thanks to the sponsors of the workshop for their valuable supports. We are grateful to the invited speakers and the members of the organizing committee for their contributions and help to make the event successful.

Puebla, October 10, 2016.

Umapada Pal (Chairman)

On behalf of the Organizing Committe

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COURSES

Fabricación electroquímica de nanoestructuras porosas

Carmen Magdalena Reza San Germán

Instituto Politécnico Nacional, UPALM, Zacatenco, ESIQIE edif. Z-5, 2º piso.

E-mail: creza@ipn.mx

Existen infinidad de métodos de síntesis para la fabricación de membranas porosas, dividiensose estos en métodos químicos y electroquímicos, los cuales a su vez se pueden calisifcar en medios acuosos y no-acuosos. Siendo estos últimos los más empleados para tal efecto.

De entre los métodos acuosos existen aquellos basados a la primera Ley de Faraday, la cual establece que: la masa de una sustancia depositada en un electrodo es directamente proporcional a la cantidad de electricidad que pasa a través de la disolución electrolítica [1]. Por lo que, de acuerdo a dicha ley, se puede realizar la síntesis de membranas nanoporosas por un medio electroquímico, este método es comúnmente llamado: anodizado electroquímico o polarización positiva, en donde, al contrario de un método electroquímico convencional, la membrana crece en el ánodo de la celda electroquímica y en el cátodo habrá desprendimiento de hidrógeno. Aunado a esto, en dicho método en lugar de utilizar una sal como electrolito se emplea un ácido, y cuando se controlan los parámetros de síntesis (voltaje, densidad de corriente, concentración, tipo y concentración del electrolito, temperatura) es posible generar membranas con diferentes espesores y tamaños de poro.

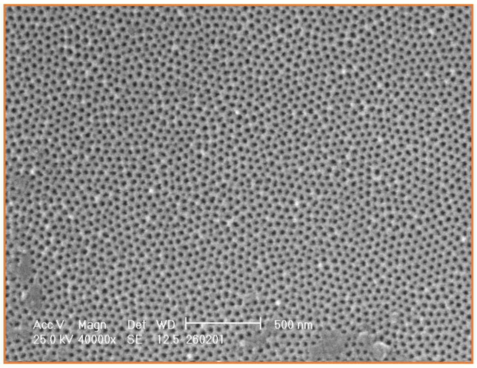

Figure 1. Micrografía típica de membrana de Al_2O_2.

[1] Ríos Dolores, Teoría básica de Electroquímica por objetivos. Instituto Politécnico Nacional. 1978. p-73

Análisis de imágenes obtenidas por TEM de alta resolución

Patricia Santiago Jacinto

Instituto de Física, UNAM, Circuito de la Investigación s/n, Ciudad Universitaria,

México, D.F., Mexico.

E-mail: paty@fisica.unam.mx

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INVITED TALKS

Plasmonic analytical tools for sensing and targeting biomolecules

Eduardo A. Coronado, Pablo Mercadal and Juan C Fraire

INFIQC-CONICET Departamento de Fìsioquimica, Facultad de Ciencias Químicas,
Universidad Nacional de Córdoba, Córdoba, (5000), Argentina.

E-mail: coronado@fcq.unc.edu.ar

The combination of the extraordinary optical properties of noble metal nanoparticles (NPs) (specially Ag and Au) with the capabilities of target recognition given by biomolecules has given rise in recent years to the interdisciplinary field called Bionanoplasmonics. In this presentation, I will give our recent research performed in our group concerning this issue. In particular I will discuss the design of plasmonic probes for localizing and quantifying receptors in neural cells, using a convenient functionalization of Au NPs and the development of a novel analytical tool for antigen quantification in real samples using conventional UV-Vis spectroscopy based on the change of the optical properties of biofunctionalized colloidal Au NPs in the presence of specific antigens. This last technique for antigen quantification will be demonstrated to be over 100 times more sensitive and 5 times less expensive than the conventional ELISA (Enzime Linked Immunosorbent Assay) methodology used for this purpose in clinical biochemical laboratories, without the need of any additional expensive equipment.

We acknowledge the financial supports from CONICET, FONCYT and SECYT-UNC.

[1] J.C. Fraire, M. Lujan Masseroni, I. Jausoro, E.Perassi, A.M. Diaz Anel and E.A. Coronado, *ACS Nano* **2014**, *8*, 8942.
[2] J.C. Fraire, R.D. Motrich and E.A. Coronado, *Nanoscale*, **2016**, in press.

Controlling the assembly and welding of gold nanorods by means of femtosecond laser pulses

O. Peña-Rodríguez[1], G. González-Rubio[2,3], J. González-Izquierdo[2],
L. Bañares[2], G. Tardajos[2], Antonio Rivera[1], T. Altantzis[4], S. Bals[4],
A. Guerrero-Martínez[2] and Luis M. Liz-Marzán[3,5]

[1]Instituto de Fusión Nuclear, Universidad Politécnica de Madrid, Spain; [2]Departamento de Química Física I, Universidad Complutense de Madrid, Spain; [3]BioNanoPlasmonics Laboratory, CIC biomaGUNE, Spain; [4]EMAT-University of Antwerp, Belgium; [5]Ikerbasque, Basque Foundation for Science, Spain.

E-mail: ovidio@bytesfall.com

Directed assembly of gold nanorods using dithiolated molecular linkers is one of the most efficient methodologies for the morphologically controlled tip-to-tip assembly of this type of anisotropic nanocrystals but this process is characterized by difficulties in chain-growth control over nanoparticle oligomers. We have devised a light-controlled synthetic procedure where selective inhibition of the formation of gold nanorod trimers is attained by exciting the longitudinal localized surface plasmon resonance with 800 nm femtosecond laser pulses, allowing efficient trapping of the dimers by hot spot mediated photothermal decomposition of the interparticle molecular linkers. Laser irradiation at higher energies produces near-field enhancement at the interparticle gaps, which is large enough to melt gold nanorod tips, offering a new pathway toward tip-to-tip welding of gold nanorod oligomers. Optical and electron microscopy characterization indicates that plasmonic oligomers can be selectively trapped and welded, which has been analyzed in terms of a model that predicts with reasonable accuracy the relative concentrations of the main plasmonic species.

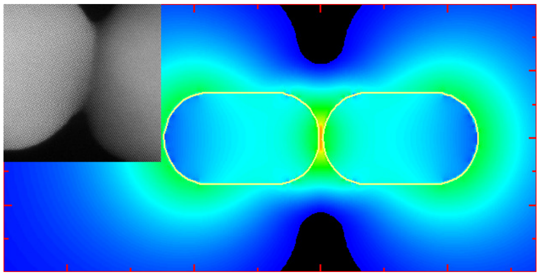

Figure 1. Local field enhancement contour plots in the middle plane for Au nanorod dimers and (inset) high resolution HAADF-STEM images of the connection points between the rods.

This work has been funded by the Spanish MINECO (MAT2012-38541, MAT2013-46101-R, MAT2014-59678-R and CTQ2012-37404-C02-01) and the European Research Council under the Seventh Framework Program (ERC Grant No. 335078 COLOURATOMS).

Sensing applications of porous silicon-metal oxide hybrid structures

V. Agarwal

Centro de Investigación en Ingeniería y Ciencias Aplicadas, UAEM, Av. Universidad
1001, Col. Chamilpa, Cuernavaca, Morelos, CP 62209, Mexico.

E-mail: vagarwal@uaem.mx

Different metal oxide- porous silicon hybrids (VO_2-PS, SnO_2-PS and ZnO-PS) have been synthesized, characterized and tested as optical/electrical sensors. An effective optical response of VO_2-PS hybrid structure was studied in terms of red/blue shift of the reflectance spectra, as a function of temperature. As compared to VO_2 film over crystalline silicon substrate, the hybrid structure (PS-VO_2) is found to demonstrate up to 3-fold increase in the change of reflectivity with temperature for its potential application as a thermally-triggered optical sensor. On the other hand, gas sensing properties of SnO_2/MPS and ZnO/MPS nanostructures were studied as a function of CO_2 gas concentration and operation temperature (upto 300 °C). Porous silicon templates greatly improve the gas-sensing properties of metal oxides at low temperatures with respect to the metal oxide thin films over c-Si/glass substrates. Irrespective of the deposition method, the ZnO/MPS sensor showed higher gas response values than SnO_2/MPS device due to its high specific surface area resulting from the porosity dependent micro/nanostructures formed in the former case. Such silicon-based hybrids represent an exciting class of cost effective, multifunctional materials and sensing devices compatible with standard (integrated circuit) IC technology.

Designing the plasmonic modes in nanoparticles and radiative heat transfer

Cecilia Noguez

Instituto de Física, Universidad Nacional Autónoma de México, Cd. México, México.

E-mail: cecilia@fisica.unam.mx

Metal nanoparticles (NPs) exhibit remarkable physical and chemical properties, which are morphology-dependent [1]. Particular interest has been paid in the optical response of NPs because their surface plasmon excitations strongly couple with external light. At the nanoscale, this physical property conducts to new phenomena because these surface plasmon resonances are localized and consequently they enhance the near electromagnetic field [2]. This latter can be used for significantly increasing the sensitivity of optical spectroscopies, and can be of importance in heat transfer at the nanoscale. In this presentation, we present a formalism to obtain the plasmonic response of isolated NPs with complex morphologies, where morphology and composition are varied at the same time [3,4]. Then, we extend our formalism to study the near field between two NPs. Finally, we discuss how it can be employed to calculate the radiative heat transfer between two or more spherical NPs.

[1] C. Noguez, Surface Plasmons on Metal Nanoparticles: The Influence of Shape and Physical Environment, J. Phys. Chem. C 111, 3806 (2007).

[2] C. Noguez, C. J. Villagómez, and A. L. González, Plasmonics of multifaceted metallic nanoparticles, field enhancement, and TERS, Phys. Status Solidi b 252, 56 (2015).

[3] C. E. Román-Velázquez, C. Noguez, Designing the plasmonic response of shell nanoparticles: spectral representation, J. Chem. Phys. 114, 044116 (2011).

[4] R. Díaz-HR, R. Esquivel-Sirvent, C, Noguez, Plasmonic Response of Nested Nanoparticles with Arbitrary Geometry, J. Phys. Chem. C 120, 2349 (2016).

Local Atomic structural changes detected through X-ray Absorption Spectroscopy in Nanostructured Materials

Juan S Lezama Pacheco, John R. Bargar, Scott E. Fendorf and Julio Villanueva Cab

Stanford Univesity, Stanford CA, USA; SLAC National Accelerator Laboratory, Menlo Park CA, USA; Benemerita Universidad Autonoma de Puebla, Puebla, Mexico.

E-mail: jlezama@stanford.edu

Over the past two decades, X-ray Absorption Fine structure spectroscopy (XAFS) has emerged as a powerful technique for the characterization of materials, Recent advances in X-ray generation and instrumentation have allowed to obtain structural atomic details, in nano-structured and other complex materials, that are not readily available through more conventional techniques. Moreover, the element specificity of the technique allows the analysis of the same material from the perspective of each one of the elements present. This opens the possibility of studying materials not only from the perspective of its main components, but also from the point of view of dopants, mono-atomic layer coatings, to mention a few.

In this talk I will present some examples in an effort to illustrate the applicability of XAFS to nano-structured materials, not only relevant to materials but also to environmental sciences. In addition to these specific examples, I will present some guidelines, in order to "demistify" the experience of using these techniques. These guidelines could potentially help establish a research program that takes advantage of X-ray spectroscopies, opening up a new set of answers in the solution of complex inquires in materials science research.

Nanomaterials for solar energy conversion systems

Gerko Oskam

Department of Applied Physics, CINVESTAV-IPN, Mérida, Yucatán 97310, México.

E-mail: gerko.oskam@cinvestav.mx

In this presentation, an overview will be given of the research in our group in the Department of Applied Physics at CINVESTAV-Mérida (Yucatán, México) on the application of nanomaterials in a variety of solar energy systems, including photovoltaics, solar fuels, and solar-thermal energy conversion.

In photovoltaics, the efforts in our group are focused on the dye-sensitized solar cell (DSC), which is based on a mesoporous, nanostructured metal oxide substrate. We have investigated the influence of the nanomaterials properties on the performance of the solar cells, using TiO_2 in both the anatase and brookite form, and ZnO prepared by a variety of methods and with a range of morphologies. We also are making progress in the scale-up of the technology fabricating mini-modules of 24 cm^2, reaching an efficiency of 4.8% for the DSCs based on anatase (in active area).

In the solar fuels research project, we use a combinatorial technique to find new metal oxide nanomaterials for solar water splitting. In addition, we use advanced (photo)electrochemical methods in order to study the fundamental processes taking place in promising nanomaterials. Recent work has shown interesting results for the p-type semiconductor $CuBi_2O_4$, and we have analyzed the hole transport and recombination properties using intensity-modulated methods, including photovoltage (IMPV) and photocurrent spectroscopy (IMPS). In addition, we have investigated water oxidation on WO_3 electrodes in detail, using the same techniques for electron transport measurements.

In the solar-to-thermal project, we focus on selective coatings that efficiently absorb sunlight but with a low thermal emittance, thus optimizing the conversion efficiency and minimizing loss processes. We use both electrodeposition and sputtering to prepare selective coatings, using cermet and multilayer stack approaches in order to tailor the optical properties of the thin films. Specific examples for Ni and Co black, and Al_2O_3-MoO_x-Al_2O_3 systems will be presented.

Thermally and optically stimulated luminescence in strontium aluminates long persistent phosphors

N.J. Zúñiga-Rivera[1], P. Salas-Castillo[2], L.A. Díaz-Torres[3], R. Meléndrez[4], V. Chernov[4], R. García[4], A. N. Aldaco-Gastélum[4] and M. Barboza-Flores[4]

[1]Departamento de Física, Posgrado en Nanotecnología, Universidad de Sonora, Hermosillo, Sonora 83100, México; [2]Departamento de Nanotecnología. Centro de Física y Tecnología Aplicada y Tecnología Avanzada, UNAM. Juriquilla, Qro. México; [3]Centro de Investigación en Óptica, Lomas del Bosque 115, Lomas del Campestre, 37150 León, Gto. México; [4]Departamento de Investigación en Física, Universidad de Sonora, Hermosillo, Sonora, 83000, México.

E-mail: mbarboza@cifus.uson.mx

We report on the thermally and optically stimulated luminescence properties of $Sr_4Al_{14}O_{25}$:Eu/Dy:$B_{0.4}$ and $Sr_4Al_{14}O_{25}$:Eu/Nd:$B_{0.4}$ long persistent phosphors synthetized by the combustion method using urea (CH_4N_2O) as fuel. The highly exothermic redox reaction between the metal nitrates and organic fuel is in excess more convenient than using solid reaction method. After exposure to low dose beta radiation the phosphors exhibit ultra-long strong afterglow with a typical multiple exponential decay curve, which is attributed to the thermal activation of holes from a trap distribution followed by the emission of $4f^{6}5d \rightarrow 4f^{7}$ transition of Eu^{2+} ion. We investigate the thermoluminescence (TL), optically stimulated luminescence (OSL) and afterglow (AG) properties in powder samples of $Sr_4Al_{14}O_{25}$:Eu/Dy:$B_{0.4}$ and $Sr_4Al_{14}O_{25}$:Eu/Nd:$B_{0.4}$ exposed to beta radiation using a Risø TL/OSL-DA-20 reader. The TL glow curve of $Sr_4Al_{14}O_{25}$:Eu/Dy:$B_{0.4}$ consist of two broad peaks located around 125°C and a lower intensity peak at 325°C, while the TL of $Sr_4Al_{14}O_{25}$:Eu/Nd:$B_{0.4}$ exhibits a main peak at 225°C and low intensity one around 100 °C. The samples exhibit green persistent luminescence or afterglow (AG) due to thermal emptying of trapped charge carriers at low temperature trapping levels. The integrated TL as a function of dose shows a linear behavior for doses below 1.0 Gy and saturates for doses higher than 30 Gy. A strong OSL signal is observed in previously irradiated samples after stimulation with 870 nm IR light with a similar dose behavior. In conclusion both phosphors were successfully synthesized by the combustion method and exhibit strong persistent luminescence features as well as integrated TL/OSL linear low dose behavior.

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Cathodoluminescence of nanomaterials

M. Herrera-Zaldivar

Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México,
km 107 carretera Tijuana-Ensenada, Ensenada, Baja California C.P. 22800, México.
E-mail: zaldivar@cnyn.unam.mx

In this work, we present some results of the cathodoluminescence (CL) technique used for characterization of point defects in GaN, SnO_2, ZnO, and hydroxyapatite (HAp) nanostructures, generated by incorporation of different impurities. CL results of GaN nanowires doped with oxygen, at several concentrations, show the generation of an emission of 2.68 eV that increased in intensity with the oxygen content. We have attributed this band to the electronic transitions between donor substitutional-oxygen (ON) and acceptor interstitial-oxygen (O_i) states [1]. CL results of N-doped SnO_2 nanowires show the generation of a defect-related emission centered at 2.0 eV, which decreases in intensity with the nitrogen content in samples. We have assigned this behavior to the decreases of oxygen vacancies in SnO_2 [2]. A CL study of ZnO:Ag nanowires reveals that Ag incorporation does not generate a significant amount of point defects in the wurtzite structure. Furthermore, we have used the CL technique to determinate the valence state of Eu and Yb ions incorporated in HAp nanocrystals. Monochromatic CL images obtained from Eu-doped HAp reveal that Eu^{2+} ions are distributed homogeneously in the entire crystal volume, while the Eu^{3+} are present mainly at the crystal edges [3]. CL spectra of Yb^{2+} ions incorporated in HAp nanocrystals show a series of sharp peaks centered at 3.27, 2.98, 2.85, 2.53, 2.27, 2.09 and 1.06 eV, corresponding to transitions between multiple levels produced by a trigonal distortion of the regular octahedral crystal field of the Yb^{2+} $4f^{13}5d$ configuration. Similarly, CL spectra of Yb^{3+} ions show three emissions centered at 1.16, 1.22 and 1.26 eV, generated by interconfigurational transitions between the $^2F_{5/2}$ and $^2F_{7/2}$ states of Yb^{3+} ions.

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References.
[1] Guzman G, Herrera M, Silva R, Vásques G C and Maestre D (2016) *Semicond. Sci. and Technol.* **31**, 055006. DOI: 10.1088/0268-1242/31/5/055006.
[2] Montalvo D and Herrera M (2016) *AIMS Materials Science* **3**, 525. DOI:10.3934/matersci.2016.2.525
[3] Zavala L, Hirata G, Novitskaya E, Karandikar K, Herrera M and Graeve O. (2015) *ACS Biomater. Sci. Eng.* **1** 1305. DOI: 10.1021/acsbiomaterials.5b00378

Bicontinuous microemulsions as templates for the synthesis of hierarchical Pt nanostructures and their electrochemical characterization

M. Sánchez-Domínguez[1], L. Khalil-Cruz[2] and M. Videa[2]
[1]*Centro de Investigación en Materiales Avanzados, S. C. (CIMAV), Unidad Monterrey; GENES-Group of Embedded Nanomaterials for Energy Scavenging. Monterrey, México;*
[2]*Departamento de Química y Escuela de Ingeniería y Ciencias. Instituto Tecnológico y de Estudios Superiores de Monterrey (ITESM). Monterrey, México.*
E-mail: margarita.sanchez@cimav.edu.mx

In contrast to the use of W/O and O/W microemulsions for the synthesis of inorganic nanoparticles [1], reports on the use of bicontinuous microemulsions are more scarce. Few examples include the synthesis of ZnO and Pt NPs [2,3]. The motivation was to increase the yield of nanoparticles obtained per microemulsion volumen, whilst keeping a narrow particle size distribution (usually below 10 nm). In all of these investigations, the precursors used were incorporated in the aqueous phase. Usually, well-dispersed, isolated spherical NPs were formed; in some cases, random agglomeration was observed. Since in a bicontinuous microemulsion, both the oil phase and the aqueous phase have nanometric channels, it is feasible to use oil-soluble precursors and still obtain nanoparticles or a nanostructure. In this investigation, we used bicontinuous microemulsions based on the system water / Synperonic 91/5 / isooctane for the synthesis of Pt nanostructures. The use of both water-soluble and oil-soluble Pt precursors were compared. A hierarchical nanostructure made by interconnected NPs and nanoneedles was obtained with the oil-soluble precursor. Cyclic voltammetry carried out between 1.3 V and -0.3 V vs. Ag|AgCl allowed to estimate the surface area of these materiales in the hydrogen adsorption region, resulting in values of 27 and 29 m^2/g for materials obtained using water-soluble and oil-soluble precursors, respectively. These results demonstrate the usefulness of employing certain bicontinuous microemulsion systems for the synthesis of hierarchical nanostructures.

[1] Sanchez-Dominguez, M.; Pemartin, K.; Boutonnet, M. *Curr Opin Colloid Interface Sci* **2012**, *17*, 297.
[2] López-Cuenca, S. Pérez, L.; Rabelero, M.; Díaz, R.; Saade, H.; López, R.; Mendizábal, E.; Puig, J. *J Nanomater* **2011**, Article ID 431382.
[3] Latsuzbaia, R.; Negro, E.; Koper, G. *Faraday Discuss.* **2015**. 181, 37.

Ag-Bi and Pd-Ag nanoalloys: experimental approach

Víctor-Fabián Ruiz-Ruiz[1], Rebeca Díaz-Pardo[3], David Díaz[1], Israel Betancourt[3],
Inti Zumeta-Dubé[1], Rodrigo González-Olvera[2], Norberto Farfán[2],
María Josefina Arellano-Jiménez[4] and Miguel José Yacamán[4]

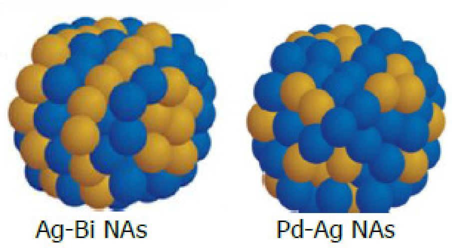
[1]Departamento de Química Inorgánica y Nuclear, Facultad de Química; [2]Departamento de Química Orgánica, Facultad de Química; [3]Departamento de Materiales Metálicos y Cerámicos, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Coyoacán, Ciudad de México, C.P. 04510, México; [4]Department of Physics and Astronomy, University of Texas at San Antonio, One UTSA Circle. San Antonio, TX 78249.

E-mail: david@unam.mx

In this contribution the characterization of several $M_{(100-x)}Ag_x$ nanoalloys, where M = Bi or Pd, is discussed. These nanostructured $M_{(100-x)}Ag_x$ alloys are prepared by a novel mechano-chemical pathway, using a conventional reducing agent, under room conditions and without large amounts of solvents.

The bulk Bi-Ag alloy system comprises a wide forbidden range of Ag solubility limited to a negligible molar fraction. In this work it is unambiguously demonstrated that Ag and Bi, elements with various in-common potential applications, can be alloyed at the nanoscale, which is quite different from the bulk form. The characterization of this sort of nanoparticles by combination of UV-visible absorption and Raman spectroscopies as well as SEM, HR-TEM, XRD, XPS and DSC lead to the finding of these sui-generis nanoalloys and the unprecedented proposal of a predominantly atomic mixed alloyed structure for the $Bi_{(100-x)}Ag_x$ $(0.1 \leq x \leq 0.5)$ clusters.

Furthermore, palladium nanoparticles have been widely studied mainly because of their magnetic properties different from bulk palladium and also, due to their catalytic properties. Here the structural and magnetic properties, as well as the catalytic activity of $Pd_{(100-x)}Ag_x$ nanoalloys are disclosed. Pd-Ag nanoalloy particles were produced with sizes ranging within 5 - 20 nm, according to HR-TEM. The incorporation of Ag atoms into the Pd unit cell was verified by X-ray diffraction analysis and UV-visible absorption spectroscopy. The magnetic response at room temperature was paramagnetic for all the studied compositions nevertheless, a mixed ferromagnetic-paramagnetic behavior was observed for low temperature measurements (5 K). The catalytic activity of these Pd-Ag nanoparticles was evaluated in a Suzuki-Miyaura reaction, in an aqueous media. In all cases, Pd-Ag nanoparticles show excellent catalytic activity with low palladium catalyst loading and the catalyst can be reused for five cycles without any significant loss of activity.



Synthesis, morphology and applications of iron oxide nanocomposites

M. A. G. Soler

Universidade de Brasília, Institute of Physics, Nanofilms and Nano Devices Laboratory,
70910-900, Brasília, DF, Brazil.

E-mail: soler@unb.br

The development of hybrid systems comprising nanoparticles and polymers is opening pathways for engineering nanocomposites exhibiting outstanding mechanical, optical, electrical, and magnetic properties. Among inorganic counterpart, superparamagnetic iron oxide particles exhibit high magnetization, controllable surface chemistry, spintronic properties, and biological compatibility. These characteristics enable them as a platform for biomedical applications and building blocks for bottom-up approaches, such as the layer-by-layer (LbL) [1]. LbL technique comprises the alternate adsorption of oppositely charged entities, being a versatile tool to produce nanostructures at very low cost with tailored properties. Further, these assemblies can be designed as erodible multilayers to be applied in transcutaneous drug delivery. Nanocomposites comprising ION and polymers can exhibit collective magnetic properties arising from inter-particle interactions. These interactions may be tuned by a fine control of particle characteristics, as well as its spatial distribution inside the matrix. This talk will summarize new initiatives taken in the area of colloidal IONs and its arrays in polymeric matrix related research for understanding fundamental issues such as the effect of nanocomposite morphology on the collective magnetic properties, through experimental and simulations, performed to assess both, the nanofilm's morphology and the corresponding magnetic signatures. Applications leading to future developments comprising these nanomaterials, as for instance chemical sensors, capacitor electrodes, and drug delivery systems, will also be highlighted.

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[1] Alcantara, G.B. et al., *Phys. Chem. Chem. Phys.* **2011**, 13, 21233.
[2] Neumann, R.F. et al. *J. Magn. Magn. Mater.* **2013**, 347, 26.

Improved activity and stability in CO oxidation and water splitting of bimetallic Au-Cu/TiO_2 catalysts

R. Zanella, A. Sandoval and Socorro Oros
Centro de Ciencias Aplicadas y Desarrollo Tecnológico, Universidad Nacional Autónoma de México, Ciudad de México, México.
E-mail: rodolfo.zanella@ccadet.unam.mx

Au-Cu bimetallic catalysts supported on TiO_2 were prepared by sequential deposition-precipitation with the urea method, copper first then gold. Au-Cu catalysts with four different Au:Cu atomic ratios were synthesized (1:0.4 to 1:1.2). This method allowed quantitative deposition of both copper and gold and the formation of small metal particles. Characterization by TPR and by DRIFTS coupled with CO adsorption showed that when the samples were activated in air at 300°C gold was present in metallic form, copper in the form of an oxide, and Au and Cu were in interaction, probably forming a Au/CuO/TiO_2 system. When the catalysts were activated in hydrogen at 300 °C, the metal particles were smaller (2 nm) and bimetallic. The activation of Au-Cu catalysts in air at 300°C produced more active catalysts than the activation under hydrogen at the same temperature. However, whatever the activation procedure, the highest catalytic activity in CO oxidation was obtained for the catalyst with an Au:Cu ratio of 1:0.9. This calcined catalyst also presented a TOF almost 3 times higher and a better temporal stability than monometallic gold catalysts in the reaction of CO oxidation at 20°C. Compared to monometallic catalysts, the better catalytic results obtained with calcined Au-Cu/TiO_2 indicate a promoting effect between gold and copper oxide in the reaction of CO oxidation [1]. The Au–CuO_X/TiO_2 samples were also evaluated in the photocatalytic water splitting reaction. It was shown that Au–CuO_x/TiO_2 effectively increased the hydrogen production (2064 $\mu mol.h^{-1}.g^{-1}$) obtained by Au/TiO_2 (1204 $\mu mol.h^{-1}.g^{-1}$). The higher photoactivities achieved by Au–CuO_x nanoparticles deposited on TiO_2 were attributed to an enhancement of the electron charge transfer from TiO_2 to the Au–M_xO_y systems and the effect of surface plasmon resonance of gold nanoparticles [2, 3].

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[1] A. Sandoval, C. Louis, R. Zanella, Appl. Catal. B. 140-141 (2013) 363-377

CONTRIBUTED TALKS

Shape and size effects on the near-field optical properties of Au and Ag nanoparticles

M. A. Ibarias and A. L. González

Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apartado Postal J48, 72570, Puebla, México.

E-mail: anagr@ifuap.buap.mx

For Surface Enhanced Raman Scattering (SERS) applications, Au and Ag are the mostly used metals due to the high Raman response observed in their presence. Particularly, at nanoscale, the Raman response of the molecules is enhanced when they are very close to the surface of plasmonic nanoparticles. This effect is related to the high intensity of the near-field associated to the plasmonic excitation and hot spots on acute vertices of the particle [1,2]. In this work, we present a numerical study of the near-field intensity of Au and Ag nanoparticles with different size and shape, using the well-known discrete dipole approximation method. Some of the studied shapes are spherical-like such as the decahedron and cuboctahedron. Also Au and Ag nanorods of various aspect ratios were studied.

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[1] E. C. Le Ru and P. G. Etchegoin, Principles of Surface-Enhanced Raman Spectroscopy, Elsevier, 2009, Oxford, UK.
[2] C. Noguez, C. Villagómez and A. L. González, Plasmonic of multifaceted metallic nanoparticles, field enhancement, and TERS, Phys. Stat. Solidi B, 252, 1, 56-71, 2015.

Functionalized gold-silica nanoparticles as a platform for enhanced direct electron transfer in enzymatic biosensor

Siva Kumar-Krishnan[1], María Guadalupe-Ferreira García[1], Evgen Prokhorov[2],
M. Estevez-González[1] and Rodrigo Esparza[1]

[1]*Centro de Física Aplicada y Tecnología Avanzada, Universidad Nacional Autónoma de México, Boulevard Juriquilla 3001, Santiago de Querétaro, Qro., 76230, México;*
[2]*Cinvestav Querétaro, Querétaro QRO, 76230, México.*
E-mail: skumar@fata.unam.mx

Engineering the nanoparticles (NPs) surface has been emerged as a promising approach for design and enhancing the direct electron characteristics in the enzymatic biosensors and microbial fuel cells applications. However, the lack of control over nanoparticles aggregation and instability of enzyme immobilization process limits their application. In this work, we demonstrate that the facile and green deep eutectic solvent (DES) mediated synthetic strategy to integrates smaller gold nanoparticles (AuNPs) on the silica (SiO_2) nanoparticles for enzymatic electrochemical biosensing. Surface decoration with small AuNPs (average size 5.2 nm), which promotes direct electron transfer (DET) process for the efficient enzymatic glucose biosensor. Moreover, we directly compare the DET characteristics of Au-SiO_2 NP system by immobilizing the GOx enzymes either physically adsorbed or covalently linked to Au-SiO_2 NPs. Interestingly, the covalently functionalized GOx onto Au-SiO_2 NPs significantly enhance the charge transfer about two order of magnitude compared to physically absorbed state. The enhanced charge transfer can be ascribed due to the effective site-specific conjugation of GOx by suppressing the steric hindrance at the Au-SiO_2NPs interface and long range 'electrical wiring" between active FAD active co-factor in the GOx and the electrode surface *via* covalent conjugation. The presented green DES-mediated synthetic approach expands the possibilities to support different metal NPs on the SiO_2 as a potential platform for biosensor applications.

Fabrication of a MIS structure based on two-dimensional ZnO nanostructures by chemical routes

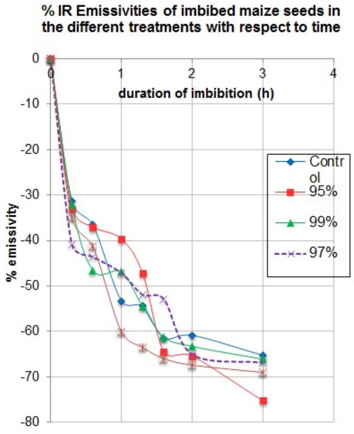
Rubén Jonatán Aranda García[1], Alejandro Escobedo Morales[2],
José Alberto Luna López[1], and José Antonio Rivera Marquez[1]
[1]Centro de Investigación en Dispositivos Semiconductores-ICUAP, Benemérita Universidad Autónoma de Puebla, Puebla, Pue., México; [2]Facultad de Ingeniería Química, Benemérita Universidad Autónoma de Puebla, Puebla, Pue., México.
E-mail: alejandro.escobedo@correo.buap.mx

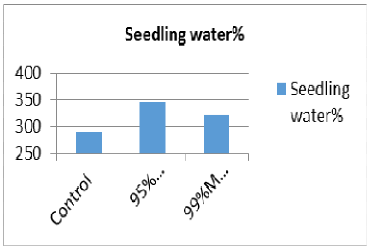
Because its physical properties, ZnO is considered a potential semiconductor compound for fabricating electronic and optoelectronic devices. In this regard, several growth techniques have been developed to ensure the required control for manufacturing commercial devices based in this material. On the pathway for improving the performance of the current devices, low-dimensional ZnO structures seem to be a promising alternative. Here, we report the fabrication of a metal-insulator-semiconductor (MIS) structure based on ZnO nanostructures grown on the surface of an anodized aluminum substrate ($ZnO/Al_2O_3/Al$) by chemical routes. While the ZnO nanostructures were obtained through a low-temperature hydrothermal route, the Al_2O_3/Al substrate was obtained by electropolishing and subsequent anodizing of aluminum foil. The obtained $ZnO/Al_2O_3/Al$ architecture was studied by x-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and electrical measurements. The voltage-time plot acquired during the anodizing process indicates formation of an insulating barrier (Al_2O_3) on the metallic substrate (Al). The SEM analysis reveals that a nanostructured layer is grown on the anodized substrate, constituted by interconnected leaf-like ZnO nanostructures with average thickness of ~100 nm. The formation of the MIS structure was observed using focused ion beam technology (FIB). The EDS analysis suggests the presence of ZnO, Al_2O_3 and Al phase; formation of these phases was confirmed definitely by XRD. Finally, the characteristic rectifying response of a metal-oxide-semiconductor junction is observed in the acquired curves I-V and C-V of the obtained architecture, demonstrating that it is possible to fabricate a MIS heterojunctions based on ZnO nanostructures using exclusively chemical routes.

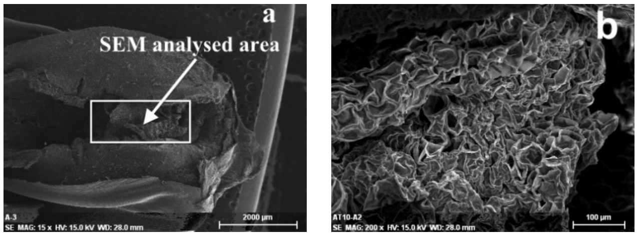
Plant responses to nano and micro structured carbon

Dhirendra K. Tiwari[1], Iris Serrato[2], Juan A. Casimiro[3], Pablo G. Martínez[1],
and Nabanita Dasgupta-Schubert[3]
[1]Instituto de Física y Matemáticas; [2]Facultad de Biología; [3]Facultad de Ciencias Físico-Matemáticas; Universidad Michoacana de San Nicolás de Hidalgo, Cd. Universitaria, Morelia, Michoacán 58060, México.
E-mail: nita@ifm.umich.mx

Carbon nanotubes (CNT) have been seen to dramatically improve seed germination, plant growth and the delivery of water and certain mineral nutrients to the plant. While the exact mechanism is unknown, several researchers suggest that the physical entry of the CNT into plant cells is a key driving factor behind the aforesaid phenomenon. Given the fact that plant cells are surrounded by relatively thick cell walls and the seed testa is ~ 500-1000 μm thick, Ficksian diffusion of the large-sized and high molecular weight CNT/AC would seem to be precluded. This work explores the response of the maize (Zea *mays* L.) seed when imbibed in an aqueous suspension of 10 and 20 mg/kg of 95-99% pure multi-walled CNT or AC. Seed imbibition kinetics of the maize seed in the presence or absence of MWCNT/AC was followed for 14 hours by Infrared Thermography (IRT) and later the 7 day germination phase was investigated. IRT provided a non-destructive assay of seed water uptake as well as the change of seed surface topography due to emissivity changes as water content increased (Figure 1). The SEM images of Figure 2 show an extensive corrugation of the seed-coat by the MWCNT. First order water absorption kinetics was seen to be followed in all the treatment types. The increased water uptake by the seedling could be a consequence of the MWCNT entering the porous root through apoplastic vias thereby avoiding the penetration of the cell wall and membrane. However, the absence of significant differences in water absorption between the Control and the MWCNT treatments at the imbibitions stage (Figure 1) suggests that the MWCNT is not able to penetrate the testa. Calculations of MWCNT/AC diffusion using Fick's equations confirmed this premise.







Evaluación de la actividad bactericida de nanopartículas de CuO y ZnO obtenidas por mecanosíntesis en presencia de disolventes

B. Paz-Diaz[1], A. R. Vázquez-Olmos[1], A. Almaguer-Flores[2], R. Y. Sato-Berrú[1],
A. L. Fernández-Osorio[3]

[1]Centro de Ciencias Aplicadas y Desarrollo Tecnológico-UNAM; [2]Laboratorio de Genética Molecular. División de Estudios de Posgrado e Investigación de la Facultad de Odontología-UNAM; [3] Facultad de Estudios Superiores Cuautitlán-UNAM.

E-mail: blankpazd@gmail.com

Cada año se presentan millones de casos de infecciones por agentes bacterianos, terminando muchos de ellos en decesos. El desarrollo de medicamentos a pesar de ser constante, resulta inútil cuando los microorganismos se vuelven resistentes. Por tal razón, existe un gran interés en generar materiales que sean bioseguros, efectivos contra diversos tipos de infecciones y de fabricación sencilla y barata. En este sentido, los óxidos metálicos nanoestructurados resultan buenos candidatos ya que presentan propiedades antimicrobianas importantes.

En este trabajo se presenta el estudio preliminar de la actividad bactericida de nanoestructuras de CuO y de ZnO frente a 2 cepas de bacterias Gram (-) *Escherichia coli* y *Pseudomonas aeruginosa* y 2 cepas de bacterias Gram (+) *Staphyloccocus epidermidis* y *Staphylococcus aureus*. Las nanopartículas fueron obtenidas por mecanosíntesis en presencia de disolventes polares próticos (agua y etanol) y polares apróticos (dimetilformamida y dimetilsulfóxido) y presentan diámetros promedio de 30 nm para ZnO y de 22 nm para CuO. Dichas nanoestructuras fueron caracterizadas por difracción de rayos-x de polvos (DRX), microscopía electrónica de transmisión (MET), por las espectroscopías UV-Visible, infrarroja (IR) y Raman así como por resonancia paramagnética electrónica (RPE). A partir de los resultados obtenidos se sugiere que la formación de diferentes defectos como la presencia de vacancias de oxígeno ionizado (O^+) o incluso intersticios de oxígeno, juegan un papel determinante en la actividad bactericida de las nanopartículas.

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Use of hydroxyapatite nanoparticles for developing bone tissue engineering scaffolds

Sudip Mondal[1], Apurba Dey[2] and Umapada Pal[1]

[1]*Instituto de Física, Universidad Autónoma de Puebla, Apdo. Postal J-48, Puebla, Pue. 72570, Mexico;* [2]*Department of Biotechnology, National Institute of Technology Durgapur, M.G. Avenue, Durgapur-713209, WB, India.*

E-mail: mailsudipmondal@gmail.com

We There has been a growing interest in developing structurally, mechanically and bio-functionally suitable implants for applications in tissue engineering. In this study, an attempt has been made to synthesize hydroxyapatite (HAp) nanoparticles and their appliance in scaffold development for tissue engineering application. A low temperature (40°C) chemical precipitation technique was employed to synthesize HAp nanoparticles using calcium nitrate tetrahydrate [$Ca(NO_3)_2 \bullet 4H_2O$] and di-ammonium hydrogen phosphate [$(NH_4)_2HPO_4$] at pH 11. The synthesized HAp powder was characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), thermo-gravimetric and differential thermal analysis (TG-DTA), scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS) analysis. The synthesized HAp powder was further used to develop porous scaffolds through gel casting technique. Compared to natural cortical bone, the porous HAp scaffold sintered at 1200ºC facilitates similar mechanical properties such as hardness (0.95-1.06 GPa), compressive stress (0.76-0.88 GPa) and tensile stress (178-186 MPa) with adequate porosity (25-30%). The *in vitro* assays [Trypan blue and 3-(4, 5-dimethythiazol- 2-yl)-2, 5-diphenyl tetrazolium bromide (MTT)] on MG63 osteoblast cell lines suggests that the implanted biomaterials are non-toxic and bioactive. The *in vivo* histological analysis of developed scaffold revealed the osteoconductive property of implanted HAp scaffold. The results suggest that mechanically stable biocompatible porous scaffolds can be developed using this technique which would perceive a key role in future for tissue engineering application.

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[1] Harley, B.A. et al., *Acta Biomaterialia.* **2007**, 3, 463.
[2] Mondal, S. et al., *Bulletin of Materials Science*. **2012**, 35, 683.

Efecto de la morfología y dopaje en las propiedades ópticas y magnéticas de nanoestructuras de ZnO sintetizadas sonoquímicamente

G. Saavedra Rodríguez, R. Sanchez Zeferino and M.E. Álvarez Ramos

Posgrado en nanotecnología, Universidad de Sonora, Blvd. Luis Encinas y Rosales
C.P.8300, Hermosillo, Sonora, México.

E-mail: gerardo.saavedra@correo.fisica.uson.mx

En los últimos años ha incrementado el interés en nanomateriales de óxidos semiconductores con propiedades magnéticas aplicables, tanto en el ramo de la espintrónica como en el diagnóstico de imágenes [1]. De la misma manera, son de gran interés los materiales cuyas propiedades ópticas, como luminiscencia visible, pueden ser controladas e incluso mejoradas variando parámetros como la morfología y dimensiones nanométricas. Además, se ha hecho relevante el uso de métodos de síntesis menos dañinos al ambiente y energéticamente menos costosos.

Se sintetizaron nanoestructuras de óxido de zinc (ZnO) y ZnO:Mn mediante el método sonoquímico, utilizando $ZnO(NO_3)_2$, agua desionizada, una solución de NaOH y diferentes concentraciones de $Mn(NO_3)_2$ (1.0, 1.5 y 2.0 mol%), para observar el efecto en las propiedades ópticas y magnéticas.

Mediante microscopía electrónica de barrido (SEM) se observó que la muestra de ZnO sin dopar presenta una morfología no homogénea con tamaño de partícula en el rango de 80 y 400 nm, mientras que las muestras con Mn presentaron una morfología esférica con tamaños entre 30 y 60 nm. Los espectros Raman mostraron modos normales de vibración característicos de ZnO para todas las muestras. Los espectros de fotoluminiscencia muestran una emisión excitónica característica centrada alrededor de 383 nm y una banda muy ancha (400-700 nm), relacionada a defectos estructurales. El estudio de magnetización muestra un comportamiento diamagnético con dominios paramagnéticos para una muestra de ZnO y un comportamiento ferromagnético para las muestras de ZnO:Mn.

[1] Ü. Özgür, Y. I. Alivov, C. Liu, a. Teke, M. a. Reshchikov, S. Doğan, V. Avrutin, S. J. Cho, and H. Morkọ, J. Appl. Phys., vol. 98, no. 4, pp. 1–103, 2005.

Enhanced heat generation capacity of bi-magnetic nanoparticles for hyperthermia applications

F. Arteaga-Cardona[1], E. Santillán-Urquiza[1], U. Pal[2], A. Angulo-Molina[3],
C. Torres-Duarte[4], M.A. Méndez-Rojas[1]

[1]Departamento de Ciencias Químico-Biológicas, Universidad de las Américas Puebla, 72810 Puebla, México; [2]Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apdo. Postal J-48,Puebla, 72570, México; [3]Departamento de Ciencias Químico-Biológicas/DIFUS, Universidad de Sonora, Colonia Centro, 83000, Hermosillo, Sonora, México; [4]Bodega Marine Laboratory 2099 Westshore Rd. Bodega Bay, CA 94923-0247.

E-mail: fernando.arteagaca@udlap.mx; miguela.mendez@udlap.mx

Cancer has been, historically, one of the most studied diseases. Among the novel methods for its early diagnosis and treatments that have been explored, one of the most promising is hyperthermia therapy, which relies on the ability of nanostructured magnetic materials to generate heat at the affected region. Although it is a promising therapy, utilization of magnetic nanostructures for this purpose is frequently inconvenient due to low heat generation and toxicity of these nanostructures [1]. We synthesized bi-magnetic nanoparticles ($Zn_{0.5}Mn_{0.5}Fe_2O_4$-Fe_3O_4) through commonly used co-precipitation method, followed by a seed-mediated precipitation method, using zinc doped manganese ferrite nanoparticles as seeds [2]. Those nanoparticles generate an exchange coupling between layers, increasing their magnetic saturation up to 30%, without spin blocking. Although the mechanism of heat generation by nanoparticles is not yet fully understood, magnetic saturation of used material is seen to play an important role, as an increase in M_s enhances the heat generation [3]. The toxicity was evaluated using mussel hemocytes, which resembles the immune system. MTT assays were used to test the viability of the nanoparticles in L929 cells. Both biocompatibility studies showed that the magnetic nanoparticles could be considered potentially safe for biomedical applications for periods up to 24 hours.

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Enhanced mechanosynthesis of MFe_2O_4 (M=Co, Ni, Zn) magnetic nonoparticles for Pb removal from aqueous solution

America R. Vazquez-Olmos[1], Mohamed Abatal[2], Roberto Y. Sato-Berru[1],
Gabriela K. Pedraza-Basulto[1], Valentín Garcia-Vazquez[3], Arianee Sainz-Vidal,
R. Perez-Bañuelos[4] and A. Quiroz[2]

[1]Centro de Ciencias Aplicadas y Desarrollo Tecnológico, UNAM, Circuito Exterior S/N, Ciudad Universitaria, A.P. 70-186, Delegación Coyoacán, CP 04510 México, DF, México; [2]Facultad de Ingeniería, UNACAR, C.P. 24180, Ciudad del Carmen, Campeche, México; [3]Instituto de Física Luis Rivera Terrazas, BUAP, Apartado Postal J-48, Puebla, Pue. 72570, Mexico; [4]Facultad de Ciencias de la Electrónica, BUAP, 18 Sur y Av. San Claudio, Edif. 109, Puebla, Pue. 72570, México.

E-mail: mabatal@pampano.unacar.mx

Adsorption of Pb(II) from aqueous solution using MFe_2O_4 nanoferrites (M = Co, Ni, Zn) was studied. Nanoferrite samples were prepared via mechanochemical method and were characterized by X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), micro-Raman, and vibrating sample magnetometry (VSM). XRD analysis confirms the formation of pure single phases of cubic ferrites with average crystallite sizes of 23.8, 19.4, and 19.2 nm for $CoFe_2O_4$, $NiFe_2O_4$, and $ZnFe_2O_4$, respectively. Only $NiFe_2O_4$ and $ZnFe_2O_4$ samples show superparamagnetic behavior at room temperature whereas $CoFe_2O_4$ is ferromagnetic. Kinetics and isotherm adsorption studies for adsorption of Pb(II) were carried out. A pseudo second-order kinetic describes the sorption behavior. The experimental data of the isotherms were well fitted to the Langmuir isotherm model. The maximum adsorption capacity of Pb(II) on the nanoferrites was found to be 20.58, 17.76, 9.34 $mg.g^{-1}$ for M = Co, Ni, and Zn, respectively.

POSTER CONTRIBUTIONS

Síntesis y caracterización de nanomateriales de grafeno-titania como fotocatalizadores en la degradación de azul de metileno asistida con luz ultravioleta

I. Andrade Hernández y E. Rubio Rosas

Centro Universitario de Vinculación y Transferencia de Tecnología, Prolongación de la 24 Sur y Av. San Claudio, Ciudad Universitaria, Col. San Manuel, 72570 Puebla.

E-mail: efrain.rubio@correo.buap.mx

El óxido de Grafeno (GO) es un material que exhibe una química, óptica y propiedades eléctricas fascinantes debidas tanto a la estructura de Grafeno como al oxígeno que contiene en sus grupos funcionales, situados en el plano basal o en los bordes de la hoja. Además, es de fácil obtención y es precursor para la obtención de Grafeno.

Los casos más exitosos de reducción química en las cuales se ha obtenido Grafeno a partir de Óxido de Grafeno se han llevado a cabo usando hidracina o hidrato de hidracina como agente reductor. Sin embargo, estos son reactivos altamente venenosos y explosivos. Por otra parte el ácido L-ascórbico (L-AA), tiene una capacidad reductora suave y es un agente reductor no tóxico, por lo cual se ha probado su capacidad para reducir GO en una solución acuosa a temperatura ambiente. Además de la capacidad reductora del L-AA, los productos oxidados del L-AA obtenidos en el proceso también desempeñan un papel importante como agente estabilizante durante la reacción, evitando el uso de reactivos adicionales.

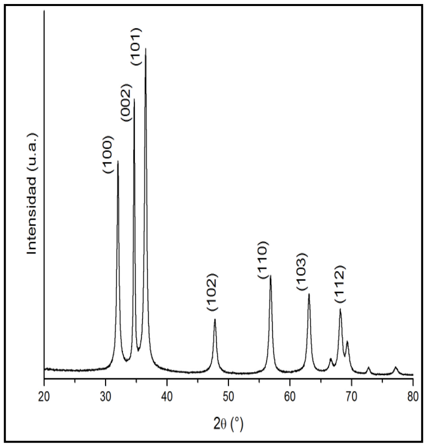
Por otra parte el TiO_2 ha sido intensamente investigado como fotocatalizador para la limpieza del medio ambiente. Sin embargo, el TiO_2 sólo puede descomponer compuestos orgánicos aromáticos en CO_2 y H_2O bajo iluminación UV y sufre de una barrera en la respuesta a la luz visible a longitudes de onda superiores a 387 nm debido a una gran brecha de banda de 3.2 eV. Como un método prometedor para mejorar el rendimiento fotocatalítico y extender el umbral de absorción del TiO_2 a la región de la luz visible se ha sugerido el dopaje con elementos orgánicos entre los cuales se encuentra el Carbono.

En el presente trabajo se realizó la síntesis de Óxido de Grafeno siguiendo el método modificado de Hummers, el producto obtenido se utilizó para la síntesis de un nanocompuesto con Dióxido de Titania para evaluar sus propiedades fotocatalíticas. Paralelo a esto se realizó la reducción del Óxido de Grafeno previamente obtenido con ayuda de Ácido Ascórbico. Tanto al Óxido de Grafeno, Óxido de Grafeno Reducido y los nanocompuestos se les dio seguimiento con ayuda de los métodos de Difracción de rayos X, Espectrometría infrarroja y Microscopía Electrónica de Barrido, que nos indicaron la obtención del producto. Mientras que la prueba de fotocatálisis fue realizada con ayuda del espectrofotómetro ultravioleta-visible.

Aproximación biotecnológica para la obtención de ZnO nanoestructurado mediante el extracto acuoso de *kalanchoe pumila*

R. Ángeles Sierra[1], M.A. Flores-González[1], M.A. Hernández-Pérez[2],
P.N. Olvera-Venegas[1] and M. Villanueva-Ibáñez[1]
[1]Universidad Politécnica de Pachuca, Carr. Pachuca - Cd. Sahagún km 20 Ex-Hda de Santa Bárbara Zempoala Hidalgo, México; [2]Instituto Politécnico Nacional, Depto. de Ingeniería en Metalurgia y Materiales-ESIQIE, Ciudad de México 07738, México.
E-mail: villanueva@upp.edu.mx

Las propiedades únicas del ZnO nanoestructurado han propiciado el incremento en su demanda en distintos sectores industriales. Los métodos físicos y químicos generalmente empleados para su obtención se estiman costosos, además de producir partículas recubiertas por residuos de los reactivos utilizados, limitando sus aplicaciones. Adicionalmente, las biosíntesis reportadas mediante extractos vegetales, indican que se requiere de un tratamiento térmico posterior para lograr el material deseado en una sola fase y composición. En este proyecto se proponer una alternativa biotecnológica para su obtención sin tratamiento térmico posterior, mediante el extracto acuoso vegetal de *kalanchoe pumila* que es una planta de fácil cultivo cuyos metabolitos secundarios participan en la formación de ZnO. Al variar el pH del medio de síntesis se obtuvo ZnO nanoestructurado libre de fases adicionales sin tratamiento térmico posterior. Espectroscopia UV-vis evidenció la absorción de ZnO ubicada a 375 nm. La caracterización estructural mediante DRX y espectroscopia Raman mostraron su estructura hexagonal tipo wurtzita. En MEB se observaron partículas homogéneas semiesféricas. Ensayos preliminares en placa indican que el extracto presenta activiad antibacteriana frente a las cepas estudiadas (*S. aureus* y *E. coli*).



Agradecimientos. Se agradece al MM. R. Gonzalez-Montes de Oca por las observaciones en MEB

Magnetic behavior of SiO_2 opals with embedded Fe

C. Avila-Crisóstomo, E. Sánchez-Mora, V. García-Vázquez
and F. Pérez-Rodríguez

Benemérita Universidad Autónoma de Puebla, Instituto de Física, Apartado Postal J-48,
Puebla, Pue., 72570, México.

E-mail: cavila@ifuap.buap.mx

Using the Stöber method, silica spheres were obtained and arranged in an fcc lattice. Metallic Fe was introduced in opal voids by means of the reduction of precursor salts with different reducing agents. Magnetization curves of the as synthesized metallic nanoparticles and of the artificial opals with infiltrated nanoparticles were measured by using the vibrating sample magnetometry (VSM) technique with an applied magnetic field oriented along the [111] direction of the opal matrix. Moreover, the Landau-Liftschitz-Gilbert [1] equation was solved, in order to reproduce the experimental results qualitatively, using Ewald summations [2] to take into account the dipolar interaction between the spatially arranged magnetic nanoparticles.

We acknowledge the partial financial supports of VIEP-BUAP.

[1] L. Landau, E. Liftschitz, Phys. Z. Sowjetunion 8, 153 (1953).
[2] P. P. Ewald, Ann. d. Phys. 369, 253 (1921).

Síntesis verde de nanopartículas de ZnO/Ag usando el extracto acuoso de *jatropha dioica*

V.P. Camargo-Pérez[1], M.A. Flores-González[1], M.A. Hernández-Pérez[2],
P.N. Olvera-Venegas[1] y M. Villanueva-Ibáñez[1*]
[1]Universidad Politécnica de Pachuca, Carr. Pachuca - Cd. Sahagún km 20 Ex-Hda de Santa Bárbara Zempoala Hidalgo, México; [2]Instituto Politécnico Nacional, Depto. de Ingeniería en Metalurgia y Materiales-ESIQIE, Ciudad de México 07738, México.
E-mail: villanueva@upp.edu.mx

ZnO es un material prometedor dadas sus variadas ventajas como biocompatibilidad, biodegradabilidad, bajo costo y toxicidad, es usado en empaques de comida dadas sus propiedades antimicrobianas. Del mismo modo, Ag presenta actividad antibacteriana cuando se encuentra en nanoescala. Cabe resaltar que al momento son escasos los reportes del efecto antibacteriano de las partículas de ZnO/Ag. Existen varias estrategias para la preparación de ZnO/Ag; sin embargo, aun son requeridos métodos verdes. En este documento se propone un medio de síntesis con el extracto acuoso de *Jatropha dioica* (Dragon's blood) [1]. Se propusieron dos métodos de obtención y se estudió el efecto de la variación del volumen del extracto acuoso y de la concentración del precursor en la síntesis de ZnO/Ag mediante seguimiento de la banda de absorción UV-vis característica para ambos componentes. El tamaño de las partículas suspendidas registrado mediante granulometría laser fue entre 375 y 530 nm dependiendo del método. Por espectroscopia infrarroja se identificaron grupos funcionales característicos de las biomoléculas que recubren las nanopartículas. Mediante Microscopía Electrónica de Barrido se encontró que las nanopartículas obtenidas forman agregados conformados por entidades más pequeñas de 37 nm que mostraron actividad antibacteriana contra *E. coli* y *S. aureus.*

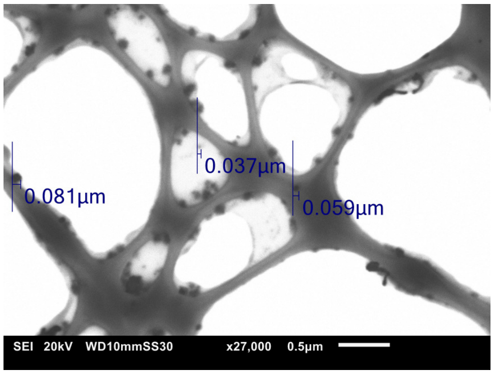


Figura 1. Ejemplo de observación en MEB de las partículas ZnO/Ag obtenidas con extracto de Jatropha dioica.

Agradecimientos. Se agradece al MM. R. González-Montes de Oca por las observaciones en MEB.

[1] Wong, J. E., Castillo, M. l., López, L. I., Contreras, J. C., Nevárez, G. V., & Aguilar, C. N. *Revista científica de la Universidad Autónoma de Coahuila*, 2.

Síntesis y caracterización de sílice mesoporosa funcionalizada con grupo tiol y su aplicación en la adsorción de iones cromo

F.J. Chimal Moreno[1], R.D. Hernández Perez[1], D.G. Mitre Martinez[1],
J. Varela Caselis[2] y E. Rubio Rosas[2]
[1]Facultad de Ingeniería Química, Benemérita Universidad Autónoma de Puebla Ciudad Universitaria, Blvd. 14 sur y Av. San Claudio, Col. San Manuel. C.P. 72450, Puebla México; [2]Centro Universitario de Vinculación y Transferencia Tecnológica, Benemérita Universidad Autónoma de Puebla Ciudad Universitaria, Prolongación 24 sur y Av. San Claudio, Col. San Manuel. C.P. 72450, Puebla México.
E-mail: chimal_123@hotmail.com

La contaminación del agua por metales pesados ha representado un gran problema desde hace tiempo, lo que ha generado conciencia como consecuencia de los elevados niveles de toxicidad observados en las últimas contingencias ambientales [1]. Por tal motivo el desarrollo de materiales con cualidades benéficas para el tratamiento de metales pesados es de suma importancia. En particular, la implementación de materiales adsorbentes es uno de los procesos más prometedores para la remoción de metales pesados por su rapidez y bajo costo. De modo que un material con buenas cualidades adsorbentes debe poseer alta capacidad de adsorción, desorción nula bajo condiciones ambientales y bajo costo de operación. La sílice (SiO_2), es un sólido constituido por una red tridimensional (de un átomo de silicio enlazado covalentemente a 4 átomos de oxigeno) generando una estructura porosa de elevada superficie especifica [2] convirtiéndolo en un excelente candidato como material adsorbente. En este trabajo se sintetizó y caracterizó sílice mesoporosa mediante la técnica sol-gel y como agente director de estructura el bromuro de cetiltrimetilamonio (CTAB), se llevó a cabo su funcionalización con grupos tiol con la finalidad de favorecer la adsorción de iones metálicos. Se llevó a cabo la caracterización por difracción de rayos X, microscopia electrónica de barrido, espectroscopia en el infrarrojo, microscopia electrónica de transmisión, Asimismo, se evaluó su desempeño en la adsorción de iones cromo en una solución acuosa.

[1] M. Ali, R. Ali, K. Rao, M. Ajmal, Khan, Heavy metal pollution and its control through nonconventional adsorbents (1998-2007): a review, J. Int. Environ. Appl. Sci. 3 (2008) 101–141.
[2]. E.Vunain, AK Mishra, BB Mamba, Dendrimers, mesoporous silicas and chitosan-based nanosorbents for the removal of heavymetal ions: A Review, International Journal of Biological Macromolecules.

Isoelectronic effect of Cu^{1+} and Ga^{3+} on Zn^{2+} in diesel particulate matter oxidation

G. Corro[1], S. Cebada[1], F. Bañuelos[1], U. Pal[2], A. Flores[1] and J.L.G. Fierro[3]
[1]Instituto de Ciencias, [2]Instituto de Física, Benemérita Universidad Autónoma de Puebla, Mexico;[3]Instituo de Catálisis y Petroleoquímica, Madrid, Spain.
E-mail: griselda.corro@correo.buap.mx

Inside a diesel engine, the complete combustion of the fuel would only generate CO_2 and H_2O, to the exclusion of any other harmful product. However, the very short time allowed for chemical oxidation processes integration in combustion chambers, the lack of homogeneity in the carbureted mixtures, and the heterogeneity and rapid variations in the temperature do not allow for the state of ideal thermodynamic equilibrium to be reached. Thus, the incomplete combustion of a hydrocarbon results in the formation of a wide range of organic and inorganic compounds being the particulate matter (PM) the most dangerous for human health and environment [1].

Diesel particulate filter (DPF) is commonly used as PM controller. However, as with other filters, they require a regeneration system to eliminate the accumulated PM, in order to consistently maintain the filter performance [2]. Therefore, the presence of an oxidation catalyst in the diesel exhaust is highly needed.

The presence of Cu^{1+} has been related to the high performance of ZnO supported catalyst [3]. On the other hand, literature research shows that Ga doped on ZnO mostly concentrates on its electrical and optical properties [4-6]. Nevertheless, Ga has not been tested in PM oxidation reaction.

This investigation reports the activity of Gallium and Copper supported on ZnO in the PM oxidation reaction. The samples were prepared by the impregnation of $Cu(NO_3)_2$ and $Ga(NO_3)_3$ precursors. The powder was reduced at 500°C in pure H_2.

The catalysts were characterized by XPS and UV-Vis spectroscopies before and after the PM oxidation reaction in order to determine the electronic state.

Results obtained from the PM oxidation reaction over Cu/ZnO and Ga/ZnO catalyst showed a strong activity at low temperatures (150°C and 200°C respectively) even after several oxidation cycles. These results can be explained by the XPS and UV-Vis analysis where it was found Cu^{1+} and Ga^{3+} were the active species. Thus, it is believed the high stability of the catalyst is due to the isolectronic interaction of Cu^{1+} and Ga^{3+} with Zn^{2+} present in the catalyst support.

[1] R.Prasad,V.Rao Bella Bull. Chem. React. Eng. Catal. 5 (2010) 69-86
[2] G.C. Koltsakis, A.M. Stamatelos, Prog. Energy Combust. Sci. 23 (1997) 1-39
[3] J. Toyir, P. Ramirez de la Piscina, J. L. G. Fierro, N. Homs Appl. Catal B: Environ, 34 (2001) 255-266
[4] R.P. Wang, A.W. Sleight, D. Cleary Chem. Mater. 8 (1996) 433–439
[5] S.W. Yoon Cryst. Growth Des. 12 (2012) 1167–1172
[6] V. Bhosle, A. Tiwari, J. Narayan J. Appl. Phys. 100 (2006) 1-6

Biosíntesis de nanopartículas metálicas mediante el extracto de café verde para su evaluación bactericida

J. F. Cruz-Hernández, B. E. Jaramillo-Loranca, M.A. Flores-González
y M. Villanueva-Ibáñez
Universidad Politécnica de Pachuca, Carretera Pachuca-Cd. Sahagún, Km. 20, Rancho Luna, Ex-Hacienda de Sta. Bárbara, Zempoala, Hidalgo, México.
E-mail: villanueva@upp.edu.mx

Las nanopartículas metálicas (NPs-M), especialmente las de plata (NPs-Ag) y de oro (NPs-Au), juegan un papel importante en áreas de la salud y medicina [1] por la creciente necesidad de contar con nuevos agentes antimicrobianos. Actualmente su obtención se basa en métodos físicos y/o químicos que no son escalables o generan subproductos tóxicos limitando su aplicación. Por esta razón se desarrollan métodos alternativos de síntesis que permitan su aplicación en dominios de la salud [2], como los que usan sistemas biológicos o sus derivados como las plantas y sus extractos. Se propone en este trabajo el uso del extracto acuoso de los granos de café verde debido a su gran contenido de antioxidantes que ayudará en la reducción de iones y formación de las partículas en un medio de baja toxicidad para el fisiológico. Este trabajo se enfoca en la síntesis de las NPs-Au y NPs-Ag las cuales fueron caracterizadas mediante espectrofotometría UV-vis, donde se observó la absorción correspondiente a estos materiales (525 y 430 nm, respectivamente). Además, microscopia electrónica de barrido y granulometría láser evidenciaron partículas semiesféricas inferiores a 20nm. Finalmente, se realizaron las pruebas antibacterianas contra patógenos humanos (*E. coli* y *S. aureus*) y se obtuvieron halos de inhibición aplicando NPs-Ag, mientras que en las pruebas realizadas con NPs-Au no se observó este efecto debido a que solo lo presentan a concentraciones muy elevadas.

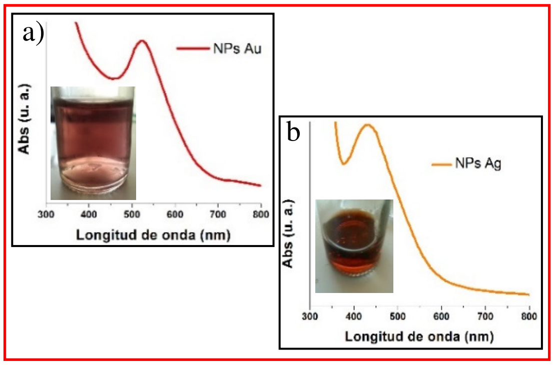


Figura 1. Espectro UV-vis de a) NPs Au y b) NPs Ag en sus respectivos viales de síntesis; t=3h.

[1] Bhattacharya, R. & Mukherjee, P. *Advanced Drug Delivey Reviews*. **2008** 60: 1289-1306.
[2] Ramanathan, V.; Kalimuthu, K.; Shubaash, G., & Sangiliyandi, G. *Biotechnology Advances.* **2009**, 27, 924–937.

Au-Fe_3O_4 core-shell nanoparticles orchestrated carbon dots as nanoflotillas for bioimaging and drug delivery

Goldie Oza[3], M. Ravichandran[2], S. Velumani[1,2] and Jose Tapia Ramirez[3]
[1]Department of Electrical Engineering (SEES); [2]Program on Nanoscience and Nanotechnology; [3]Department of Genetics and Molecular Biology, [4]Department of Cell Biology, CINVESTAV-IPN, Avenida IPN 6508, San Pedro Zacatenco, D.F., Mexico.
E-mail: goldieoza@gmail.com

Carbon dots (CDs) are proving to be an effective Imaging paraphernalia for the comprehension of morphological alterations in the cellular membrane due to high absorption coefficients and Quantum efficiency. Such CDs can be used in drug/delivery vehicles, Biolabelling as well as in PCR. An upsurge of expanded interest in the field of Magnetic nanotechnology has led us to allow indepth exploitation of magnetic nanoparticles in nanomedicine. Encapsulating the core made up of magnetic nanoparticles by Gold nanoshell leads to the development of a proficient biocompatible and stabilized drug/delivery system under physiological conditions. Further creating a nanocomposite by allowing conglomeration of Au- Fe_3O_4 core-shell with CDs, is the main requirement.

This modular design enables Au-Fe_3O_4-CDs to perform multiple functions simultaneously, such as in multimodal imaging, drug delivery and real-time monitoring, as well as combined therapeutic approaches. The ability of MNPs to enhance proton relaxation of specific tissues and serve as MR imaging contrast agents is one of the most promising applications of nanomedicine. In the present work, Au-Fe_3O_4 nanoparticles are used as able cargo for the docking of anti-cancer drug such as Doxorubicin (DOX) using cysteamine as a linker for the attachment. The attachment could be monitored using UV-visible spectroscopy. The stability of Au-Fe_3O_4 nanoparticles was scrutinized by measuring the flocculation parameter, which was found to be in the range of 0–0.65. Further, zeta potential measurements confirmed the pH of 7.4 at which maximum drug attachment can take place. The amalgamation of the drug along with activated folic acid as a navigational molecule is the critical phase for targeted drug delivery. Attachments were verified using FTIR and NMR, which confirmed the formation of non-covalent interactions. The drug loading capacity of the Au-$Fe_3O_4$was found to be 76%. Drug-release was studied using the AC magnetic field generator and was found to be temperature dependent phenomena. CDs were found to be effective players in tracking the drug-delivery vehicle around the miscreant cell and inside them. Au-Fe_3O_4-CD-FA-DOX complex was found to be comparatively non-toxic for normal cells and considerably toxic for Hep-2 cells due to hyperthermal properties of SPIONS and targeted-mechanism of folic acid.

Catalizadores heterogéneos de óxidos metálicos nanoestructurados en la síntesis de biodiesel por transesterificación de triacilglicéridos

K. M. Talavera Sánchez[1], M. Estrada Flores[1, 2], C. M. Reza San Germán[1],
y M. E. Manríquez Ramírez[1]

[1]Instituto Politécnico Nacional ESIQIE, Laboratorio de Fundamentos de Nanotecnología, Edif. Z-5, 2do. Piso, 07738, CDMX, México; [2]Instituto de Investigaciones en Materiales, Circuito Exterior S/N, Zona de Institutos, Ciudad Universitaria, C.P. 04510, México, D.F.

E-mail: kevintalavera20@gmail.com

El agotamiento de las reservas de petróleo y el aumento progresivo de su precio ha dado gran importancia a la utilización de combustibles alternativos como el biodiesel. La síntesis de biodiesel se lleva a cabo mediante la transesterificación de triacilglicéridos (aceites vegetales y grasas animales) y la utilización de un alcohol liviano como el metanol en presencia de catalizadores. [1] La síntesis de biodiesel se logra mediante el uso de catalizadores homogéneos como son los hidróxidos de sodio y potasio, se pueden utilizar catalizadores heterogéneos como óxidos de metales, alcalinotérreos, zeolitas y heteropoliácidos. En este artículo se presenta un estudio de la catálisis heterogénea para la síntesis de biodiesel por transesterificación, además se dan algunas consideraciones sobre qué tipo de catalizador se recomiendo para producción industrial de biodiesel. Se sintetizaron materiales nanoestructurados de óxido de aluminio por el método de anodización y dopados con diferentes óxidos. Se realizó la caracterización estructural por Microscopía Electrónica de Barrido y Difracción de Rayos X de los materiales sintetizados.

[1]. G.Castellar, E.R.Angulo, B.M.Cardozo, “Transesterification vegetable oils using Heterogeneous catalysts”, Prospect, Vol 12, N° 2, 90-104, 2014.

Calcium containing photocatalysts: an alternative in water treatment

A.B. Galindo-Rodríguez[1], M. Sánchez-Cantú[1*], M.L. Ruiz Peralta[1],
E. Puente-López[1] and F. Tzompantzi[2]
[1]Benemérita Universidad Autónoma de Puebla, Facultad de Ingeniería Química, Avenida San Claudio y 18 Sur, C.P. 72570 Puebla, Puebla, México; [2]UAM-Iztapalapa, Departamento de Química, Av. San Rafael Atlixco # 186, C.P. 09340.
Ciudad de México, México.
E-mail: manuel.sanchez@correo.buap.mx

The industrial development and population growth have generated an increased environmental contamination caused by organic pollutants (dyes), with a total annual production of more than $7x10^5$ tons [1]. Photocatalysis is considered as an alternative for cleaning wastewater. In this aspect, semiconductor materials such as TiO_2 and ZnO have been extensively studied as photocatalysts in the degradation of a wide variety of dyes.

Recently, materials not considered as semiconductors due to their dielectrical nature have been evaluated successfully in the photodegradation of distinct organic molecules. Such materials include Al_2O_3, layered double hydroxides and spinel, among others. It is worth mentioning that among these non-semiconductor compounds the calcium-containing catalysts have attracted especial attention due to their low cost, availability and their photoactivity. For instance, Shujuan Zhang [2] evaluated $Ca(OH)_2$ as photocatalyst in methylene blue (MB) decomposition under visible light radiation and he proposed that reaction was conducted by indirect dye photosensitization. In this sense, also CaO has been used in the photodegradation of methylene blue [3], Violet GL2B [4], and Rhodamine B [5].

In this work, four calcium-containing materials (calcium hydroxide, commercial hydrated lime, calcium oxide and calcium carbonate) were evaluated as non-conventional catalysts in the photodegradation of Rhodamine 6G (Rh6G) under UV radiation. Materials were characterized by X-ray powder diffraction, thermogravimetric analysis, and diffuse reflectance and Uv-vis absorption spectroscopy. In the photodegradation reaction, variables such as catalyst nature and amount were investigated. Materials evaluation indicated that among the calcium-containing catalysts Ca(OH)2 was the most active material showing a 50% degradation. An indirect dye sensitization mechanism was proposed to explain the photoactivity of these not-semiconductor materials.

[1] Ajmal, A.; Majeed I.; Naseem-Malik R. RSC Adv., **2014**, 4, 37003-37026.
[2] Shujuan, Z.; RSC Adv., **2014**, 4 ,15835-15840.
[3] Ameta, R.; Kumar, D.; Jhalora, P. Acta Chim. Pharm. Indica., **2014**, 4, 20-28.
[4] Madhusudhana, N.; Yogendra, K.; Mahadevan, K. IJERA., **2012**, 2, 1300-1307.
[5] Kornprobst, T.; Plank, J.; Int. J. of Photoenergy, **2012**, 1, 1-6.

Nanostructured porous silicon microparticles for controlled delivery of theophylline

G. García, J.J. Barrios, A. Guerra and G. Palestino
Universidad Autónoma de San Luis Potosí, Facultad de Ciencias Químicas, Av. Dr. Manuel Nava No.6 - Zona Universitaria, C.P. 78210. San Luis Potosí, S.L.P., México.
E-mail: palestinogabriela@fcq.uaslp.mx

Porous materials have been used over the past decade in biomedical field due its inherent physicochemical and biological properties such as good biocompatibility, biodegradability, intrinsic luminescence, pore size tunability and chemical surface compatibility [1]. Recently, nanostructured porous silicon (pSi) has been developed as a novel material for drug delivery since it has several outstanding advantages compared with other specialized drug carriers [2]. Specifically, the ability to tailor particle from bio-inert to bioactive and to biodegradable by varying pore size and porosity, as well as surface chemistry has led to these nanostructured particles to be considered not only as an appealing platform for drug delivery systems but also, theranostic nanovectors if its diagnostic imaging possibilities are combined with therapeutic payload delivery at specific target [3]. In the present work, pSi nanostructured microparticles were produced by electrochemical etching followed by thermal oxidation for stabilization. Additionally, the surface chemistry of the pSi carriers was tailored by surface alkylation using thermal hydrosilylation of undecylenic acid, followed by physical adsorption or covalent attachment of theophylline to the particle. Size and morphology of microparticles were analyzed by transmission electron microscopy (TEM) and high resolution scanning electronic microscopy (HR-SEM), respectively. Formation of oxide layer and covalent binding was confirmed by FT-IR spectra. The loading of theophylline into the microparticles and its subsequent in vitro drug release behavior was also studied by means of UV-Vis and thermogravimetric analysis (TGA).

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We also acknowledge I.Q. Yatzil Avalos Quiroz (Biopolymers and Nanostructures Laboratory) and M.C. Concepción López Padilla (Bromatology Laboratory) for technical support.

[1] Shresth, N.; Shahbazi, M.; et al. *Biomaterials* **2014**, 35, 7172-7179
[2] Tzur-Balter, A.; Gilert, A.; et al. *Acta Biomaterialia* **2013,** 9, 6208–6217
[3] Wang Ch.; Sarparanta, M.; et al. *Biomaterials* **2015**, 48, 108-118

Mexican natural zeolite applied to CO_2 adsorption

R. García Franco[1], M.A. Hernández[2] and V. Petranovskii[3]

[1]*Chemical Engineering Faculty, BUAP;* [2]*ICUAP-BUAP Zeolites Research Department;*
[3]*Nanoscience and Nanotechnology Centre, UNAM.*
E-mail: rodo_gf@hotmail.com

Climate change has become one of humanity's biggest problems nowadays, this is boosted by the continuous demographic and industrial growth which has significantly accelerated over the recent decades [1]. Such phenomenon has resulted in a continuously growing consumption of fossil origin fuels, increasing greenhouse effect gasses concentration on the atmosphere, being CO_2 the one with the highest concentration. Atmospheric contaminants do not just affect air quality near their emission sources, but also have effect on other areas away from where they were generated due to their transportation facility.[2]

Nanotechnology has contributed to develop environmental remediation such as gas adsorption on nanoporous materials using their high specific surface, with zeolites being an example of such materials, which feature high nanoporosity properties and the possibility for modifications through chemical or physical methods.[3]

The purpose of this paper is to evaluate the carbon dioxide adsorption capacity on a natural zeolite from San Luis Potosí, Mexico under different chemical treatments.

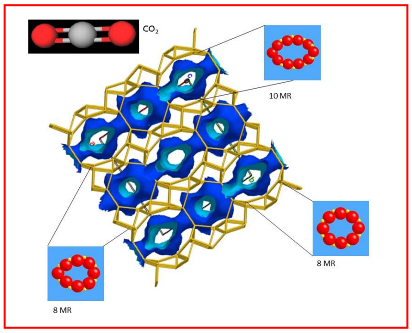

Figure 1. CLI zeolite structure and channel system.

We acknowledge the partial financial supports of CONACyT, through the project P43984-Q.

[1] Hernández, M.A.; Portillo, R.; Salgado, M.A.; Rojas, F.; Petranovskii, V. *Superfices y vacío.* **(2010)**, 23, 67-72.
[2] Molina, M.; Molina, L. T. *Journal of the Air & Waste Mnagement Association.* **(2004)**. 644-680.
[3] Bhawana, P.; Fulekar, M.H. *Research Journal of Chemical Sciences.* **(2012)**. 2, 90-96.

Surface modification of glass ceramic TiO_2 sol-gel nanoparticles with amino groups and PABA functionalization

M. L. Carrera Jota[1,2], M. García Hernández[3], E. Rivera Becerril[2],
Á. de J. Morales Ramírez[4], J. A. Melo Banda[3] and L. Aguilera Vázquez[3]
[1]Posgrado en Ciencias Naturales e Ingeniería; [2]Departamento de Ciencias Naturales, Universidad Autónoma Metropolitana, Unidad Cuajimalpa, Av. Vasco de Quiroga 4871, Col. Santa Fe, Delegación Cuajimalpa de Morelos, Cd. de México, C.P. 05300, México; [3]Tecnológico Nacional de México - Instituto Tecnológico de Ciudad Madero, Av. 1º. de Mayo esq. Sor Juana Inés de la Cruz s/n Col. Los Mangos, Cd. Madero Tamaulipas, C.P.89440, México; [4] Centro de Investigación e Innovación Tecnológica-IPN. Cerrada de Cecati S/N. Col. Santa Catarina Azcapotzalco, Cd. de México, CP.02250, México.
E-mail: mlcj1812@gmail.com

Nanostructured materials have been extensively studied since they offer an incomparable route to control material properties and functionalities for several applications. For this reason, nanomaterials that fulfil requirements for being used in a wide range of applications are denominated multifunctional materials, titanium oxide and silicon oxide are examples of them. Both matrix are known for their physicochemical properties and they are used in chemistry, biology, optical areas, etc., specifically as photocatalysis in environmental remediation, dye-sensitized solar cell, gas sensor, biomedical applications, etc. Recently, SiO_2 and TiO_2 are candidates to be used as drugs carriers, due to its low toxicity and compatibility with the organism. In this paper nanostructures of TiO_2, SiO_2 and $TiO_2@SiO_2$ were obtained by the sol-gel route adding APTES (3-aminopropyltrimethoxysilane) in order to promote the amino groups on the surface of the particles to facilitate the subsequent PABA (para-aminobenzoic acid) functionalization in nanostructured systems of $TiO_2@SiO_2$ -APTES. Particles of titanium and silicon oxides were obtained from titanium diisopropoxide bis(acetylacetonate) and tetraethylorthosilicate (TEOS). The molar ratios of titanium oxide particles into silicon oxide matrix were TiO_2:SiO_2 25:75, 20:80, 80:20, 60:40, 50:50, 75:25, 40:60 0:100 and 100:0. The obtained sols were stable for two months after para-aminobenzoic acid (PABA) functionalization were done. Typical absorption bands were observed from the ceramic, glass-ceramic and functionalized system by means of Fourier Transform infrared spectroscopy; the structural changes as a function of different molar ratio of TiO_2:SiO_2 were studied by X-ray diffraction. The particle morphology was observed by electron scanning microscopy and finally by nuclear magnetic resonance spectroscopy was analysed ^{1}H and ^{13}C. Glass ceramic matrix are promising and innovative materials in the field of chemistry and pharmacology specifically as drug carriers.

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Efecto del pH en la biosíntesis de nanopartículas de oro a partir del extracto de *Jatropha dioica*

D. L. García-Rubio[1], R. Álvarez-García[2], M. A. Flores-González[1],
G. Vargas-Hernández[2], M.A. Hernández-Pérez[4], B.E. Jaramillo Loranca[1],
O. Tillement[3] y M. Villanueva-Ibáñez[1]
[1]Laboratorio de Nanotecnología y Bioelectromagnetismo Aplicado, Universidad Politécnica de Pachuca, Zempoala, Hidalgo 43830, México; [2] Departamento de Biotecnología, Universidad Politécnica de Pachuca, Zempoala, Hidalgo 43830, México;
[3]Institut Lumière Matière Equipe FENNEC - UMR CNRS 5306 - Univ. Lyon 1, 69622 Villeurbanne, Francia.
E-mail: villanueva@upp.edu.mx

Las nanopartículas de oro (AuNPs) son de gran interés debido a sus propiedades ópticas, electrónicas y catalíticas, además sus propiedades de superficie facilitan su funcionalización [1]. Para su obtención se emplean tanto métodos físicos como químicos y recientemente, métodos biológicos. La reducción química de sales metálicas es uno de los modos de obtención más empleados y actualmente se lleva a cabo mediante métodos químicos y biológicos [2]; en este proceso, el pH es un parámetro muy importante para la formación y distribución del tamaño final de las nanopartículas ya que tiene influencia en los potenciales de óxido reducción de los complejos de oro, los cuales de igual forma varían en abundancia dependiendo del pH de la dilución acuosa [3]. En este trabajo se presenta la influencia de la variación del pH en la biosíntesis de nanopartículas de oro mediante el extracto acuoso de *Jatropha dioica*, el cual contiene compuestos antioxidantes con capacidad de llevar cabo la biorreducción de los iones en solución dando lugar a la formación y estabilización de nanopartículas de oro. El tamaño de las AuNPs obtenidas es notablemente dependiente del pH del precursor en solución acuosa, esto debido a la variedad de complejos iónicos y su presencia en diferentes proporciones en función de su valor, el pH cercano a 6.0 proporciona condiciones para la formación de las AuNPs. Las AuNPs fueron polimórficas de tamaños menores a 100 nm y con baja polidispersidad (Figura 1).

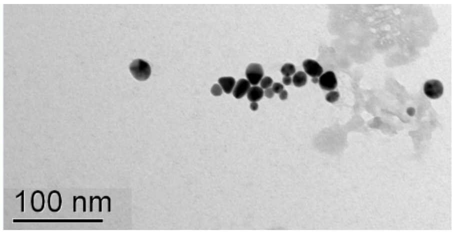

Figura 1. Las AuNPs son polimórficas, se aprecian partículas ovoides, triangulares, alargadas y hexagonales todas ellas de tamaños por debajo de 100 nm

[1] González AL., Noguez C., Barnard AS. (2102) *Map of the Structural and Optical Properties of Gold Nanoparticles at Thermal Equilibrium*. J. Phys. Chem. 116(26):14170–14175.
[2] Iravani S., Korbekandi H., Mirmohammadi SD., Zolfaghari B. (2014) *Synthesis of silver nanoparticles: Chemical, physical and biological methods*. Res. Pharm. Sci. 9(6): 385–406.
[3] Goia D., Matijevic E. (1999). Tailoring the particle size of monodispersed colloidal gold. Colloids and surfaces: A: Physicochemical and Engineering Aspects, 146: 139-152

Synthesis, characterization and evaluation of adducts of C_{60} as inhibitors of amyloid-β peptide aggregation

M. Martínez[1], J.A. Lerma[1,2], M.L. Mendoza[1,2], H.I. Beltran[1], P.Y. López[1],
A. Rojas[3] and G. Basurto[2]

[1]*Universidad Autónoma Metropolitana, DCN, Unidad Cuajimalpa, Av.Vasco de Quiroga 4871, Col. Santa Fe Cuajimalpa, Ciudad de México, 05300, Mexico;* [2]*Universidad de Guanajuato, Campus León, DCI, Loma del Bosque No. 103 Col. Lomas del Campestre, León, Guanajuato, 37150, México;* [3]*Centro de Investigación y de Estudios Avanzados del IPN, Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Ciudad de México, 07360, Mexico.*

E-mail: pylc62@hotmail.com

Carbon nanostructures are one of the most prevalent types of nanomaterials present in the environment which having at least one dimension between 1 and 100 nm. Fullerenes, such as C_{60} or C_{70} are small carbon nanostructures with spherical cage shape and diameter ~ 1 nm. Increasing experimental studies indicate that fullerene derivatives have remarkable anti-amyloid properties for Alzheimer's disease and other neurodegenerative diseases [1a-d]. For example, *in vitro* experiments showed that 1,2-(dimethoxymethano)fullerene, inhibits strongly the amiloyd-β (Aβ) peptide aggregation at the early stage [1a]. Other fullerene derivatives were also found to be able to inhibit amyloid fibrillation and reduce the cytotoxity of Aβ peptides [1b-d]. In this study, we have synthetized adducts of C_{60}, specifically ethyl fullerenmalonates and the corresponding fullerenmalonic acid sodium salts $C_{60+x}(COOR)_{2x}$ (x=1-6 and R= ethyl, Na) and were evaluated by thioflavin T fluorescence assay, demonstrating the fullerenes derivatives properties as inhibitors of Aβ peptide aggregation. The fullerenmalonates were synthesized by cyclopropanation of C_{60} starting from diethylmalonate and purified by chromatographic column; while the sodium salts by alkaline hydrolysis of the respective ethyl fullerenmalonates [2]. All compounds were characterized by IR, UV-Vis and ^{1}H-NMR spectroscopy and mass spectrometry. The ability of some adducts of C_{60} in disrupting Aβ peptide aggregation stablish the basis to generate a new therapeutic approach for Alzheimer´s disease treatment.

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[1] a) Kim, J. E. ; Lee, M. *Biochem. Biophys. Res. Commun.,* **2003**, *303*, 576. b) Podolski, I.; Podlubnaya, Z.; Klochkov, V. *J. Nanosci. Nanotechnol.,* **2007**, *7*, 4. c) Bobylev, A.; Podlubnaya, Z. *Org. Biomol. Chem.,* **2011**, *9*, 5714. d) Makarova, E.; Gordon, R.; Podolski, I. *J. Nanosci. Nanotechnol.,* **2012**, *12*, 119.

[2] a) Camps, X.; Hirsch, A. J. Chem. Soc. Perkin Trans. 1, 1997, 1595. b) Straface, E.; Natalini, B.; Malorni, W. *FEBS Letters*, **1999**, *454*, 335.

Controlled in-situ synthesis of nanosilver on cotton fibers toward highly hydrophobic textiles

L. Macuil Cuautle[1], Z. Morales Vásquez[1], J.U. Tlaminci Marquez[1], J.A. Juárez Torres[1], N. Ortega Hernandez[2], J. Águila-López[2], M.P. Gonzales Araoz[2] and J.F. Sánchez-Ramírez[2]

[1]Ingeniería Textil, Facultad de Ingenieria, Benemérita Universidad Autónoma de Puebla, Puebla, 72570, México. Blvd. Valsequillo y Av. San Claudio, S/N, Edif. 108c Col. San Manuel, Ciudad Universitaria. Puebla, Pue. C.P. 72570; [2]CIBA-Instituto Politécnico Nacional. San Juan Molino Km 1.5 de la Carretera Estatal Sta. Inés Tecuexcomac-Tepetitla, Tlaxcala, 90700. México.

E-mail: jfsanchez@ipn.mx.

The preparation of functional cotton textiles using nanosilver is presented in this work. The synthesis of nanoparticles was performed by the *in-situ* method on the surface of cotton textiles through the pre-activation with potassium hydroxide and silver nitrate. The metal reduction was carried successfully using the ascorbic acid and borohydride of sodium at room temperature. Surface energy on cotton fabric were modified using hexadecyl-trimethoxysilane. Textiles with properties, superhydrophobic and UV protection were obtained. The results of the characterization of the samples using techniques SEM, EDS, DRX, transmittance spectroscopy and contact angle measurement are presented in this research. The results showed that silver nanoparticles uniform were anchored on the surface of cotton textile fibers with high crystalline quality. The modification of the surface composition of the textile was carried out successfully. Blocking ultraviolet light was measured by transmittance data in 280-400 nm and shown ultraviolet protection factor taller than pristine cotton, also it exhibits a static water contact angle > 150° for a 5 µl droplet.

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Síntesis y caracterización de las propiedades fotoluminiscentes del ZnO:Eu^{3+} obtenido por un método biológico

E. Marcelino-Pérez, M.A. Flores-González y M. Villanueva-Ibáñez
Universidad Politécnica de Pachuca, Carretera Pachuca-Cd. Sahagún, Km. 20, Rancho Luna, Ex-Hacienda de Sta. Bárbara, Zempoala, Hidalgo, México.
E-mail: villanueva@upp.edu.mx

Los óxidos metálicos cobran especial atención, particularmente el ZnO gracias a sus propiedades ópticas. Se ha reportado que mediante la inserción de átomos dopantes dentro de su estructura, especialmente átomos de tierras raras, se logran potenciar sus propiedades [1]. Su creciente uso ha ocasionado una alta demanda; sin embargo, los métodos actualmente utilizados para su obtención resultan costosos y hacen uso de reactivos que pueden limitar sus aplicaciones. Por este motivo, surge la necesidad de buscar métodos ecoamigables como los que proporcionan los sistemas biológicos como bacterias, hongos, algas, levaduras y plantas, así como sus derivados [2]. Este trabajo describe la obtención de partículas sub-micrométricas de ZnO dopadas con Eu^{3+} usando como medio al extracto acuoso de *Schoenoplectus californicus*. Espectroscopia UV-vis mostró la banda de absorción de la matriz en un rango de 342-348 nm, propia del ZnO; asimismo, el análisis DRX mostró que ZnO tiene estructura hexagonal tipo wurzita. Por fotoluminiscencia se identificaron cinco bandas de emisión a 579, 591, 613, 650 y 699 nm correspondientes a las transiciones electrónicas $^5D_0 \rightarrow {}^7F_J$ (J=0-4) del Eu en la matriz ZnO [3], la de mayor intensidad ubicada en 613 nm (Fig. 1a). Figura 1b muestra la emisión de 615 nm correspondiente al color rojo-naranja característico del elemento dopante.

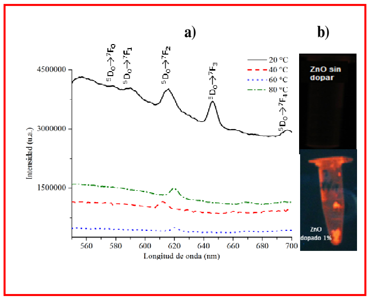

Figura 1. ZnO dopado con Eu a) espectro de fotoluminiscencia de ZnO:Eu (λ_{exc}=375 nm) b) polvos de ZnO sin (superior) y con (inferior) dopaje al 1 %at bajo radiación UV.

[1] Robak, E.; Kotkowiak, M.; & Drozdowski, H. *Nanotechnology*. **2016**, 27(17), 1-13.
[2] Thakkar, K. N.; Mhatre, S. S.; & Parikh, R. Y. *Nanomedicine: Nanotechnology, Biology and Medicine.* **2010**, 6(2), 257-262.
[3] Zhong, M.; Shan, G.; Li, Y.; Wang, G.; & Liu, Y. *Materials Chemistry and Physics*. **2007**, 106(2-3), 305-309.

Effect of sputtering temperature on the growth kinetics and CO_2 sensing properties of ZnO deposited over porous silicon

L. Martínez[1], J.T. Holguín-Momaca[2], T. V. K. Karthik[1], S.F. Olive-Méndez[2],
J. Campos-Alvarez[3] and V. Agarwal[1]
[1]Center for Engineering and Applied Sciences (CIICAp-UAEM), Av. Universidad 1001. Col. Chamilpa, Cuernavaca, Morelos 62209, México; [2]Centro de Investigación en Materiales Avanzados (CIMAV) Av. Miguel de Cervantes 120, Complejo Industrial Chihuahua, C.P. 31136, Chihuahua, México; [3]Institute for Renewable Energy (IER-UNAM), Priv. Xochicalco S/N Temixco, Morelos 62580 México.
E-mail: vagarwal @uaem.mx

ZnO is a versatile functional semiconductor with broad attention in technological applications due its wide direct band gap of 3.37 eV and a large excitation binding energy of 60 meV [1]. Diverse group of morphologies of ZnO nanostructures have been synthetized by different techniques, such as: RF magnetron sputtering [2], chemical vapor deposition [3], sol-gel process [4], homogeneous precipitation [5], etc. We report the growth kinetics and sensing properties of ZnO deposited over macro-porous silicon substrates at 400 and 600°C using magnetron-sputtering technique. Scanning electron microscopy (SEM) was employed to investigate the morphology and the particle size of the ZnO nanoparticles (NPs). The grain growth kinetics were analyzed with the help of the phenomenological equation $r^n = k_0 t \, exp(-Q/RT)$. As well, the sensing response of the complete structure has been tested at different temperatures. The highest sensitivity, S ~ 10, was obtained at a sensor temperature of 300°C on the ZnO NPs sputtered on to the porous silicon substrate at 400 °C. The high response is attributed to the infiltration, uniform and homogenous distribution of the ZnO NPs into the pores. ZnO NPs sputtered at 400°C are found to be smaller than those grown at 600°C, exhibiting a larger surface-area/volume ratio and hence increasing the oxygen adsorption resulting in an enhanced CO_2 sensitivity.

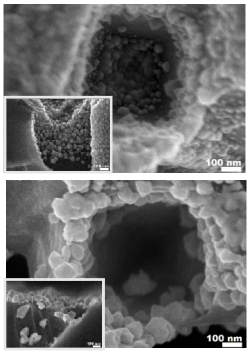

Figure 1. Top-view SEM micrographs of ZnO NPs deposited on PS substrate at 400 (a) and 600 °C (b). The insets are their corresponding cross-sectional view.

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[1] C. Shaoqiang, Z. Jian, F. Xiao, W. Xiaohua, L. laiqiang, S. Yanling, X. Qingsong, W. Chang, Z. Jianzhong, Z. Ziqiang. *Appl. Surf. Sci*. **2005**, 241, 384–391.

[2] S. Flickyngerova, K. Shtereva, V. Stenova, D. Hasko, I. Novotny, V.Tvarozek, P. Sutta, E. Vavrinsky, *Appl. Surf. Sci.* **2008,** 254, 3643–3647.

[3] P. Hu, N. Han, D. Zhang, J.C. Ho, Y. Chen, *Sensors Actuators B Chem*. **2012**, 169, 74–80.

[4] L. Martínez, Y. Kumar, D. Mayorga, N. Goswami, V. Agarwal, *Superlattices Microstruct*. **2014**, 67, 72–81.

[5] T.V.K. Karthik, M. de la L. Olvera, A. Maldonado, Sensor Letters, **2014**, 1513-1518.

Promoting effect of Nb on NiMo/MCM-41 nanostructured catalysts for dibenzothiophene hydrodesulfurization

Franklin J. Méndez, Oscar E. Franco-López and Tatiana E. Klimova
Laboratorio de Nanocatálisis, Facultad de Química, Universidad Nacional Autónoma de México, Ciudad Universitaria, Coyoacán, Ciudad de México 04510, México
E-mail: frankmendez.mz@gmail.com

New environmental regulations on fuels' quality, especially S and N contents, impose a drastic improvement to hydrodesulfurization processes, which can be achieved through the development of more efficient catalytic formulations. In this work, a series of NiMo/MCM-41 nanostructured catalysts modified with Nb were prepared and tested in dibenzothiophene hydrodesulfurization (1300 ppm of S) at 300°C and 7.3 MPa in a batch reactor. Catalysts were denoted as NiMo*x*NbM, where *x* represents Nb loading in the catalysts (*x* = 0, 3, 5 and 10 wt.%). The MCM-41 support was synthesized according to a well-known procedure described elsewhere [1], using a molar gel composition: Na_2SiO_3 = 1 (NaOH = 2 and SiO_2 = 1), TEA = 0.2, CTAB = 0.25 and H_2O = 40. The metal species were deposited by successive impregnation using aqueous solutions of ammonium niobate(V) oxalate hydrate, nickel(II) sulfate hexahydrate and ammonium heptamolybdate tetrahydrate. Catalysts were dried at 100°C for 6 h and calcined at 500 °C for 4 h. The samples were characterized by SA- and WA-XRD, N_2 physisorption, SEM-EDX, UV-Vis DRS, TPR-H_2 and HRTEM. The results showed that the incorporation of small amounts of Nb (3-5 wt.%) to the NiMoM catalysts improved their activity and, in addition, increased their HYD selectivity, as it can be seen in Figure 1 for different DBT conversions. It seems that the above behavior of Nb-containing catalysts is due to a decrease in the temperature of reduction of Mo oxide species that facilitates formation of a better sulfided MoS_2 active phase with a larger amount of active sites.

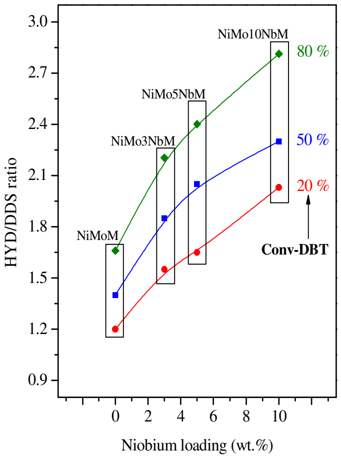

Figure 1. Catalytic performance of the catalysts.

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[1] Méndez, F.J.; Bastardo-González, E.; Betancourt, P.; Paiva, L.; Brito, J.L. *Catal. Lett.* **2013**, *43*, 93.

Visible light photocatalytic activity of gold loaded hydroxyapatite nanoparticles

Sudip Mondal, María Eunice De Anda Reyes and Umapada Pal

Instituto de Física, Universidad Autónoma de Puebla, Apdo. Postal J-48, Puebla, Pue. 72570, Mexico.

E-mail: mailsudipmondal@gmail.com

The study investigates visible light photocatalytic activity of gold loaded hydroxyapatite (HAp) nano particles. HAp nanoparticles were synthesized by wet precipitation method followed by microwave assisted hydrothermal treatment to synthesize different concentration gold (Au) loaded HAp (Au-HAp) nanocomposites. The XRD (X-ray Diffraction) and UV-Vis DRS (Ultraviolet- Visible- Diffuse Reflectance Spectroscopy) analysis revealed the phase purity and Plasmon effect of gold nanoparticles in the synthesized composite materials. The effect of different concentration gold loading on HAp surface influences the surface area and porosity of the composite materials which is confirmed by Brunauer–Emmett–Teller (BET) surface area measurement. These Au-HAp nanocomposites are further used to degrade methylene blue (MB) model dye under visible light at neutral pH 7.0 at 25°C. The photocatalytic degradation of MB obeyed pseudo first order kinetics. Incorporation of Au nanoparticles is seen to be very much effective to activate photocatalytic activity of HAp under visible light.

The work was financially supported by VIEP-BUAP (VIEP-EXC/2016), and PRODEP–SEP (Offer No. DSA/103.5/15/8164), Mexico.

[1] Haslinda Shariffuddin, J; Ian Jones, M; Alec Patterson, D. *Chem. Eng. Res. Des.* **2013,** 91, 1693.

[2] Domínguez, M.I., Romero-Sarria, F, Centeno, M.A, Odriozola, J.A. *Appl. Catal. B: Environ.* **2009**. 87, 245.

Recuperación de nanopartículas de hierro mediante extractos de plantas a partir de un lixiviado de origen vegetal

R. Córdova-Rivera, P. Olvera-Venegas, M. Villanueva-Ibáñez
y M. Flores-González
Laboratorio de Nanotecnología y Bioelectromagnetismo Aplicado, Universidad Politécnica de Pachuca. Ex-Hacienda de Santa Bárbara, carretera Pachuca-Cd. Sahagún, Km 20, Zempoala, Hidalgo, México. CP 43830, Tel. 01 (771) 5477-510.
E-mail: pattytolvera@gmail.com

Durante los últimos 50 años, la actividad humana ha provocado la contaminación de los recursos hídricos en una magnitud sin precedentes históricos. Entre los diversos contaminantes, los metales pesados se encuentran como unos de los más peligrosos [1]. Uno de los metales pesados de uso frecuente es el hierro, es el cuarto elemento más abundante en la corteza terrestre [2]. En este sentido, en el proceso de purificación de arcillas, como resultado de su beneficio se obtienen licores ricos en hierro y otros metales, los cuales no pueden ser vertidos debido a su alta concentración, por ello, es importante buscar alternativas que permitan recuperar estos metales valiosos y a la vez disminuir la descarga de contaminantes. Actualmente, se ha puesto gran atención a las nanopartículas o nanoestructuras base hierro sintetizadas mediante compuestos orgánicos, para la remediación de diversos contaminantes acuosos [3]. Por lo anterior, en este trabajo se busca recuperar nanopartículas de hierro provenientes de residuos acuosos, mediante extractos vegetales, para reducir la cantidad de residuos generados. Se realizó un análisis fotoquímico del extracto para conocer los metabolitos presentes. Los experimentos se realizaron adicionando el extracto y el lixiviado derivado de la purificación de arcillas, se utilizó agitación constante y se evaluó pH y volumen de lixiviado. Se monitoreo la síntesis mediante Espectrofotometría UV- Vis para comprobar la formación de las nanopartículas de hierro, observándose la banda característica de las mismas. Además, con la finalidad de corroborar los resultados y determinar la formación de la especie de hierro obtenida, se caracterizaron las nanopartículas en Espectrofotómetro de transformada de Fourier (FTIR), Espectroscopia de Energías Dispersivas (EDS), Microscopía Electrónica de Barrido (MEB) y Espectroscopia Raman. Mediante este estudio fue posible recuperar nanopartículas semiesféricas a base hierro a partir del lixiviado de la purificación de arcillas y con ello disminuir los residuos generados del proceso de beneficio.

[1] Aloma-Vicente, I., Blázquez-García, G. (2013). Panorama general en torno a la contaminación del agua. La biosorción como tecnología de tratamiento. Revista Cubana De Química, 25(3), 266.
[2] García-Lobato, M., Martinez, A. (2009). Desarrollo de los óxidos de hierro en la nanotecnología. Primera Revista Electrónica en América Latina Especializada, (68), 10-12.
[3] Iravani, S. (2011). Green synthesis of metal nanoparticles using plants. Green Chemistry, 13(10), 2638.

Structural and Optical Characterization of ZnO:Eu nanoparticles for applications in photocatalysis

M.A. Hernández-Carrillo, G. Pérez-Hernández, E. Ramírez-Morales,
L. Rojas-Blanco, C. Ricardez-Jiménez, M. González-Solano, J.G. Álvarez-Ramírez
and L.L. Díaz-Flores

Universidad Juárez Autónoma de Tabasco, Avenida Universidad S/N, Zona de la Cultura,
Col. Magisterial, Villahermosa, Centro, Tabasco 86040, México.

E-mail: german.perez@ujat.mx

ZnO and ZnO:Eu nanoparticles were prepared by simple forced hydrolysis technique. Influence of concentration of Eu doping in physical properties of ZnO on its photocatalytic performance has been investigated. In this work, we are presenting the results of structural and optical investigations of ZnO and Eu doped ZnO films using XRD, EDX, UV-VIS transmittance spectroscopy, and the application of these films in photocatalysis is demonstrated. Eu doped ZnO films were prepared by forced hy method. The concentration of Eu utilized for doping ranged from 1 to 5 % by atomic weight. The nanoparticles possesses good crystallinity and the preferential orientation of the grains is along the (101) plane. The average grain size for 0-5% Eu doped sample was in the range of 15-25 nm. The optical band gap was found to decrease with Eu concentration. The 1-3 % Eu doped ZnO films showed an increased photocatalytic activity for the decomposition of methylene blue.

Preparation of Poly (vinyl alcohol) fibers containing silver nanoparticles by electrospinning and evaluation of their antibacterial activity

S. Pichón Posada[1], J. M. Pérez Porras[1], R. Agustín Serrano[2], E. Reyes Cervantes[2], G. Landeta Cortés[2] and E. Rubio Rosas[2]

[1]Facultad de Ingeniería Química, Benemérita Universidad Autónoma de Puebla Ciudad Universitaria, Blvd. 14 sur y Av. San Claudio, Col. San Manuel. C.P. 72450, Puebla México; [2]Centro Universitario de Vinculación y Transferencia Tecnológica, Benemérita Universidad Autónoma de Puebla Ciudad Universitaria, Prolongación 24 sur y Av. San Claudio, Col. San Manuel. C.P. 72450, Puebla México.

E-mail: efrain.rubio@correo.buap.mx

In recent years, electrospinning technology has received much interest in fabricating bioengineering materials which have high specific surface areas. Electrospinning is a process by which a polymer solution is charged to a high voltage to produce fibers with a diameter ranging from 10 nm to 500 nm.

In this study, antimicrobial Poly (vinyl alcohol) fibers containing silver nanoparticles were prepared by electrospinning.

Polyvinyl alcohol (PVA) was dissolved in deionized water under stirring at 80 °C. Silver nitrate dissolved in water is added drop-wise under stirring to PVA solution thus achieving final concentrations of silver nitrate in the solution. This solution was stirred at room temperature and then aqueous solution of glucose was added and was stirred for 10 min. After that, aqueous solution of NaOH was added (the color was turned brown).

The electrospinning setup used in this study consisted of a hypodermic syringe, an aluminum collecting drum, and a high voltage supply. The syringe pump connected to the hypodermic syringe controlled the flow rate. The PVA aqueous solution was electrospun at a positive voltage of 10 kV, a tip-to-collector distance of 10 cm, and a solution flow rate of 0.5 mL/h. After that the fiber obtained was characterized using x-ray diffraction, transmission electron microscopy, UV-visible spectroscopy, Fourier transform infrared spectroscopy, and atomic absorption spectrometer.

The antibacterial activities of the Ag/PLA-NC films were examined against Gram-negative bacteria (Escherichia coli) by diffusion method using Muller–Hinton agar.

[1] L. Li, Y.L. Hsieh, Polymer, 46 (2005), p. 5133
[2] W.K. Son, J.H. Youk, T.S. Lee, W.H. Park, Polymer, 45 (2004), p. 2959

1D nanostructures of CuO and ZnO as adsorbents for biogas desulfurization

F. Pola-Albores, K. Zambrano-Solís and E. Ríos-Valdovinos
Universidad de Ciencias y Artes de Chiapas. ICBA-Centro de Investigación y Desarrollo Tecnológico en Energías Renovables, Libramiento Norte Poniente 1150, Colonia Lajas Maciel. C.P. 29039. Tuxtla Gutiérrez, Chiapas.
E-mail: francisco.pola@unicach.mx

Synthesis, structural characterization and chemical evaluation (desulfurization) of removal was also realized using non nanostructured materials in order to compare size effects in the reaction. The materials were synthesized by wet chemical routes. CuO nanowires were obtained mixing copper chloride and sodium hydroxide precursor solutions at 60°C. The ZnO nanorods were prepared by seed assisted nucleation in chemical bath deposition at 90 °C by 3h with hexamethylenetetramine and zinc nitrate as reactants and finally it was thermally treated at 360 °C for 2 hours. In both cases, PEG was added into solutions as stabilizer agent. Grazing incidence X-ray diffraction shows wurtzite hexagonal phase for ZnO and monoclinic tenorite for CuO with domains ranging between 180-200 and 10-30 nm, respectively. X-ˇray energy and wavelength dispersive spectroscopies show elemental analysis in concordance with stoichiometric phases, although the purity in non nanostructured materials were lower, ca. to 92 % w/w. The desulfurization reactions were performed at atmospheric pressure and room temperature using a fixed-bed glass reactor (i.d.= 5 mm, L/D=30) loaded with 4 g of material for each test. H_2S 100 ppm (N_2 as balance) was used as reactant, and it was feed at 450 ml/min (GHSV 9120 h-1). The effluent gas analysis was realized using a M-560 (Sewerin) biogas detector, coupled with electrochemical H_2S sensor (0-2000 ppm, ± 2). Results show that CuO and ZnO are feasible adsorbents for hydrogen sulfide removal but they have saturated at ca. 5 min. after the reaction begins. The characterization of wasted adsorbents shows evidence of the sulfur presence (obtained by WDXRF, SEM and TEM) at amounts less than 0.2% w/w, but no phase was detected neither FTIR nor XRD analysis. An effort to explain the chemical nature of the sulfur was done.

[1] Escobedo-Morales, A.; Pal, U. *Appl. Phys. Lett.,* **2008**, *93*, 193120.
[1] Parra, M. R.; Haque, F. Z. *J. Mater. Res. Technol*., **2014**, 3 (4), 363–369.
[2] Hwang, C.-C.; Wu, T.-Y. *Mater. Sci. Eng. B,* **2004**, 111 (2-3), 197–206.
[3] Liu, X. M.; Zhou, Y. C. *J. Cryst. Growth,* **2004**, 270 (3-4), 527–534.
[4] Habibi, R.; Rashidi, A. M.; Daryan, J. T.; Zadeh, A. M. Ali. *Appl. Surf. Sci*., **2010**, 257 (2), 434–439.
[5] Fan, H.; Yang, L.; Hua, W.; Wu, X.; Wu, Z.; Xie, S.; Zou, B. *Nanotechnology,* **2003**, 15 (1), 37–42.
[6] Z.F. Zhang, B.S. Liu, F. Wang, W.S. Wang, C. Xia, S. Zheng, R. Amin, *App. Surf. Sci.* **2014**, 313, 961–969.

Evaluation of calcium oxide in the photodegradation of Rhodamine 6G using ultraviolet light

E. Puente López, A. Galindo Rodríguez, María de Lourdes Ruíz Peralta
and M. Sánchez Cantú

Benemérita Universidad Autónoma de Puebla, Facultad de Ingeniería Química, Avenida San Claudio y 18 Sur, CP 72570 Puebla, México.

E-mail: lourdes.ruiz@correo.buap.mx

In this work, calcium oxide (CaO) was evaluated as catalyst in the photodegradation of Rhodamine 6G (Rh6G) under UV radiation. The effect of the calcination, dose of catalyst, dye concentration and pH were evaluated. Materials were characterized by X-ray powder diffraction, thermogravimetric analysis, Scanning Electron Microscopy and Diffuse Reflectance Spectroscopy.

CaO samples were obtained from the calcination of calcium hydroxide at different temperatures (500-800°C). The X-ray powder patterns of CaO show intense and defined diffraction peaks, which correspond to CaO and $CaCO_3$ in calcite form; the cell parameters and average crystal sizes, were calculated. SEM micrographs showed cuasi-espherical microparticles and aggregation is observed. Furthermore, DRX analysis of the CaO (700°C) at the beginning and end of the photocatalysis revealed that the active phase during the reaction was calcium hydroxide, whereby the photocatalytic activity was attributed to an indirect dye sensitization [1]. The optimum parameters as calcination temperature of 700°C and 0.075 g of catalysis were found reaching a photocatalytic efficiency of 48%.

Band gap values of calcined-CaO samples were lower than the value of the single crystal (6.8 eV) due to surface states associated with oxide ions coordinated incompletely on the surface as a result of calcination temperature [2].

We acknowledge the partial financial supports of VIEP through the Consolidation Subprogram for Young Researchers 2016

[1] Chen, C., Ma, W. & Zhao, J., 2010. Semiconductor-mediated photodegradation of pollutants under visible-light irradiation. Chemical Society Reviews, Volumen 39, pp. 4206–4219.

[2] Zecchina, A., Lofthouse, M. G. & Stone, F. S., 1975. Reflectance Spectra of Surface States in Magnesium Oxide and Calcium Oxide. J. Chem. Soc., Faraday Trans. 1, 71(0), pp. 1476-1490.

Green synthesis of silver nanoparticles from MGYP fungal culture medium and its constituents

D. Roa-Velazquez, M. A. Flores-González, R. Álvarez-García, X. Tovar-Jiménez, M. A. Hernández-Pérez and M. Villanueva-Ibáñez

[1]*Universidad Politécnica de Pachuca, Carr. Pachuca - Cd. Sahagún km 20 Ex-Hda de Santa Bárbara Zempoala Hidalgo, México;* [2]*Instituto Politécnico Nacional, Depto. de Ingeniería en Metalurgia y Materiales-ESIQIE, Ciudad de México 07738, México.*

E-mail: villanueva@upp.edu.mx

Fungi are currently being evaluated for its ability to form silver nanoparticles (AgNPs), however fungal culture media are another practical alternative. This work carried out the green synthesis of silver nanoparticles by MGYP and its constituents (malt extract, glucose, yeast extract, and casein peptone). The complex culture medium and all its constituents, except dextrose, showed ability to obtain silver nanoparticles. UV-vis spectra showed the absorption characteristic band attributed to AgNPs, at 390 nm with MGYP, 406 nm with casein peptone, 410 nm with yeast extract and 453 nm in malt extract. The functional groups responsible of silver ions reduction were evidenced by infrared Fourier transform spectroscopy; principally amino groups of the culture media are possibly involved in this reduction process and formation of nanoparticles. The analysis by scanning electron microscopy showed spherical particles. All the as-synthesized AgNPs had antibacterial activity against the two bacteria under study, nevertheless AgNPs synthesized from casein peptone and yeast extract showed better effect against *S. aureus* than *E. coli*.

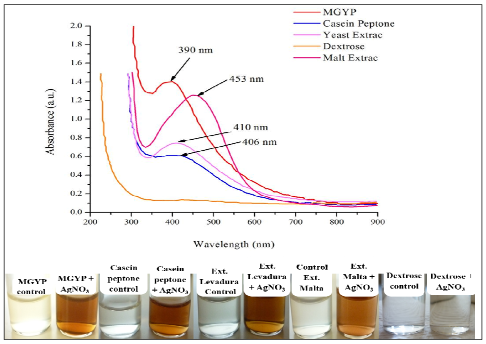

Figure 1. UV–vis absorption spectra of NPsAg obtained with MGYP and all its constituents. The figure shows the characteristic color of culture media mediated synthesis of NPsAg and their respectively control.

Authors would like to thank MM. R. Gonzalez-Montes de Oca for SEM analysis.

Silver 1D nanoestructures and its adsortion on cotton fabric

A. Rodríguez Juárez[1], A. Netzahual Lopantzi[1,2], E. Sánchez Mora[3],
F. Díaz Monge[4], P. Rodriguez Cuamatzi[5], R. Luna García[6]
and J. F. Sánchez Ramírez[2]

[1]Instituto Politécnico Nacional-UPIITA, Av. Instituto Politécnico Nacional 2580. Barrio Laguna Ticomán, 07340. México D.F.; [2]Centro de Investigación en Biotecnología Aplicada, Ex-Hacienda San Juan Molino Carretera Estatal Tecuexcomac-Tepetitla Km 1.5, Tlaxcala C.P. 90700, México; [3]Instituto de Física, Av. San Claudio y Blvd. 18 Sur, Col. San Manuel Edificios 110 'A', 110 'B' y 110 'C', Ciudad Universitaria, C.P. 72570, Puebla, Pue.; [4]Ingeniería en materiales. Instituto Tecnológico Superior de Tlaxco, Predio Cristo Rey Ex Hacienda de Xalostoc s/n Carretera Apizaco Tlaxco Km. 16.8 C.P.90250 Tlaxco Tlaxcala, México; [5]Ingenieria Quimica, A. Universidad Politecnica No. 1 San Pedro Xalcaltzing 90180 Tepeyanco, Tlaxcala, México; [6]Metapol, S.A. de C.V., Carretera a Veracruz Km 144, San Cosme Xaloztoc, C.P. 90460, Tlaxcala, México.

E-mail: alexrj3@hotmail.com

We report a systematic study of the synthesis of Ag NWs with high rate in a simple and scalable preparation method. Using glycerol as a reducing agent and a solvent with a high boiling point, the reaction is rapidly heated to 210°C in air to synthesize Ag NWs with a very high yield in gram level. The obtained Ag NWs are highly crystalline, monodisperse and exhibit two absorption peaks at 350 and 3378 nm. By simply varying the temperature of reaction, the formation of Ag NWs can be controlled. Visual color changes between 40 - 140°C were observed in the colloidal dispersions. A possible growth mechanism of the Ag NWs is given. The Ag Nws were assembly on cotton fibers through a one-step simple dip and dry process to fabricate superhydrophobic cotton fabrics. The formation and assembly of Ag NWs has been confirmed using the techniques UV-Vis spectroscopy, XRD, SEM.

Chemical and surface structure evolution of the as-milled powders of a ductile-ductile system: Effects of ethanol as a process control agent

H. Rojas-Chávez[1,2], J.A. Andraca-Adame[3], N. Cayetano-Castro[3]
and J. Santoyo-Salazar[1]

[1]Departamento de Física, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Del. Gustavo A. Madero, México, CDMX, 07360; [2] Instituto Tecnológico de Tláhuac II - Tecnológico Nacional de México, Camino Real 625, Col. Jardines del Llano, San Juan Ixtayopan. Del. Tláhuac, México, CDMX. 13508;[3]Centro de Nanociencias y Micro y Nanotecnologías - IPN, Av. Luis Enrique Erro s/n, U.P.A.L.M. México, CDMX. 07738.

E-mail: hrojas@fis.cinvestav.mx; rojas_hugo@ittlahuac2.edu.mx

To analyze the effect of ethanol as a process control agent during high-energy milling of a ductile-ductile system, experimental studies were proposed. The chemical structure evolution of ethanol molecules defines the pathway by which these interact on Pb (111), Sn (101) and Pb/Sn (001) powder surfaces during the effects of the mechanochemical treatment. As-milled reaction products were traced via surface (XPS and HRTEM) and bulk characterization techniques (XRD). Dynamic light scattering method demonstrates that as-milled reaction products have particle size distributions in the nanometric scale. Moreover, nitrogen adsorption results ensure that powders' reactivity was increased; therefore, the chemical reactions during high-energy milling process will be promoted via generation of chemical composition gradients.

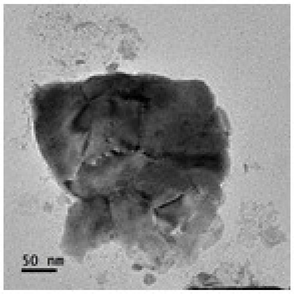

Figure. TEM image obtained from the as-milled products. The effects of ethanol on surface structure of the as-milled powders.

One of the authors (H. Rojas-Chávez) gratefully thanks Consejo Nacional de Ciencia y Tecnología (CONACyT) de México for the Postdoc Scholarship.

Eu doped ZnO thin films by sol-gel method: effect of doping concentration on photo catalytic activity

M. Sánchez, Y. Kumar, N.R. Mathews and X. Mathew

Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Temixco, Morelos 62580, México.

E-mail: xm@ier.unam.mx

Doping concentration driven effect on the morphological, electrical and optical properties of ZnO films prepared by sol gel method have been studied systematically. The prepared films were characterized by X-ray diffraction (XRD), Atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), photoconductivity measurements (PC) and photoluminescence spectroscopy (PL). Debye-Scherrer analysis of XRD patterns reveals a decrease in crystallite size with the increase in doping concentration. Incorporation of europium into the ZnO lattice is confirmed by XPS analysis. Photoluminescence analysis showed that the red emission intensity was altered with the europium doping, 6% Eu doped film showed the maximum PL intensity. The photoconductivity measurements showed maximum photosensivity at 4% Eu doped film. The photocatalytic activity of Eu- doped films was evaluated for methylene degradation and is found to be maximum for 6% Eu doped film.

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Biocompatible magnetic nanoparticles as intranasal drug delivery carriers for the brain

M. F. Veloz-Castillo[1], J. Cordero-Arreola[2], S. Hidalgo-Tobón[3], O. Arias-Carrión[2],
and M.A. Méndez-Rojas[1]

[1]Departamento de Ciencias Químico-Biológicas, Universidad de las Américas Puebla, Ex Hacienda Santa Catarina Mártir, San Andrés Cholula, 72820, Puebla, México; [2]Unidad de Trastornos del Sueño y Movimiento, Hospital General "Dr. Manuel Gea González, 14080, Ciudad de México, México; [3]Hospital Infantil de México "Dr. Federico Gómez" y Universidad Autónoma Metropolitana-Iztapalapa, Ciudad de México, México.

E-mail: maria.velozco@udlap.mx; miguela.mendez@udlap.mx

Magnetic nanoparticles, in particular of magnetite (Fe_3O_4), have been explored for their potential use as drug delivery systems, contrast agents for magnetic resonance imaging (MRI) and hyperthermal therapy [1, 2]. We have evaluated the use of nearly monodispersed, water soluble and stable Fe_3O_4 nanoparticles (~30 nm) modified with a biocompatible polysaccharide coating as novel drug delivery carriers to the brain. The nano-platform used was characterized using FTIR and Raman spectroscopy, SEM and TEM electron microscopies; drug loading and release (dopamine) was followed in a closed vessel until a pseudo-equilibrium was reached during periods up to 48 hours using a UV-Visible spectrophotometer. The biocompatible magnetic nanoparticles were administered via intranasal to a set of male Wistar rats and the biological response at different concentrations as well as its biodistribution in the brain was evaluated as a preliminary test. The presence of nanoparticles distributed in different regions of the rats brains was confirmed by histopathological analysis, using Perls' Prussian blue staining to detect exogenous Fe(III) and verified by MRI tracking [3] Our results suggest that this biocompatible, nanostructured system may become an interesting, non-invasive method to introduce therapeutics into the brain for the potential treatment of several neurodegenerative disorders such as Parkinson or Alzheimer diseases.

We acknowledge partial financial supports from CONACyT, Mexico, through grants CB-2010/154602 and INFR-2014-02-230530.

[1] Veloz-Castillo, MF; West, R.; Cordero-Arreola, J.; Arias-Carrión, O.; Méndez-Rojas, MA. *CNS & Neurol. Dis.*. **2016**, *93*, 193120.

[2] F. Arteaga-Cardona, E. S. Urquiza, et.al- *RSC Adv.,* **2016**, 6, 77558–77568.

[3] F. Arteaga-Cardona, S. Hidalgo-Tobón, U. Pal, and M. Á. Méndez-Rojas *AIP Conf. Proc.,* **2016**, 1747.

Characterization method of the microstructure using the compositional gradient by diffusion couple

C.D. Hernández-Jiménez[1], R. Borja-Urby[2], J.L. González-Velázquez[1],
D. Rivas-Lopez[1], H.J. Dorantes Rosales[1] and N. Cayetano Castro[2]
[1]Instituto Politécnico Nacional, ESIQIE, Departamento de Metalurgia, C.P.07300, CMX, México; [2]Centro de Nanociencias y Micro y Nanotecnologías - IPN, Av. Luis Enrique Erro s/n, U.P.A.L.M. México, CDMX. 07738.
E-mail: ncayetanoc@ipn.mx

A new experimental method was used to determine the morphological evolution of precipitation and phase equilibria using a diffusion couple Cu/Cu-Ti alloy was prepared in order to obtain a compositional gradient in the Cu-Ti system. The diffusion-couple was solution treated at 1223 K for suitable duration, after the specimens were aged at 873 K for 600 s. SEM and TEM analyzed the precipitation process. The gradient method enabled us to construct a T-t-c diagram, which shows the composition, morphology and volume fraction of precipitates for different alloys composition. Besides, it was possible to determine the temperature for the equilibrium solvus-line at 600 ºC.

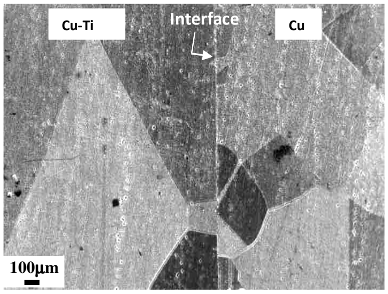

Figure 1. Typical SEM micrographs of diffusion couple after heat treatment.

We acknowledge the financial support of SIP-IPN registry 20161032 and Transmission Electron Microscopy in CNMN-IPN.

Decomposition process in furnace cooled Zn-22%Al-2%Cu alloy with Ag additions

O. Hernández-Nava[1], H.J. Dorantes-Rosales[1], A.A. Torres-Castillo[2], N. Cayetano-Castro[3], J.L. González-Velázquez[1], C. Ferreira-Palma[1], K.I. Morales-Bolaños[1]

[1]Instituto Politécnico Nacional, ESIQIE-DIMM, Del. GAM, Ciudad de México, 07738, México; [2]Facultad de Ingeniería-Instituto de Metalurgia UASLP, Sierra Leona 550, SLP, 78210, México; [3]Instituto Politécnico Nacional, CNMN, Del. GAM, Ciudad de México, 07738, México.

E-mail: cferreirap1200@alumno.ipn.mx; cferreira1089@gmail.com

Furnace cooled Zn-22%Al-2%Cu and Zn-22%Al-2%Cu with 1, 2 and 4%Ag alloys were subjected to aging treatments at 200°C for different times to control the kinetic of the four phase reaction $\alpha + \varepsilon \rightarrow \eta + \tau$, which is responsible of the dimensional instability in this alloy [1, 2]. X-ray Diffraction (XRD), High Resolution Scanning Electron Microscopy (HR-SEM), Conventional transmission electron microscopy (CTEM) and Vickers microhardness measurements (HV), respectively carried out the structural, microstructural and mechanical characterizations. The alloys were homogenized at 350°C for 15 days and then furnace cooled. Subsequently, the alloys were aged at 200°C for different times. The microstructure in the as-annealed condition consists in lamellar structure of the α and η phases, with embedded particles of the ε and φ phases, for alloys with and without addition of Ag, respectively. During aging treatments at 200°C, in the ZAC alloy the development of the four phase reaction, $\alpha + \varepsilon \rightarrow \eta + \tau$ is promoted, as the appearance of the X ray diffraction peaks of the τ and τ' phases after 3.5 h suggest. This fact is accomplished with the intensity decrease and disappearance of the peaks corresponding to the ε phase after 25 h. The 1 and 2% Ag additions retard the four-phase reaction for 7 and 28 times, in comparison with the ZAC alloy, respectively. In the alloy with 4% Ag, the four-phase reaction is completely inhibited [3]. All alloys showed a coarsened cellular decomposition reaction with the increase in aging time. The dimensional stability of the annealed Zn-22%Al-2%Cu alloy could be improved with the Ag additions.

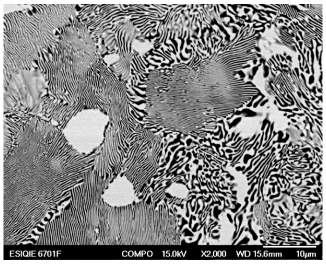

Figure 1: Characteristic BSE SEM micrographs of a furnace cooled Zn-22%Al-2%Cu alloy.

Acknowledgements: the authors would like to thank, CONACYT, IPN-SIP-PIFI and GAID for their financial support.

[1] Savaskan, T.; Mat. Sci. Tech. **1990**,6, 695-703.
[2] Ciach, R.; Bull. Acad. Pol. Sci. **1969**¸18, 371-378.
[3] Flores, A.; Rev. Metal. **2014**, 50 (4).

Design of non-stoichiometric silicon carbide fullerene: analysis of structural and electronic properties

F. G. Bernal Texca and E. Chigo Anota

Benemérita Universidad Autónoma de Puebla, Facultad de Ingeniería Química, Ciudad Universitaria, San Manuel, Puebla, C.P. 72570, Puebla, México.

E-mail: franbertex@gmail.com; ernesto. chigo@correo.buap.mx

We present the results of first-principles molecular orbitals calculations (HSEh1PBE/6-31g(d) [1]) describing the structural and electronic properties of a new silicon carbide fullerene (SiCF) rich in carbon with a chemical composition of $C_{36}Si_{24}$ for the pristine case (in analogy to Boron Nitride fullerene [2]) and doped with nitrogen atoms ($C_{36-n}N_nSi_{24}$; N=1,5,10,15,20). The results of the simulation indicate that no complex frequencies are obtained; this guarantees the stability of the structure 0D. Also, it present non-magnetic semiconductor characteristics (HOMO-LUMO gap of 0.89 eV), high polarity, 1.16 D, and low chemical reactivity ($\mu = -5.75$ eV), which It makes it viable for applications such as drug delivery.

On the other hand, when it is doped with nitrogen atoms shows a transition semiconductor-conductor due to reduction of HOMO-LUMO gap and work function. This behavior indicates their possible usefulness for device design.

We thank the National Supercomputing Laboratory stayed in the BUAP and VIEP-BUAP Project: CHAE-ING16-G.

[1] Heyd J, Scuseria G (2004) J Chem Phys 121: 1187-1192

[2] Chigo Anota E, Escobedo Morales A, Cocoletzi Hernández H, López y López J G (2015) Physica E 74: 538-543

Biosíntesis de nanopartículas de plata a partir del filtrado libre de células de *mucor fragilis*

G. Marcelino-Pérez, Y. Mercado-Flores, M. A. Flores-González,
M. A, Anducho-Reyes, X. Tovar-Jiménez and M. Villanueva-Ibáñez
Universidad Politécnica de Pachuca, Carr. Pachuca - Cd. Sahagún km 20 Ex-Hda de Santa Bárbara Zempoala Hidalgo, México.
E-mail: villanueva@upp.edu.mx

En los últimos años, las nanopartículas de plata (NPs-Ag) han recibido gran atención debido a que presentan propiedades antimicrobianas [1]; sin embargo, su obtención por métodos convencionales exhibe diversos inconvenientes, una alternativa de síntesis propuesta es el uso de microorganismos [2]. Es así como en este trabajo, a partir de un muestreo realizado en el jal de la mina Dos Carlos (Hidalgo), se aisló un hongo filamentoso (H6) que al exponer su biomasa y filtrado libre células (FLC) a $AgNO_3$ 1 mM, llevó a cabo la biosíntesis de NPs-Ag, tal y como lo demuestra el análisis de espectroscopia UV-vis y granulometría láser. Dado que H6 realizó la biosíntesis de NPs-Ag, se procedió a identificar molecularmente amplificando la región ITS por la reacción en cadena de la polimerasa (PCR) dando como resultado el hongo zigomiceto *Mucor fragilis*. Nuevamente se realizó la biosíntesis de NPs-Ag con el FLC de *M. fragilis* variando cuatro factores mediante el diseño de experimentos Box-Behnken. A partir de estos experimentos se determinaron las mejores condiciones con las cuales se obtienen NPs con tamaños inferiores a 50 nm, y mediante el análisis complementario con UV-vis, granulometría láser, MEB (Figura 1), FL, FTIR y DRX. Las NPs obtenidas serán utilizadas para el control de hongos fitopatógenos.

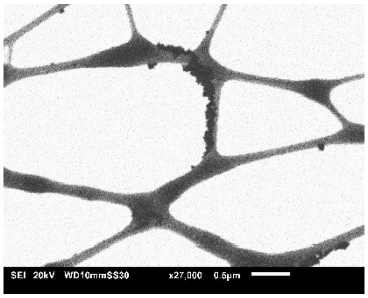

Figura 1. Micrografía de MEB de las NPs-Ag obtenidas a partir del FLC de Mucor fragilis.

[1] Li, G., He, D., Qian, Y., Guan, B., Gao, S., Cui, Y., Yokoyama, K. y Wang, L. *International Journal of Molecular Sciences*. **2012**, 13, 466476.
[2] Chauhan, R., Reddy, A. y Abraham, J. *Appl Nanosci*, **2015**, 5, 6371.

Heterojunctions bulk of organic semiconducting materials and carbon nanotubes to build ofets

J. P. Aguliar-González[1], R. Gómez-Aguilar[2] and G. Ortega-Cervantez[1]

[1]Departamento de Física, Instituto Politécnico Nacional, ESFM, Edificio 9, UPALM, Av. IPN s/n, 07738 Ciudad de México, México; [2]Instituto Politécnico Nacional, UPIITA, Ave. IPN Núm. 2580, Col. La Laguna Ticomán, 07340 Ciudad de México, México.

E-mail: norbac_pablo@hotmail.com

The new technologies of (organic) transistors field effect (OFET) have been trying to use inexpensive materials such as some types of substances rich in carbon, including certain polymers to create organic semiconductors capable of performing the same functions as technologies silicon-based. In order to design, build and analyze OFET, in this work the design of the device is proposed on flexible substrate with a different architecture using thin films of polymer MEH-PPV and Multi -Wall Carbon Nanotubes (MWNTs) as a bulk heterojunction. The current-voltage characteristic (I-V), and the combined effects of the source-drain voltage and gate voltage are analyzed in the range of 0.12 volts and 0-20 respectively. The OFETs based on MEH-PPV and MWNTs show great potential for technological applications in optoelectronics. MWCNTs were synthesized using a mixture of graphite powder, acetate Co and acetate Mo by microwave irradiation technique [1]. The architecture used is vertical stacking, ITO / PEDOT:PSS / MEHPPV:MWNTS / GaIn / PMMA / ITO. One of the important results is that these transistors exhibit a linear behavior in a source-drain current below 300mV and a regime of saturation below 1 volt, these results allow us to think of devices that modulate the current at low gate voltage. Other result is the importance of the sensitivity to ambient light, which makes it a candidate to be an opto-transistor competent.

[1] G. Ortega-Cervantez, R. Gómez-Aguilar, G. Rueda-Morales, J. Ortiz-López, J Mater Sci: Mater Electron, DOI 10.1007/s10854-016-5397-1

Thermal vacuum evaporation ZnO films applied in quantum dot sensitizer solar cells

Jose Alberto Alvarado[1], Z. Neale[1], H. Juarez[2], G. Escalante[2], Jun Luo[1,3] and Guozhong Cao[1]

[1]*Department of Materials and Engineering, University of Washington, Seattle, WA 98195-2120, USA;* [2]*Centro de Investigaciones en Dispositivos Semiconductores, Benemérita Universidad Autónoma de Puebla, Ciudad Universitaria Avenida San Claudio y 14 Sur, 72570, Puebla, México;* [3]*School of Materials Science and Engineering, Jingdezhen Ceramic Institute, JiangXi province, Jingdezhen 333403, P. R. China*

E-mail: alvarja@u.washington.edu; jalvarado@cinvestav.mx

Nowadays, solar energy has become an important renewable source, using promising novel nanomaterials such as quantum dots to convert sunlight into electricity. In this work, ZnO photoanodes deposited by thermal vacuum evaporation and CdS/CdSe co-sensitized quantum dots deposited by SILAR technique are reported. ZnO nanostructured film is used as photoanode due to its high surface area that can allow a well attached zero dimensional nanoparticles (OD) contributing for light absorption. ZnO nanostructured film (~ 2µm of thickness) tested under a solar simulator (1.5M) obtaining a total efficiency of 1.4 %. Films properties such as morphological, structural and optical were carried out by SEM, XRD and UV-Vis techniques respectively. I-V technique was used in order to analyze, the solar cell electrical properties.

Characterization of carbon nanotubes oxidized to form composites

N. Calzada Dorantes[1], P. Román Cuevas[1] and R. Cruz Silva[2]
[1]Centro de Investigación en Ingeniería y Ciencias Aplicadas, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Col. Chamilpa, C.P. 62209, Cuernavaca, Mor. México; [2]Aqua Center of Innovation Shinshu University, Faculty of Engineering; 4-17-1 Wakasato, Nagano, 380-8553- Japan.
E-mail: xiang_551@hotmail.com

Carbon nanotubes (CNTs) tend to agglomerate due to the strong interactions π-π stacking between neighboring CNTs, hindering its handling and application. Likewise it has been demonstrated that nanotubes treated with strong oxidants results in the formation of functional groups (C = O, OH, = O) on the surface of the nanotube improving dispersion and interaction with other molecular species [1]. For this reason it is interesting to assess how it influences the degree of oxidation of the carbon nanotubes in the formation of composite materials; based on microwave assisted oxidation. As part of the results of oxidation, we observed by FTIR new absorption bands and intensifying other associated with a higher concentration of oxygen-containing functional groups. These differences will be evaluated in the formation of composites.

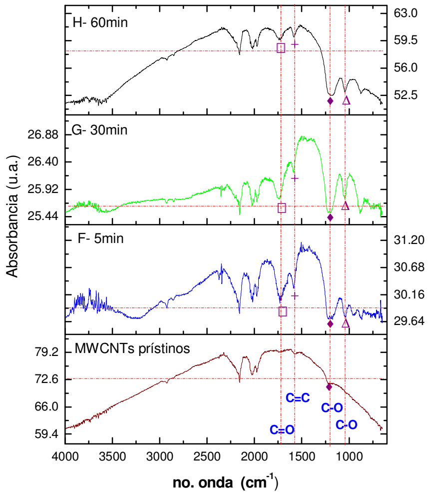

Figure 1. Comparison of the absorption bands obtained by FTIR pristine and oxidized MWCNTs.

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[1] Iwona Pelech, Urszula Narkiewicz, et.al.Separation and Purification Technology. 136 (2014) 105-110.

ZnS-ZnO thin films with Cu, Ga and Ag dopants prepared by ZnS oxidation in different ambient

R. B. Cortés Herrera[1], T. Kryshtab[2] and J. A. Andraca Adame[3]
[1]Instituto Politécnico Nacional-ENCB, Prolongación de Carpio y Plan de Ayala s/n, Col. Santo Tomás, C.P. 11340, Ciudad de México; [2]Instituto Politécnico Nacional-ESFM, Av. IPN, Ed. 9 U.P.A.L.M., 07738 Mexico D.F., Mexico; [3]Instituto Politécnico Nacional-CNMN, Av. Luis Enrique Erro S/N, U.P.A.L.M.,07738, Ciudad de México.
E-mail: benjiii93.bc@gmail.com; kryshtab@gmail.com

ZnO:[Cu, Ga, Ag] thin films were obtained by oxidization of ZnS:[Cu, Ga] films deposited onto glass substrates at 120 ºC by electron-beam evaporation from ZnS:[Cu,Ga] target and of some ZnS:[Cu, Ga] films additionally doped with Ag by the closed space sublimation technique at atmospheric pressure. The film thickness was about 1 μm. The oxidation was carried out in the air or in an atmosphere containing the water vapor at 600-650 ºC during 1 hour. Structural characteristics were investigated by X-ray diffraction and atomic force microscopy. Photoluminescence (PL) spectra of the film were studied at 300 and 77 K using the excitation wavelengths 405 and 457.9 nm.

XRD pattern of as-deposited ZnS films revealed only cubic crystal structure with strong preferred grain orientation in <111> direction. The annealing in the air of ZnS:Cu, Ga film leaded to complete phase transition from ZnS cubic structure to ZnO hexagonal structure with feebly marked texture in <0002> direction and average grain size about 30 nm. The presence of water vapor resulted in the increase of texture in <0002> direction and grain size of 38 nm. ZnS:Cu, Ga, Ag films with strong texture in <0002> direction and grain size of 44 nm were obtained by oxidation in the air.

As-deposited doped ZnS thin films did *not* emit *luminescence* neither at 300 K, nor at 77 K temperatures. Luminescence appeared after the ZnO formation. An intensive green luminescence at excitation by λ=405 nm was observed uniformly in the whole area of the sample at 300 K and at 77 K the intensity increased noticeably. The additional Ag doping resulted in the increase of PL intensity with respect to ZnS:[Cu, Ga] films. The strongest increasing of PL intensity was observed after oxidation process of the films in an atmosphere containing the water vapor.

Synthesis of Au/SiO_2 core- shell nanoparticles, SERS probe for glucose detection

K. de Lázaro- Gasca[1], Ma. de L. Ruiz- Peralta[1] and E. Rubio- Rosas[2]
[1]Facultad de Ingeniería Química- BUAP, Av. San Claudio, S/N, C. P. 72570, Ciudad Universitaria, Cd. de Puebla, Puebla, México; [2]Centro Universitario de Vinculación y Transferencia de Tecnología, Benemérita Universidad Autónoma de Puebla. Av. San Claudio, S/N, C. P. 72570, Ciudad Universitaria, Cd. de Puebla, Puebla, México.
E-mail: lavig_124@hotmail.com; luluza3@hotmail.com

The core-shell nanoparticles have significant advantages over monometallic nanoparticles leading to improved properties such as less cytotoxicity, better conjugation with other bioactive molecules, greater thermal, and, chemical stability [1]. The sensitivity in detection of biological molecules by Raman spectroscopy can be strongly driven and, in some cases, extending to the level of single molecule detection. An example of this is the SERS effect is the appearance of an electromagnetic field located around the nanostructures, providing additional energy for signaling the reagents present [2]. In this work Au / SiO_2 core-shell nanoparticles were fabricated by two–step method. First, gold nanoparticles were synthetized using chemical reduction and the shell was growth using Stober method [3], varying the amount of water, and, ammonium hydroxide it was possible control the hydrolysis and condensation reactions, as a result, the shell thickness was from 15 to 100 nm approximately.

The synthesized samples were analyzed by XRD in order to determinate the crystallinity and present phases, ICP was carried out to identify elemental composition, SEM and TEM microscopies to determinate the morphology and size of Au/SiO_2 nanoparticles. The change in the Au nanoparticles Surface Plasmon positon due to the different shell thickness was determined by diffuse reflectance spectroscopy. Au/SiO_2 core-shell nanoparticles were applied as biosensor in glucose detection by micro-Raman technique using similar concentrations to the human body blood ranging from 2 mM to 6 mM.

[1] Krishnendu Chatterjee, Sreerupa Sarkar, K. Jagajjanani Rao, Santanu Paria. Core/shell nanoparticles in biomedical applications. Advances in Colloid and Interface Science 209 (2014) 8-39.

[2] Engineering of SiO2-Au-SiO2 Sandwich Nanoaggregates Using a Building Block: Single, Double, and Triple Cores for Enhancement of Near Infrared Fluorescence. Shuping Xu, Shay Hartvickson, and Julia Xiaojun Zhao Department of Chemistry, UniVersity of North Dakota, Grand Forks, North Dakota 58202 ReceiVed February 13, 2008. ReVised Manuscript ReceiVed April 6, 2008.

[3] Ismail A.M. Ibrahim, A.A.F. Zikry, Mohamed A. Sharaf Chemistry Department, Faculty of science, Helwan University, 11795 Egypt, “Preparation of spherical silica nanoparticles: Stober silica”, Journal of American Science, 2010;6(11).

Electronic properties of Ga and As doped silicon nanowires with surface dangling bonds

F. De Santiago, A. Trejo, A. Miranda and M. Cruz-Irisson

ESIME-Culhuacán, Instituto Politécnico Nacional, Av. Santa Ana 1000, 04430, Ciudad de México, Mexico.

E-mail: varelasdf@gmail.com

The study of nanostructures with surface dangling bonds is important for the development of nanomagnets and spintronics, as the dangling bonds provide the unpaired electrons necessary for magnetic ordering. In particular, semiconductor nanowires with surface dangling bonds can show half-metallic behaviour, as they are 100% spin-polarized at the Fermi level. This effect has been theoretically investigated in boron and phosphorous doped silicon nanowires [1], however, reports of other dopants from groups III and V are missing from the literature. In this work, through density functional theory, the effect of Gallium and Arsenic doping on the electronic properties of Si nanowires with surface dangling bonds is studied. The ultra-thin nanowires are modelled in the [100] crystallographic direction by removing atoms outside a circumference with diameters of about 1 nm. The doping is made by substituting a Si atom with a dopant atom at the centre of the cross section of the nanowire, and the dangling bonds are in mutually symmetric sites on the surface. Ferromagnetic and antiferromagnetic ordering, plus a non-magnetic case, are simulated, and the ground state is obtained by comparing their total energies. The electronic states due to the dangling bonds have significant spin-splitting, and the states contributed by the dopants are expected to cause a shift in the energy of the bands, allowing some bands to cross the Fermi level for one of the spin channels. This investigation could be important to enrich the knowledge about nanostructures with possible spintronics applications.

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[1]Zhuo, X.; Yan, Q.-B.; Zheng, Q.-R.; Su, G. *Phys. Rev. B* **2009**, *80*, 081306(R).

Synthesis of cobalt nanostructures by electrochemical and thermal decomposition approaches

M. Estrada Flores[1,2], C. Reza San Germán[1], M.E. Manríquez[1]
and L. Díaz Barriga Arceo[1]

[1]Instituto Politécnico Nacional-ESIQIE, Laboratorio de Fundamentos de Nanotecnología, Edif. Z-5, 2do. Piso, Ciudad de México, 07738, México; [2]Instituto de Investigaciones en Materiales, Circuito Exterior S/N, Zona de Institutos, Ciudad Universitaria, C.P. 04510, México, D.F.

E-mail: mestradaf0400@ipn.mx

The effect of electrolysis and heat treatment conditions on the structures morphology of cobalt structures was studied. The template method was used assisted with two approaches: electrolysis and heat treatment. Cobalt electrodeposits and heat treatment samples have been produced in cobalt acetyl acetonate in DMF solutions. Depending on the electrolysis parameters applied, two different structures for the electrodeposits and structures were observed. Their characterization included microstructure exploration by Scanning Electron Microscopy and Transmission Electron Microscopy with analytic determination. The influence of structure on mechanical properties was examined. The results showed that the physical properties of the cobalt structures were highly sensitive to the synthesis method, consequently the synthesized phase. The domain structure of electrodeposited cylindrical Co nanowires with length of 10 or 50 nm and diameters ranging from 20 to 60 nm are studied and measure by means of as well as Transmission Electron Microscopy. Experimental results reveal that crystal structure changes because of the synthesis method, the shape is the approximately the same but the crystallographic phase are different although the orientation growing perpendicular to the wire, depending on whether the diameter of the wires is smaller or larger than a critical diameter of 50 nm.

P2-8

PMMA nanofibers by electrospinning synthesis: morphology and optical properties

A. Hernández-Mata[1], M. Estrada-Flores[1,2], M.E. Manriquez-Ramírez[1],
H. Martínez Gutiérrez[3], J. V. Méndez-Méndez[3] and C. M. Reza-San Germán[1]
[1]Laboratorio de Investigación en Fisicoquímica y Materiales, Departamento de Ingeniería Química Industrial, Escuela Superior de Ingeniería Química e Industrias Extractivas, Instituto Politécnico Nacional, Unidad Profesional Adolfo López Mateos, México, D.F., 07738, México; [2]Instituto de Investigación en Materiales, Circuito Exterior, Ciudad Universitaria, Coyoacán, México, D.F, 04510, México; [3] Centro de Nanociencias y micro y nanotecnologías, D.F., 07738, México.
E-mail: mestradaf7@hotmail.com

Currently the world is leaning to the study, development and application of nanomaterials. Every day are different nanomaterials that are uncovered, and this coupled with their applications are in constant development and growth, achieving increasingly lightweight, durable, versatile and cheaper finished products. In this study we evaluated the process of obtaining nanofibers composite by electrospinning via, structural analysis by Infrared and Raman spectroscopies, The morphology through Scanning Electron Microscopy and Atomic Force Microscopy, The thickness of the polymeric matrix and optical properties by Spectroscopic Ellipsometry. The results show how change the properties of the nanofiber when changes the synthesis voltage.

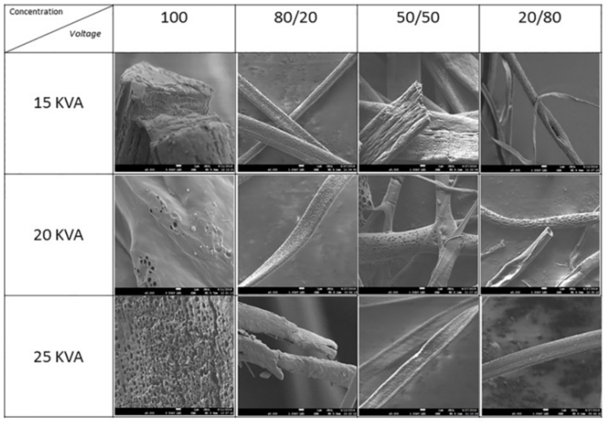

Fig. 1 Micrograph PMMA nanofibers.

Electroactive surface determination of a graphene/wireglue/silver electrode for microbial fuel cell

A. Flores-Meza[1], P.J. Sebastian[1], M. Miranda-Hernández[1]
and L. Contreras-Romero[2]

[1]Instituto de Energías Renovables de la UNAM. Privada Xochicalco S/N Colonia Centro. C.P 62580, Temixco, Morelos, México; [2]Universidad del Istmo, Campus Tehuantepec, Ciudad Universitaria S/N, Barrio Santa Cruz, 4a. Sección. C.P 70760, Santo Domingo Tehuantepec, Oaxaca, México.

E-mail: alflm@ier.unam.mx; sjp@ier.unam.mx

This paper presents the determination of the electroactive surface of an electrode (0.196 mm^2 geometric surface) made from graphene, a composite of a conductive adhesive (wireglue) based on nano-carbon and silver paint, the latter two as support, for application in a microbial fuel cell. For this purpose the electrochemical technique of chronoamperometry and the Cottrell's equation were used. In addition, the electrochemical behavior was studied using the reversible reaction $Fe(CN)_6^3 /Fe(CN)_6^4$ in aqueous solution of potassium chloride. The main objective was to develop a novel electrode material having a high electrical conductivity, high surface area by incorporating graphene in its preparation and electrochemical stability. As results of this work, we obtained an electroactive electrode area of $0.6687 cm^2$ with an electrical conductivity of 1550.3876 $ohm^{-1}m^{-1}$. The test with ferrocyanide showed that the prepared electrode favors faradaic charge transfer process and it is expected to be an alternative anode in microbial fuel cells (MFC).

A numerical modeling of the optical response of bacteria: size, shape and composition effects

M. J. Gálvez Vázquez and A. L. González

Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apartado Postal J48-72570, Puebla, México.

E-mail: mgalvez@ifuap.buap.mx; anagr@ifuap.buap.mx

A general classification of bacteria divides them in two big groups, Gram-positive and Gram-negative. The main characteristic of the bacteria in the first group is a thick peptidoglycan cell wall, while the members of the other group have a thin wall. Using some common dyes, it is possible to identify them, the Gram-positive becomes purple, while the others become pink. Therefore, their different optical properties are useful to generate a catalogue of bacteria classification [1]. From the point of view of basic science, it is interesting to study how the optical response of the bacteria is defined not only by the peptidoglycan wall even also by their size and shape.

Here we present a theoretical-numerical study of the optical properties of *S. aureus* (Gram-positive bacterium) and *E. coli* (Gram-negative bacterium), using the discrete dipole approximation. The analysis includes a simple model of the refractive index of each type of bacteria considering the peptidoglycan wall thickness [2], size and morphology. The scattering, absorption and extinction are presented varying the mentioned parameters.

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[1] Shvalov, A. N.; Soini, J. T.; Surovtsev, I. V.; Kochneva, G. V.; Sivolobova, G. F.; Petrov, A. K.; Maltsev, V. *Cytometry*, **2000**, 41, 41-45.

[2] Balaev, A. E.; Doubrovski, V. A.; Dvoretski, K. N. *Proceedings of SPIE*, **2000,** 4001, 312-316.

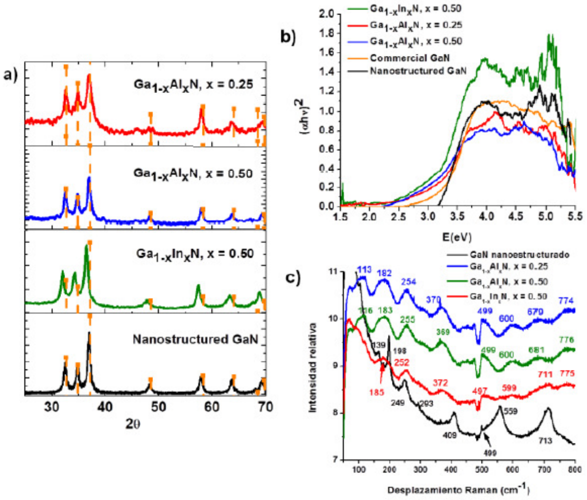
Synthesis and optical properties of nanostructures of GaN, $Ga_{1-x}Al_xN$ and $Ga_{1-x}In_xN$

Gómez - Peralta Juan I.[1], Vázquez - Olmos América R.[1],
Fernández – Osorio Ana Leticia[2] and Sato – Berrú Roberto Y.[1]

[1]Centro de Ciencias Aplicadas y Desarrollo Tecnológico, UNAM, Circuito Exterior S/N, C.U., C.P. 04510, Coyoacán, Cd. de México, México; [2]Facultad de Estudios Superiores Cuautitlán, UNAM, C.P. 54740, Cuautitlán Izcalli, Edo. De México, México.

E-mail: igoformexico@gmail.com

GaN, $Ga_{1-x}Al_xN$ and $Ga_{1-x}In_xN$ were synthesized using a simple – cheap chemical route [1] by using urea, elemental gallium and nitrate salts of Al(III) and In(III). The reagent were milled and heated in two stages under N_2 flux at 300 and 800°C. XRD patterns reveals an unique phase corresponding to the wurzite structure of GaN. The average size of the particle of all sample was determined to be about 15 nm. Raman and IR spectroscopies confirm the nature of the synthesized samples. A small presence of the doping metal within the GaN structured is suggested from XRD and the PL emission displays the presence of a high quantity of defects, these radiative centers may be helpful for applications including sensing, disinfection, and water purification [2]. The strongest emission band belongs to $Ga_{1-x}Al_xN$ with $x = 50$.



Figures: a) X – ray diffractograms of prepared samples b) UV – visible spectra c) Raman spectra.

We acknowledge the financial support CONACyT (Scholarship Number: 336003, and project 128460)

[1] Giordano, Cristina, et al., Chem. Mater. 2009, 21, 5136 – 5144
[2] Yao, Weitang et al., Chem. Eur. J. 2009, 15, 11999 – 12004

Surface Lithium effects on the structure and electronic states of porous silicon

I. González, A. Trejo and M. Cruz-Irisson
Instituto Politécnico Nacional-ESIME Culhuacán Av. Santa Anna 1000, C. P. 04430 D. F, México.
E-mail: israel.ipn.esime@gmail.com

In recent years there have been extensive studies on the development of materials to improve the performance of lithium-ion batteries. One of the most interesting alternatives is Silicon which has a theoretical capacity of about 4500 mAh/Gr, however, it has the limitation of a dramatic volume expansion (of about 300%) with the Li insertion-removal which leads to subsequent fractures and the loss of charge capacity. To overcome this limitation porous silicon (pSi) has been suggested as an alternative, nevertheless, theoretical studies of the effects of lithium on the properties of pSi are still scarce. In this work we study the electronic properties and the atomic structure of pSi with surface Li through a first principles density functional theory approach using the generalized gradient approximation and norm-conserving pseudopotentials. The porous structures were modeled according to the supercell scheme [1,2], by removing atoms of an otherwise perfect Si crystal. The surface dangling bonds were passivated with H atoms and subsequently replaced with Li atoms to observe its effects on the electronic structure of the pSi. The results show that there is a gradual decrease of the band gap energy due to trap like states induced by the Li, as more Li is inserted on the surface the adjacent H tend to shift their positions and hybridization which suggest a grade of amorphization of the surface. If the Si/Li ratio is high the deformations of the lattice are negligible, however if the ratio is Low the structure suffers a radical deformation and Li atoms begin to clusterize. The volume does not show a radical increase which could make this material suitable for Li-ion battery applications

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[1] Escobedo-Morales, A.; Pal, U. *Appl. Phys. Lett.* **2008**, *93*, 193120.
[2] Calvino, M., Trejo, A., Iturrios, M. I., Crisóstomo, M. C., Carvajal, E., & Cruz-Irisson, M. (2014). DFT study of the electronic structure of cubic-SiC nanopores with a C-terminated surface. *Journal of Nanomaterials*, *2014*, 4.
[3] Calvino, M., Trejo, A., Crisóstomo, M.C. et al. Theor Chem Acc (2016) 135: 104. doi:10.1007/s00214-016-1861-5

Modification of the mechanical properties of a polyester resin by incorporation of nanosized zinc oxide

R.N. Vázquez Chavarría[1], F. May Crespo[2], E.A. Franco Urquiza[2], P.G. González[2]

[1]*Universidad Tecnológica del Estado de Querétaro, Av. Playa Pie de la Cuesta 2501, C.P. 76148 Querétaro, Qro. México;* [2]*CONACYT-Centro de Ingeniería y Desarrollo Industrial, Av. Playa Pie de la Cuesta 702, C.P. 76125, Querétaro, Qro. México.*

E-mail: pedro.gonzalez@cidesi.edu.mx

During last years, the inorganic particle filled polymer composites have attracted considerable interest because of their good processability and tailorable characteristics by controlling the content of the filler [1]. Various nanoparticles, such as TiO_2, Al_2O_3 and ZrO_2 [2] have been employed as fillers in composite materials to modify the electrical, optical, mechanical and structural properties of some polymeric matrices. In this work, we describe the effect of incorporation of zinc oxide (ZnO) particles on the mechanical properties of a polyester resin. ZnO was prepared by the sol-gel method. Zinc oxide and oxalic acid were used as precursors of the gel, which was thermally treated at 400, 500 and 600°C to evaluate the effect of the temperature on the structure of the ZnO and the ZnO/polyester composites. The composite materials were formed at room temperature by incorporating 0.05 wt% of ZnO into the polyester resin.

The hardness of the composite increases from 83 to 87 according to the Shore D scale with the increase of the thermal treatment of ZnO. The dynamical mechanical analysis showed a decrease in modulus storage and Tan δ in comparison with polyester resin without particles. In addition, the Tan δ curves show two peaks at around 90 and 145°C for polyester resin, but for the ZnO/polyester composites inhibit the presence of second peak. The wettability test showed a decrease in the surface tension on the composite with the temperature of the incorpored ZnO.

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[1] Bouzidi, A.; et al. *Superl. Microst.* **2015**, *83*, 796.
[2] Kurahatti, R.V.; et al. *Proc. Mater. Sci.* **2014**, *5*, 274.

Synthesis and characterization of $Al_xZn_{1-x}O$

J.J. Reyes Valdes[1], C. Guarneros Aguilar[2], L.V. Ponce Cabrera[1],
C. Estrada Moreno[1], M. Pacio Castillo[3] and F. Caballero Briones[1]

[1]Instituto Politécnico Nacional, Laboratorio de Materiales Fotovoltaicos, CICATA, Altamira, Km 14.5 Carretera Tampico-Puerto Industrial, Corredor Industrial Altamira, 89600, Altamira Tamps., México; [2]CONACYT - Instituto Politécnico Nacional, CICATA, Altamira, Km 14.5 Carretera Tampico-Puerto Industrial, Corredor Industrial Altamira, 89600, Altamira, Tamps., México; [3]Benemérita Universidad Autónoma de Puebla, CIDS-ICUAP, Av. San Claudio y 14 Sur Col. San Manuel, 72570, Puebla, Pue., México.

E-mail: cguarnerosag@conacyt.mx

Aluminium doped zinc oxide ($Al_xZn_{1-x}O$) has been studied in recent years due to its chemical, structural and thermal stability, easy processing and low cost. This metal oxide has potential applications in gas sensors, solar cells, photodiodes, photodetectors, UV-light emitting diodes, transparent conductive oxides and is a promising candidate for high temperature thermoelectric devices due to its high electrical and low thermal conductivities [1-4]. In this work $Al_xZn_{1-x}O$ was synthesized by Pechini method using aluminum chloride ($AlCl_3$), zinc chloride ($ZnCl_2$), citric acid ($C_6H_8O_7$) and ethylene glycol ($C_2H_6O_2$). The samples were sintered at 900°C during 3 h, at different weight percent of Al in order to evaluate the dopant concentration effect on the optical, structural, thermal and electrical properties of $Al_xZn_{1-x}O$ to evaluate its performance for thermoelectric devices.

The authors acknowledge the financial support of SIP-IPN Multidisciplinary 20161804/0291 project.

[1] Dongsheng Chen, Yan Zhao, Yani Chen, Biao Wang, Haiyan Chen, Jun Zhou, and Ziqi Liang, *ACS Appl. Mater. Interfaces* **2015**, 7, 3224.

[2] Ahmed A. Al-Ghamdi, Omar A. Al-Hartomy, M. El Okr, A.M. Nawar, S. El-Gazzar, Farid El-Tantawy, F. Yakuphanoglu, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* **2014**, 131, 512.

[3] A. Akdağ, H. F. Budak, M. Yılmaz, A. Efe, M. Büyükaydın, M. Can, G. Turgut, and E. Sönmez, *Journal of Physics: Conference Series* **2016**, 707, 012020.

[4] B. S. Barros, R. Barbosa, N. R. dos Santos, T. S. Barros, and M. A. Souza, Inorganic Materials **2006**, 42, No. 12, 1348.

Synthesis and characterization of $Ni_{1-x}Cu_xFe_2O_4$ ferrite by Pechini type sol-gel method

Tomás Hernández and Luis Ernesto Padilla

Universidad Autónoma de Nuevo León, Facultad de Ciencias Químicas, Laboratorio de Materiales 1, Ciudad Universitaria, Av. Pedro de Alba s/n C.P. 66450, San Nicolás de los Garza, Nuevo León, México.

E-mail: tomas.hernandezgr@uanl.edu.mx

$Ni_{0.5}Cu_{0.5}Fe_2O_4$ ferrite was synthesized by Pechini type sol-gel method. Nickel nitrate, copper nitrate and ferric nitrate were used as precursors reactants. Citric acid was used as the polymerization agent and the metal nitrate- to -citric acid taken as ratio 1:5. X-ray diffraction (XRD), thermo gravimetric analysis (TGA), differential thermal analysis (DTA) and scanning electron microscopy (SEM) were used to characterize the obtained powder. XRD patterns suggests that Cu substituted Ni ferrite with chemical composition $Ni_{0.5}Cu_{0.5}Fe_2O_4$ shows cubic spinel structure. The DTA/TGA was performed at 0°C-800°C in order to determine the temperature range for growth of the ferrite. SEM images showed agglomerated spheroidal particles.

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Magnetite nanostructures growth and characterization: possible application on hyperthermia therapy

N. Hernández-Guerrero, N. Torres-Gómez and A.R. Vilchis-Nestor

Centro Conjunto de Investigación en Química Sustentable UAEM-UNAM. Carretera Toluca-Atlacomulco, km. 14.5, Toluca, Estado de México, C.P. 50200.

E-mail: nadia_9@live.com; arvilchisn@unam.mx

Hyperthermia has become a promising approach to cancer therapy, avoiding severe side effects and multidrug resistance associated with typical treatment [1]. Magnetic iron oxide nanoparticles have been explored in biomedical research and they are considered to be nontoxic and were approved by the US Food and Drug Administration (FDA) for *in-vivo* applications [2]. Magnetite has the ability to absorb energy from an electromagnetic field and dissipate it as heat to increase the temperature of a tumor up to 43–45 °C, causing its necrosis without damaging the surrounding normal tissue [3].

Herein, magnetite nanoparticles were synthetized by the co-precipitation method, this is one of the simplest and highly potential methods with low cost and control of particle size and shape. To ensure biocompatibility, nanoparticles were PEGylated to limit mononuclear phagocyte system clearance and prolonging blood circulation time for nanoparticles. [4].

TEM characterization shows magnetite nanoparticles obtained have spherical shape and average size of 2.82 nm. To evaluate the cellular response and hyperthermia applications, nanoparticles will be first proved in fungus cell culture.

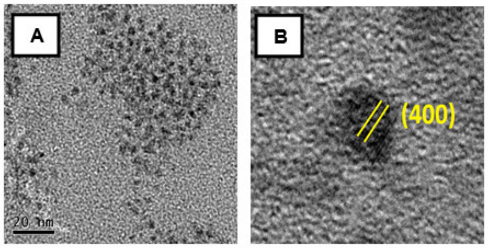

Figure 1. Magnetite micrograph A) TEM B) HRTEM plane (400) according to JCPDS # 19-0629.

We acknowledge the financial support of Universidad Autónoma del Estado de México (Grant: 3688/2014/CIB).

[1] Tietze, R.; et al. *Bioc. Biop. Rese. Comm.*, **2015**, 468, 463470.
[2] Richard, A.; et al. *Mate. Toda.*, **2016**, 19, 157168.
[3] Rodrigues, E.; et al. *Jour. of Magn. and Magn. Mate.*, **2016**, 416, 434440.
[4] Illés, E. et al. *Jour. of Magn. and Magn. Mate.*, **2015**, 380, 132139.

Junction-activation of CdTe/CdS heterostructure under controlled amount of cadmium chloride

Marisol Hernández Gutiérrez[1], Eulises Regalado-Perez[1], Leónides Rojas Gálvez[2],
N.R. Mathews[1] and X. Mathew[1]

[1]Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Temixco, Morelos 62580, México; [2]Universidad de Ciencias y Artes de Chiapas, Tuxtla Gutiérrez, Chipas 29000, México.

E-mail: xm@ier.unam.mx

In this work the effects of post-deposition thermal treatments and the resulting junction-activation of CdTe/CdS heterostructure is studied. There exist lot of discussion in the literature regarding the junction-activation and related topics, however, very little or no conclusive studies exist on the quantity of the chloride sources involved in the process or what is the relation between amount of chloride salt and the effectiveness of the junction-activation. In this work, we are reporting a very systematic study varying quantitatively the amount of $CdCl_2$ involved in the process, and optimized the amount of $CdCl_2$ based on the measured device parameters. We have identified the adequate amount of $CdCl_2$, temperature, and time duration for the junction activation process and the results will be presented. The optimization process was based on the J-V, C-V and EQE measurements of the devices fabricated with the configuration glass/TCO/CdS/CdTe/Cu-Au. We are reporting prototype devices with efficiency close to 10% measured under AM1.5 and 100 mW/cm^2 irradiance. Based on the experimental results we propose the following conditions for junction activation: 1.3 mg $CdCl_2$, anneal temperature 410° C, and 50% O_2 in the ambient.

This work is part of the project CeMIE-Sol 207450/P25, and Marisol Hernández Gutiérrez acknowledges the scholarship from the same Project.

Evaluation of nanoporosity by differential curves of adsorption in narrow pores zeolites

V.A. Hernández[1] and M.A. Hernández[2]

[1]Faculty of Chemical Engineering, BUAP, Av. San Claudio s/n C.P.72570 Puebla, Pue. México; [2]Department of Zeolites Investigation, ICUAP, Av. San Claudio s/n C.P.72570 Puebla, Pue. México.

E-mail: ame.hdzs@gmail.com

Even though there has been an increasing development in the field of nanotechnology in the last years, the equations and methods to evaluate pore size distribution (PSD) still demonstrating few modifications considering the new classification of pores in the last IUPAC report [1]. Thus, in this work we applied the differential curves of adsorption (DCCP) to evaluate the pore size distribution in zeolites of narrow pores which have been chemically modified. This empirical method is based on the experimental data of N_2 adsoprtion at 77 K to obtain later the t-plot giving the graph with the adsorbed volume changing (V) against the thickness of adsorbed layer (t) and finally applied the DCCP method [2]. The results were compared with the classic method Barrett-Joyner-Halenda [3]. In addition of the evaluation of PSD, the zeolites were analyzed by different techniques such as SEM, DRX and EDS. These techniques provided different information about the treatments effects in their structure and composition respectively. Respect to textural parameters, the information was obtained from the adsorption isotherms where the specific surface area was acquired by BET equation in the case of natural zeolite and Langmuir equation for the chemically modified zeolites, while the total pore volume was determined by the Gurvischt rule.

[1] Thommes M.; Kaneko K.; Neimark A.; Olivier J.; Rodriguez-Reinoso F.; Rouquerol J.; Sing K.; *Pure Appl. Chem.* **2015**, *87*, 1051.
[2] Zhu H.Y.; Lu G.Q.; *Stud. Surf. Sci. Catal.*, **2000**,*128*, 243.
[3] Hernández M.A.; Rojas F.; Portillo R.; Salgado M.A.; Perez G.; *J. Chem. Chem. Eng.* **2013**, *7*, 901.

Ag/ZnO nanostructured hollow spheres by hydrothermal and microwave-assisted synthesis

M. A. Herrera Pérez[1], A. Montes Mendez[1], R. Agustín Serrano[2], E. Reyes Cervantes[2] and M. Juárez Meneses and E. Rubio Rosas[2]

[1]Facultad de Ingeniería Química (Ingeniería en Materiales), Benemérita Universidad Autónoma de Puebla Ciudad Universitaria, Blvd. 14 sur y Av. San Claudio, Col. San Manuel. C.P. 72450, Puebla México;[2]Centro Universitario de Vinculación y Transferencia Tecnológica, Benemérita Universidad Autónoma de Puebla Ciudad Universitaria, Prolongación 24 sur y Av. San Claudio, Col. San Manuel. C.P. 72450, Puebla México.

E-mail: efrain.rubio@yahoo.com

ZnO is an important semiconductor with a wide direct band gap and large exciton binding energy. Due to its unique optical and electronic properties, ZnO has potential applications in many fields. Because of size- and shape-dependent properties, it is very important to control the morphology of ZnO.

In this work, a facile and rapid microwave-assisted route was reported for the fabrication of zinc peroxide (ZnO_2) nanostructured hollow spheres of 1 micrometer in diameter. In a typical synthesis of ZnO_2, zinc acetate solution was mixed with hydrogen peroxide in a flask under vigorous stirring. The resultant reaction system was sealed, heated to 150°C by microwave and maintained at this temperature for 30 min, and then cooled down naturally. The precipitate was collected by centrifugation, washed with deionized water and finally was heated at 250°C for 2 h. The material obtained was characterized by X-ray diffraction, scanning electron microscope and transmission electron microscope. The transition temperature of ZnO_2 to ZnO was determined by TG-DSC.

[1] J. Yu, X. Yu, Hydrothermal synthesis and photocatalytic activity of zinc oxide hollow spheres, Environ. Sci. Technol. 42 (2008) 4902–4907

[2] M. Mazloumi, Sh. Taghavi, H. Arami, S. Zanganeh, A. Kajbafvala, M.R. Shayegh, S.K. Sadrnezhaad, Self-assembly of ZnO nanoparticles and subsequent formation of hollow microspheres, J. Allys. Compds. 468 (2009) 303–307.

Double-negative metamaterial in optical range based on nanoscaled gold framed crosses

A. Konovalenko[1], J. Reyes-Avendaño[2] and F. Pérez-Rodríguez[1]

[1]*Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apdo. Post. J-48, Puebla, Pue., 72570, Mexico;* [2]*Instituto Tecnológico y de Estudios Superiores de Monterrey, Campus Puebla, vía Atlixcáyotl 2301, Reserva Territorial Atlixcáyotl, 72453 Puebla, Pue., Mexico.*

E-mail: anatolii@ifuap.buap.mx

Great interest in the study of modern metamaterials belongs to the artificial metal-dielectric periodic structures with negative index of refraction. In the past few years, many forms of metallic inclusions for negative index metamaterials have been proposed [1, 2]. However, the design of metamaterials exhibiting negative refraction in a wide frequency interval is still of high interest. To calculate the effective parameters of the artificial metal-dielectric periodic structures, the parameter retrieval method is commonly used [3].

In the present work, the metamaterial behavior of a golden-framed-crosses periodic structure in a polymer dielectric matrix is studied using the explicit expressions for the tensors of the effective bianisotropic response [1], applying the form-factor division approach [2]. The frequency dependencies of the effective tensors components, and of the refractive index are analyzed. A relatively wide frequency interval of negative dispersion was found.

This work was partially supported by PRODEP-BUAP-CA-250, SEP-CONACYT (grant No. CB-2011-01-166382), VIEP-BUAP.

1. J. A. Reyes-Avendaño, U. Algredo-Badillo, P. Halevi, F. Pérez-Rodríguez, "From photonic crystals to metamaterials: the bianisotropic response", *New J. Phys*. **13**, 073041, 1-33 (2011).
2. J. A. Reyes-Avendaño, M. P. Sampedro, E. Juárez-Ruiz, F. Pérez-Rodríguez, "Bianisotropic metamaterials based on twisted asymmetric crosses", *J. Opt*. **16**, 065102, 1-14 (2014).
3. D. R. Smith, D. C. Vier, T. Koschny and C. M. Soukoulis, "Electromagnetic parameter retrieval from inhomogeneous metamaterials", *Phys. Rev. E* **71**, 036617 (2005).

Optimization of chemical bath deposited CuS thin films and their characterization

F. Loranca-Ramos[1], E. Sanchez Mora[1], N.R. Mathews[2] and Mou Pal[1]

[1]Instituto de Física, BUAP, Av. San Claudio y Blvd. 18 Sur Col. San Manuel, Ciudad Universitaria, C.P. 72570 Puebla, Mexico; [2]Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Temixco, Morelos 62580, Mexico.

E-mail: mou@ifuap.buap.mx

We have reported the optimization of bath conditions to maximize the thickness of CuS films grown by chemical bath deposition. We could increase the thickness by controlling different parameters such as bath temperature, deposition time and by applying a second dip in a freshly prepared bath. Characterization results revealed that the optimized films showed improved structural and optical properties. A post-selenization process has been employed to the optimized CuS films and the preliminary result obtained from Raman scattering study indicates the incorporation of Se in CuS films. Further structural, optical and electrical characterizations of $CuSx(Se)_{1-x}$ are under progress.

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Development of Cu_2ZnGeS_4 thin films using nanoparticle precursor obtained through a wet-chemical route

A. Martínez-Ayala, N.R. Mathews and X. Mathew

Instituto de Energías Renovables, Universidad nacional Autónoma de México, Temixco, Morelos, 62580, México.

E-mail: xm@ier.unam.mx

In this work, we report the development of Cu2ZnGeS4 (CZGS) thin films using a wet chemical route. The precursor for the film deposition was obtained by mixing appropriate quantities of the binary nanoparticles CuS, ZnS and GeS with Triethanolamine (TEA) and acetic acid. Uniform thin films on glass substrates were deposited by doctor-blading. The post-deposition thermal processing was studied by annealing the films in N2-S atmosphere in the temperature range 450 to 550 oC. Using X-ray diffraction studies on the phase purity, the annealing temperature of 500 °C was identified as the optimum temperature. Further studies were carried out to determine the relation between precursor composition and required film stoichiometry matching to the CZTS phase (Cu/Zn+Ge = 0.8 y Zn/Ge = 1.2). The results of the material studies using XRD, SEM, EDXS, UV-Vis, Seebeck, and Raman spectroscopy are presented.

This work is part of the projects PAPIIT-UNAM, IN 113214, CeMIE-Sol 207450/P26 and P28. This work used some of the experimental facilities acquired through the projects PAPIIT-IN107815, and CONACyT 238869, and has collateral contribution to these projects. A. Martinez-Ayala acknowledges the postdoctoral support from the project P28.

Far-field and near-field optical properties of spherical Au@SiO$_2$ nanoparticles

J. L. Montaño-Priede[1], O. Peña-Rodríguez[2] and U. Pal[1]*

[1]Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apdo. Postal J-48, Puebla, Pue. 72570, Mexico; [2]Instituto de Fusión Nuclear, Universidad Politécnica de Madrid, José Gutiérrez Abascal 2, E-28006 Madrid, Spain.

E-mail: upal@ifuap.buap.mx

Metal nanoparticles such as gold nanospheres present interesting optical properties like high absorption and/or scattering in the far-field region and electric field enhancement in the near-field region [1]. Due to these characteristic optical properties, gold nanoparticles found several technological applications such as in surface enhanced Raman spectroscopy (SERS), chemical sensing, and plasmon-enhanced luminescence (PEL) for biomedical imaging [2, 3]. For these applications, dielectric shells should be fabricated over the nanoparticles to protect them from corrosion and/or serve as anchor for luminescence materials or atoms. In this contribution, we present the theoretically obtained near- and far-field optical properties of Au@SiO$_2$ nanoparticles of different sizes surrounded by air and corresponding experiment results for chemically synthesized spherical Au@SiO$_2$ nanoparticles. It has been seen that the maximum of the near electric field is localized outside the shell for small SiO$_2$ shell and it is near the metal core for thicker silica shell. A typical TEM image of synthetized spherical monodispersed gold nanoparticles covered with silica shell is shown in Fig. A.

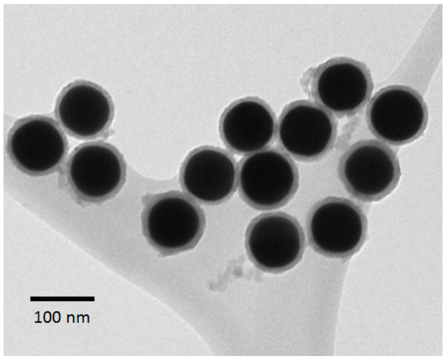

Figure A. Typical TEM image of synthetized Au@SiO$_2$ nanoparticles.

The work was supported by CONACyT, VIEP-BUAP and DITCo-BUAP, Mexico.

[1] L. M. Priede et al. *Nanoscale* **2016**, 8, 14836-14845
[2] E. L. Keller et al. *Analyst* **2015**, 140, 4922
[3] S. T. Kochuveedu et al. *Sci. Rep.* **2014**, 4, 4735

Study of thermal annealing effect under different pressures on the material properties of $Cu_2ZnSn(S,Se)_4$ thin films

I. Montoya De Los Santos[1,2], Maykel C. Piedrahita[1], A. Martinez Ayala[1], M. Pal[3], N.R. Mathews[1] and X. Mathew[1]

[1]Instituto de Energías Renovables, Universidad nacional Autónoma de México, Temixco, Morelos, C.P. 62580, México; [2]Centro Universitario de los Valles. Universidad de Guadalajara Carretera Guadalajara - Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México; 3Instituto de Fısica, BUAP, Av. San Claudio y Blvd. 18 Sur Col. San Manuel, Ciudad Universitaria, C.P. 72570 Puebla, Mexico.

E-mail: xm@ier.unam.mx

The kesterite compound $Cu_2ZnSn(S,Se)_4$ (CZTSSe) has become a promising material for solar cell applications due to its p-type conductivity, an absorption coefficient higher than 104 cm^{-1} and a band-gap value between 1.0 - 1.5 eV depending on Se/(S+Se) ratio. In this work we are reporting the development of CZTSSe thin films through a vacuum-free, lowcost method and the material characterization using different experimental tools to understand the properties and optimize the processing of this promising material for photovoltaic applications. Nanoparticles of the precursor materials ZnS, SnS and CuS were synthesized by solid-state chemical reaction. Then, Cu_2ZnSnS_4 thin films are deposited by doctor blade using a paste of these three binary compounds mixed in appropriate proportions, and submitted to a thermal treatment under Se atmosphere at different temperatures and pressures. The impact of temperature and pressure on structural, compositional, optical, and opto-electronic properties are discussed in order to optimize the physical properties CZTSSe. By increasing temperature from 450°C to 600°C, improvements in $Cu_2ZnSn(S,Se)_4$ crystalline quality as well as a better Se incorporation are found for all chamber pressures. Besides, as an interesting result, it was observed that the kesterite band-gap can be tailored as a function of thermal annealing temperature and chamber pressure.

I. Montoya De Los Santos acknowledges the scholarship from CONACyT for his doctoral studies. This work is part of the projects PAPIIT-UNAM, IN 113214, CeMIE-Sol 207450/P26 and P28. This work used some of the experimental facilities acquired through the projects PAPIIT-IN107815, and CONACyT 238869, and has collateral contribution to these projects.

Optical properties of $Bi_2Mo_xW_{1-x}O_6$ by EELS

D. Morales[1,2], F. Paraguay-Delgado[1], G. Herrera-Pérez[1], O. Salas-Torres[2]
and R. Borja-Urby[3]

[1]Centro de Investigaciones en Materiales (CIMAV) S. C. Miguel de Cervantes 120, Chihuahua, 31136 Chihuahua, México; [2]Escuela Superior de Ingeniería Mecánica y Eléctrica IPN, Unidad Prof. Adolfo López Mateos, Zacatenco, Del. Gustavo A. Madero, 07738, Cd. de México; [3]Centro de Nanociencias Micro y Nanotecnología IPN, Unidad Prof. Adolfo López Mateos, Zacatenco, Del. Gustavo A. Madero, 07738, Cd. de México.

E-mail: dmoralescr@ipn.mx; guillermo.herrera@cimav.edu.mx

The low loss region of the electron energy loss spectrum, supplies information of optical properties of materials [1]. We used electron energy loss spectroscopy (EELS) to determine the optical properties of $Bi_2Mo_xW_{1-x}O_6$. For this purpose, we made use a high resolution transmission electron microscopy in scanning mode (STEM). Kramers-Kronig analysis was performed in order to obtain the energy loss function (ELF). In this model, the response of the material is represented in terms of the dielectric function, which is described by the energy loss function. Our results suggest an increase from about 2.53 eV to about 3.0 eV in the band gap energy. These band gaps are consistent with optical band gaps determined by UV-Vis in diffuse reflectance (DRS). This work shows a parabolic fit to determine the E_g value, which suggests a direct electronic transition for this material.

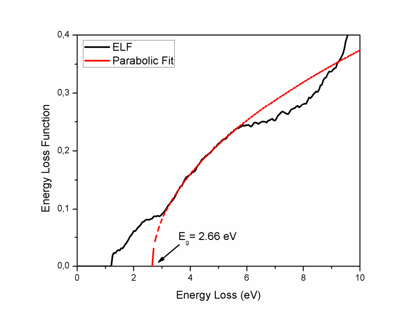

Figure 1. Parabolic fit in the Electron Loss Function to determine the Eg=2.66 eV of Bi_2MoO_6.

Thanks to the Cemisol Project P25 from Sener-CONACyT project. D. Morales thanks to CONACyT postdoctoral scholarship. G. Herrera-Pérez would like to thank CONACyT, Mexico, through the SNI 1; Basic Research grant # 253605; Catedra Research Fellow # 530 and Catedras Research grant # 2563.

[1] T. Kiguchi, N. Wakiya, K. Shinozaki, T.J. Konno, Mat. Sci. and Eng. B **161** (2009) 160-165.

Earth abundant $CuSbS_2$ thin films from electrodeposited Cu-Sb_2S_3 layers

R. Obispo-Solis, R.G. Avilés García, A. Martinez Ayala and N.R.Mathews

Instituto de Energías Renovables, Universidad nacional Autónoma de México, Temixco, Morelos 62580, México.

E-mail: nrm@ier.unam.mx

In this work, we present the preparation of $CuSbS_2$ thin films by sulfurizing a stack consisting of Sb_2S_3 and Cu layers in nitrogen atmosphere. First, the Sb_2S_3 thin films were electrochemically deposited on F: SnO_2 glass substrates from a solution containing $SbCl_3$ and $Na_2S_2O_3$. The deposition was carried out by applying potential pulses. Uniform and stoichiometric films were obtained at deposition potentials of -0.7 V and 0.1 V vs. saturated calomel electrode. The bath temperature was maintained at 40 oC. This was followed by the electrodeposition Cu layers on to these Sb_2S_3 films. The optimum annealing condition for the formation of $CuSbS_2$ was developed after testing different sulfurization temperatures. The films were characterized for structural, morphological, optical, and electrical properties. The XRD analysis confirmed pure chalcostibite with hexagonal structure. The band gap estimated from the transmittance and the reflectance measurements were about 1.5 eV. The films were p-type and photosensitive.

Angel Raymundo Obispo Solis acknowledge the scholarship from PAPIIT IN107815 for thesis. This work is part of the projects PAPIIT-IN107815, and CONACyT 238869. This work used some of the experimental facilities acquired through the projects PAPIIT-UNAM, IN 113214, CeMIE-Sol 207450/P26 and P28 and has collateral contribution to these projects.

Evolution pathway of CZTSe nanoparticles prepared by microwave-assisted chemical synthesis

Odín Reyes Vallejo, M.F. Sánchez and P.J. Sebastian
Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Temixco, Morelos, México.
E-mail: odrev@ier.unam.mx

In this study we present the reaction mechanism of Cu2ZnSnSe4 (CZTSe) nanoparticles prepared by microwave-assisted chemical synthesis. We performed reactions every 10 minutes in order to identify different phases during quaternary CZTSe formation. The powder samples were analyzed by X-ray diffraction (XRD), Raman spectroscopy, energy dispersive spectroscopy (EDS) and X-ray photoelectron spectroscopy (XPS). The results showed (Figure 9) that in the first few minutes, copper phases are predominant, then copper and tin secondary phases react to form ternary phase. The quaternary phase is formed at 50 minutes while ternary and secondary phases are consumed. At 60 minutes pure quaternary CZTSe phase is present. After 60 minutes the quaternary phase decomposes in the previous ternary and secondary phases, which indicates that 60 minutes is ideal reaction time. The EDS analysis of pure quaternary nanocrystals (CZTSe) showed stoichiometric relations similar to the reported research in the literature, which falls in the range of Cu/(Zn+Sn): 0.8 - 1.0, Zn/Sn: 1.0 - 1.20. In conclusion, the evolution pathway of CZTSe synthesized by this novel method is similar to other synthesis methods reported before. Nanoparticles synthesized in this study present desirable properties in order to use them in solar cell and photoelectrochemical cell applications.

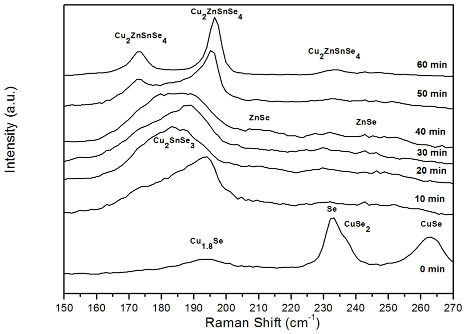

Figure 9: Raman analysis of mechanism reaction

[1] Lee, P. Y., Chang, S. P., Hsu, E. H., & Chang, S. J. (2014). Synthesis of CZTSe nanoink via a facile one-pot heating route based on polyetheramine chelation. *Solar Energy Materials and Solar Cells*, *128*, 156-165.
[2] Zhou, J., You, L., Yi, Q., & Ye, Z. (2013). One-step synthesis of Cu 2 ZnSnSe 4 microparticles via a facile solution route in triethylenetetramine reaction media and its characterization. *Materials Letters*, *107*, 225-227.
[3] Lee, P. Y., Shei, S. C., & Chang, S. J. (2013). Evolution pathways for the formation of Nano-Cu 2 ZnSnSe 4 absorber materials via elemental sources and isophorondiamine chelation. *Journal of Alloys and Compounds*, *574*, 27-32.

Design of an electronic system for the real time characterization of energy conversion devices

J. Riquelme A.[1], P. J. Sebastian[2]*, S.A. Gamboa[2] and J. Campos[2]

[1]*Instituto Tecnológico de Zacatepec-TECNAMEX, 62780 Zacatepec, Morelos México;*

[2]*Instituto de Energías Renovables-UNAM, 62580 Temixco, Morelos, México.*

E-mail: joria@ier.unam.mx

It is very important to use an accurate equipment to perform measurements of electrical signals obtained from energy conversion systems or devices [1-4]. Voltage and current are significant signals that define the characteristic curve (I-V plot) of any solar cell or fuel cell. Temperature, flow rate and concentration of the fuel are important parameters that could control the performance of fuel cells. On other hand, the temperature and irradiance are determining parameters that control the performance of solar cells. It is crucial that the mechatronic system for measuring the electrical variables could consider the acquisition of voltage, current as well as the parameters that control the electrical power of the energy conversion device. It is necessary for the plotting of electrical variables and for the calculation of other characteristics like the electrical power, the cell efficiency, fill factor of the solar cell, etc.

In this communication, it is presented an electronic system for acquiring data from experimental energy conversion devices such as solar cells and fuel cells for micro-electronic applications. The electronic system consists of a software installed in a personal computer and an electronic circuit coupled to a four-wire terminal where the electrical variables like voltage and current can be measured from experimental cells. The software contains a feedback control system for allowing the maximum power transfer from the energy conversion devices to the electrical load. It is possible to record and plot the obtained data in real time for a dynamic analysis of the experimental devices at transient or stable state conditions. It is a portable and low-cost device useful for educational purposes.

Fabricación de celdas solares sensibilizadas por tinte usando películas de TiO_2 de diferente porosidad

J. Rossainz Santos, J. Villanueva-Cab y U. Pal

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

E-mail: rossainz@ifuap.buap.mx

Las celdas solares sensibilizadas por tintes (DSSCs) consiste de una capa nanoestructurada de dióxido de titanio, sensibilizada al espectro del visible por moléculas de tinte adsorbidas en la superficie. Como las nanoestructuras y materiales porosos tienen gran área superficial específica, se espera que se absorba un mayor cantidad de colorante. De esta forma se mejoraría la capacidad de absorción de luz y la generación de más portadores eléctricos en las celdas DSSCs. Por consiguiente, utilizar nanoestructuras de TiO_2 con diferentes tamaños y porosidades puede contribuir positivamente en el rendimiento fotovoltaico de las DSSCs.En este trabajo se sintetizaron nanoparticulas de TiO_2 con diferente tamaño y se caracterizaron por las técnicas SEM, BET, DRS, XRD y micro Raman. Las nanoparticulas de TiO_2 fueron utilizadas para fabricar celdas solares, con películas de diferentes porosidades y espesores similares, posteriormente caracterizadas por medición sus curvas densidad de corriente contra voltaje (J-V). A partir de la caracterización del TiO_2 en polvo se observa que: El tamaño de la porosidad (o área superficial) depende del tamaño promedio de nanoparticula; En todos los casos se obtuvo anatasa, como fase mayoritaria; y finalmente, en dispositivos, un aumento en el área superficial de la película de TiO_2 es proporcional al aumento de su eficiencia.

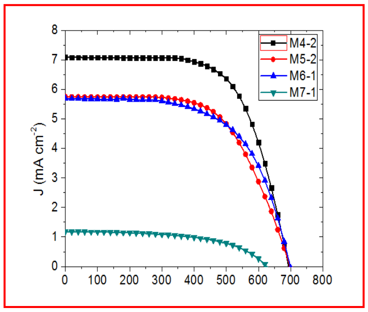

Figura 1 Curvas J-V representativas para celdas fabricadas usando peliculas de TiO_2 con diferentes porosidades.

Este trabajo fue apoyado por VIEP, PRODEP-SEP, CONACYT y CUVyTT-BUAP.

[1] Brian O'Regan, Michael Grätzel. "A low-cost high-efficiency solar cell based on dye-sensitized colloidal TiO2 films". Nature, vol. 353, 737-740 (1991).

Enhanced optical transmission through a nano-slit

Juan Sumaya-Martínez and Daniel A. Rossano-Mercado

Universidad Autónoma del Estado de México, Instituto Literario #100

E-mail: j.sumaya2011@gmail.com; rossd777@gmail.com

The anomalously-high transmission of light through nano- apertures is a phenomenon which has been observed in numerous experiments, but whose theoretical explanation is incomplete. In this work we present a numerical analysis of the power flow of the electromagnetic field near a nano-slit in a thin metal plate, and demonstrate that the enhanced transmission is accompanied by several vortices which pump the energy through the cavity.

Optical response in aperiodically modulated one-dimensional systems with left-handed materials

X. I. Saldaña

Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apartado Postal J-48, Puebla 72570, Avenida San Claudio y 18 Sur, Edificio 1F, Colonia San Manuel, Puebla, México.

E-mail: xochitl@ifuap.buap.mx

Since the predictions made by V. Veselago [1] in 1968 of novel properties of materials having dielectric permittivity and magnetic permeability simultaneously negative where the electromagnetic radiation travels in a direction opposite to the Poynting vector (left-handed materials LHM), many structures have been studied [2] showing new properties not shown by materials with a classical behavior (right-handed materials RHM). Using the transfer matrix theory [3] and the rational approximation [4] a numerical study is made of the optical response of a multilayer system constructed with bilayer units AB periodically ordered. Slab A is a RHM with modulated width da = d*(1+ D*S) where D is a fixed width's increment and S represents consecutive generations of a Fibonacci sequence constructed with the sustitutional rule: 1 -> 10, 0 -> 1 and slab B is a LHM with fixed width db. It is shown that for some values of the structure's parameters, the calculated refractive index average of the system is zero, this is a new property not found in a multilayer formed only with RHM slabs.

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[1] Veselago, V. G., *Sov. Phys. Usp*., **1968**, 10, 509.
[2] Bria, D., B. Djafari-Rouhani, A. Akjouj, L. Dobrzynski, J. P. Vigneron, E. H. El Boudouti, and A. Nougaoui, *Phys. Rev. E*, **2004**, 69, 066613.
[3] Yeh P., Optical Waves in Layered Media, **1988**, Wiley, New York.
[4] Hawrylak, P. G., G. Eliasson, and J. Quinn, *Phys. Rev. B*, **1987**, 36, 6501

Optical properties of Sb_2S_3-SiO_2 composite opals

A. G. Sánchez-Gonzalez[1], E. Sánchez-Mora[2], R. Silva-González[2],
J. Miguel Gracia y Jiménez[2], y Mou Pal[2]

[1]Facultad de Ingeniería Química, Benemérita Universidad Autónoma de Puebla, Av. San Claudio y 18 Sur, C.P. 72570, Puebla, Pue., Mexico; [2]Intituto de Física, Benemérita Universidad Autónoma de Puebla, Av. San Claudio y 18 Sur, C.P. 72570, Puebla, Pue., Mexico

E-mail: mou@ifuap.buap.mx

Photonic crystals are materials with a high ordered microstructure, hence they have a great periodical dielectric contrast distribution and, for this distribution, these materials can possess a photonic band gap (PBG) [1]. The artificial silica opals (SiO_2) are 3D photonic crystal formed by amorphous SiO_2 microsphere with close packed array as face centered cubic arrangement [2]; therefore, there are a ~26 % void space between SiO_2 spheres (figure 1). In the present work, optical properties of SiO_2 opals infiltrated with Sb_2S_3 nanoparticles were studied. The infiltration process consists of the addition of SiO_2 opals dispersed in water in a precursor solution of Sb_2S_3 with different volume and maintaining under agitation for certain time. The SiO_2 opals were synthetized following a version of Stöber-Fink-Bohn method using tetraethyl orthosilicate, ethanol, deionized water and ammonium hydroxide solution while Sb_2S_3 precursor solution was prepared with antimony trichloride, acetone, sodium thiosulfate solution and deionized water. The optical and structural properties of Sb_2S_3-SiO_2 composites were studied by scanning electron microscope (SEM), Raman spectroscopy and UV-Vis spectroscopy and photoluminescence spectroscopy.

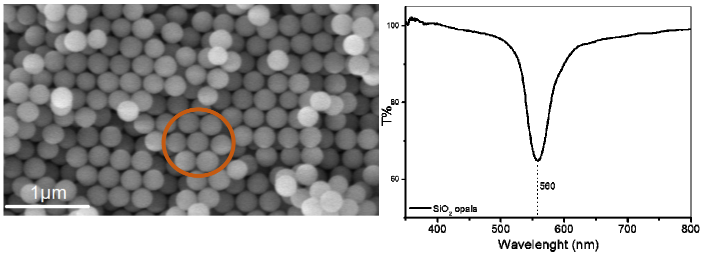

Figure 1. SEM micrographs of close packed array of SiO_2 opal with 260 nm of diameter and transmittance spectra with their characteristic photonic gap.

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[1] Sukhoivnovs, I.; Guryev, I. *Heidelberg: Spinger.* **2009**.
[2] Santamaria-Razo, D.; Pallavidinol, L. *J. Nanoparticle Research.* **2008**, *10*, 1225.

Optical and structural characterization of gold nanoparticles incorporate a porous silicon: effect of the concentration of ions of gold

F. Morales-Morales[1], G. García-Salgado[1], F. Severiano[2] and V. López Gayou[2]

[1]Centro de Investigaciones en Dispositivos Semiconductores CIDS-ICUAP, Edificios 136 y 137 Cd. Universitaria, Blvd 14 Sur y San Claudio, Col. San Manuel, C.P. 72570. Tel. 01(222) 229-5500 Ext. 7876, Puebla, Pue. México. Universidad Autónoma de Puebla, Apartado Postal J-48, 72570 Puebla, México; [2]Centro de Investigación en Biotecnología Aplicada, IPN, Ex-Hacienda San Juan Molino Carretera Estatal Tecuexcomac-Tepetitla Km 1.5, Tlaxcala C.P. 90700, México. Tels.: 01-248-48707-65 y 66 Conmutador IPN: 57296000, Ext. 87816.

E-mail: valgayou@gmail.com

Photoluminescence (PL) and scanning electron microscopy (SEM) studies of gold nanoparticles incorporated in porous silicon layers (PLS) at different concentration by electroplating method have been carried out. SEM results confirmed the presence of gold nanoparticles above and inside of PSL. Observing that since low concentrations (0.5mM) it has the presence of gold nanowire and nanoparticle and its density increases as the concentration of gold ions increases, also is observed an increase in the length of the nanowires and a decrease in isolated nanoparticles. PL analysis reveals the characteristic emissions of porous silicon (PS) i.e. a broad emission band at 450nm attributed to defects and at 610nm corresponding to porous silicon (PS). Also an increment in the PL main emission of PS is observed with the Au nanoparticles inclusion.

Band gap engineering of porous Ge for applications to lithium batteries

A.N. Sosa, I. González, A. Trejo, A. Miranda, E. Carvajal and M. Cruz-Irisson

Instituto Politécnico Nacional, ESIME-Culhuacan, Av. Santa Ana 1000, 04430 Cd. de México, México.

E-mail: asosacamposeco@gmail.com

In the last years the low dimensional systems have gathered significant attention due to their potential applications, especially Germanium nanostructures could be used in lithium-ion batteries. One of the most promising nanostructures to this end is the porous Germanium (pGe), however theoretical studies of this porous semiconductor, for this application is still rare, and would prove useful for the development of the new generation of Li batteries. In this work the effect of surface Li on the electronic properties of pGe was investigated by means of the density functional theory and the supercell scheme [1,2], where the porous structures are modeled by removing atoms of a Ge supercell along the [001] direction. The surface dangling bonds were passivated with H. To model the effects of surface Li, the H atoms were gradually replaced with Li atoms until achieving a total coverage of the pore surface. The calculations show that as Li atoms are inserted on the surface the electronic band gap decreases by effects of trap like states on the band gap energy, those states increase the overall electron conductivity favoring the conduction on these nanostructures which would be beneficial for its use on Li-ion batteries.

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[1] M. Calvino, A. Trejo, M. C. Crisóstomo, M. I. Iturrios, E. Carvajal, M. Cruz-Irisson, *Theor. Chem. Acc.* **2016**,135,104.

[2] A. Trejo, A. Miranda, L. K. Toscano-Medina, R. Vázquez-Medina, *Microelectronic Eng.* **2016**¸ 159,215.

Far field diffraction of an ultrashort laser pulse by metallic rectangular nano-slits

J. Sumaya-Martinez and A.D. Rossano Mercado

Facultad de Ciencias, Universidad Autónoma del Estado de México, México.

E-mail: j.sumaya2011@gmail.com; jsumaya2000@yahoo.com.mx

Based on a Double Fourier Transform and a Modal Theory we simulate the diffraction of ultrashort laser pulses through several metallic nano-slits. The Fraunhoffer region is analyzed as a function of several opto-geometrical parameters such as broadband width, spot size and slit width.

Electronic structure and vibrational properties of GaSb nanowires: an *ab-initio* study

M. Marthen, A. Trejo and M. Cruz-Irisson

Instituto Politécnico Nacional, ESIME-Culhuacan, Av. Santa Ana 1000, 04430 Cd. de México, México

E-mail: marthenm@hotmail.com

In recent years there has been an increasing interest on the research of the properties of binary semiconductor nanowires due to their potential applications for microelectronic and optic devices, specially GaSb nanowires (GaSbNWs) could be used for high speed electronic and optoelectronic applications due to its high hole mobility. A correct understanding of the properties of GaSbNWs crucial for the development of these new applications, however the theoretical investigations of this materials are still scarce. In this work the electronic and vibrational properties of GaSb nanowires are studied by means of the Density Functional Theory approach with the generalized gradient approximation and the supercell scheme [1,2]. The nanowires are modeled by removing atoms outside a circumference on the [111] direction of an otherwise perfect GaSb crystal, where all surface dangling bonds are passivated with H. The results show that the electronic band structure shows a quantum confinement signature since the electronic band gap energy decreases as the nanowire diameter increases. For the vibrational properties no clear quantum confinement signature was observed due to some bond bending modes (Ga–H, Sb–H) which mask the expected shift of the highest optical modes of GaSb to lower frequencies compared to their bulk counterparts. These results could be important for the characterization of these nanowires for applications on the microelectronic industry due to the possibility of band gap engineering.

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[1] Trejo A.; Ojeda M.; Cuevas J.L.; Miranda Á.; Pérez L.A.; Cruz–Irisson M. *Int. J. of nanotechnol.*¸ **2015**, 12 (3-4), 275-284

[2] Trejo A.; Miranda A.; Toscano-Medina L.K.; Vázquez-Medina R.; Cruz-Irisson M. *Microelectronic Eng,*. **2016,** 159, 215-220

Influence of time deposition of SnS thin films on stainless steel substrate by chemical bath deposition at room temperature

L. Treviño-Yarce[1], R. Romano-Trujillo[1], E. Rosendo[1], C. Morales[1], J. M. Lugo[1], A. I. Oliva[2], E. Flores[1], T. Díaz[1], G. García[1] and R. Galeazzi[1]

[1]Posgrado en Dispositivos Semiconductores, Instituto de Ciencias, BUAP 14 Sur y Avenida San Claudio, C.U. Edificio 103-C, C. P. 72750 Puebla, Puebla México; [2]Centro de Investigación y de Estudios Avanzados del IPN-Unidad Mérida, Departamento de Física Aplicada, A.P. 73-Cordemex, 97310 Mérida, Yucatán, México.

E-mail: lty_tyta@hotmail.com

In this work we show the effect of deposition time on structural and optical properties of Tin Sulfide (SnS) films. Chemical bath deposition technique was used to deposit SnS thin films on stainless steel (type 304) substrates at 25 °C, the deposition time was varied from 6 to 24 hours. Tin chloride and thioacetamide was used as source of Sn ions and S ions respectively in aqueous solution. Structural analysis was done using X-ray diffraction (XRD), and shown that the SnS films deposited exhibit an orthorhombic crystalline structure with preferred growth on (111) direction. Band gap values were obtained using reflectance measurements, and applying Kubelka Munk method [1]. The band gap values are between 1.3 and 1.9 eV, and this value depends on the time deposition. Profilometry measurements, shown an increase in the film thickness from 0.2 to 1.8 μm as the deposition time was increased from 6 h to 24 h. Using the technique of atomic force microscopy (AFM) it was observed that the morphology of the films of 6-16 hours is spherical, while the 20 and 24 hours presented wire morphology.

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[1] Francis M. Mirabella. Modern techniques in applied, Edit. John Wiley and Sons, Inc.

AMPS-1D simulation study of solar cells based on cubic $In_xGa_{1-x}N$ in green region

J.A. Santis, A. Ruiz, I. Zuñiga, J. Conde, H. Vilchis

Centro de Investigación y Desarrollo Tecnológico en energías Renovables, Universidad de Ciencias y Artes de Chiapas. Libramiento Norte #1150 Col. Lajas Maciel 29039, Tuxtla Gutiérrez, Chiapas, México.

E-mail: heber.vilchis@unicach.mx

InGaN alloys are the most investigate III-V semiconductor in the last decade due to its potential to cover the full solar spectrum by varying the In fraction. So it has been recognized as a leading photovoltaic candidate for high conversion efficiency. However, its main drawbacks is the difficulty for synthesize some In concentration and p-doping films.

In the last years several authors have reported solar cells based InGaN/GaN multi quantum wells (MQW) with hexagonal phase [1]. Nevertheless, the cubic phase has some advantages over the hexagonal phase, such as it not presents spontaneous and piezoelectric polarization, also it is easier to dope. On the other hand, I. E. Orozco et al. [2] reported this year a MQW based in cubic InGaN with different In concentrations (from 0.1 to 0.47).

Further several authors have published simulation papers about InGaN multijunction tandem and InGaN Schottky based solar cells [3,4]. Simulated works only used numerical equations and electrical parameters calculations for predict solar cells performance. Also all simulated works considering In concentrations in the infrared region despise the visible region where the sun spectra is more intense.

Considering all of the above, it is necessary to predict the InGaN solar cell performance in the visible spectrum. We simulated $In_xGa_{1-x}N$ solar cells with In concentration from 0.2 to 0.35 using Analysis of Microelectronic and Photonic Structures (AMPS-1D) code. For simulated parameters we used several experimental values reported by others authors, such as absorption coefficient, energy band gap (considering current bowing parameter) and work function of metal contacts. The thickness, the band gap energy, and the density of the states were varied in the layers for complete the study. Our results confirm an increase of efficiency with double and triple junction. The best efficiency was obtained for solar cell based on 0.25 In concentration.

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[1] H. Li, P. Li, J. Kang, Z. Li, J. Li, X. Yi, G. Wang, App. Phys. Express 6 (2013) 102103.
[2] I. E. Orozco, M. Avalos, V. D. Compeán, C. Cuellar, A. G. Rodríguez, E. López, M. A. Vidal, Journal of Crystal Growth 435 (2016) 110.
[3] A. Mesrane, F. Rahmoune, A. Mahrane, A. Oulebsir, International Journal of Photoenergy (2015) 594858
[4] A. Adaine, S.O. Saad Hamady, N. Fressengeas, Superlattices and Microstructures 96 (2016) 121.

Relation between crystallographic structure and photoluminescence emission polarization for III-V semiconductor alloys

T. Prutskij[1] and G. Attolini[2]

[1]Instituto de Ciencias, BUAP, Privada 17 Norte, No 3417, col. San Miguel Huyeotlipan, 72050, Puebla, Pue., México; [2]IMEM/CNR, Parco Area delle Scienze 37/A - 43010, Parma, Italy.

E-mail: tatiana.prutskij@correo.buap.mx

III-V semiconductor alloys, as ternary GaInP and quaternary GaInAsP alloys are important materials widely used in semiconductor lasers, solar cells, high electron mobility transistor (HEMT) and heterojunction bipolar transistors (HBT). Due to kinetic conditions in almost all ternary alloys grown by MOVPE technique, long range *atomic ordering* is observed. In particular, within GaInP epitaxial layers a superlattice structure made of alternate In-rich and Ga-rich {111} diagonal planes, with interleaving planes of P atoms, corresponding to a CuPt-type atomic ordering, is spontaneously formed during the growth. The resulting symmetry of the crystal lattice of ordered alloy causes reduction of the band-gap energy (with respect to its value in the disordered material) and splitting of the valence band. Another factor that changes the symmetry of the alloy is an internal biaxial strain due to a mismatch between the epitaxial layer and the substrate. As a consequence, the photoluminescence (PL) emission of the alloy becomes polarized.

Here we analyze the PL emission of GaInP and GaInAsP epitaxial layers grown by MOVPE on GaAs and Ge substrates. For these structures, which have different order parameters, we experimentally studied the PL spectra from the (001), (110), and (1-10) crystallographic planes of the layer as a function of the angle of linear polarization of the PL emission. We also compare the experimental and calculated PL emission intensity curves and analyze the temperature dependence of the value of biaxial strain in the layer.

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