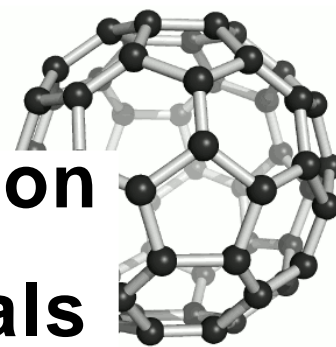


# 4th Mexican Workshop on Nanostructured Materials



March 19-22, 2013

Puebla, Mexico

## Abstract Book



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# FOREWORDS

The 4<sup>th</sup> 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, physics and chemical phenomena associated to nanometric materials, to 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. Though the first version of this event was a small gathering, the number of participants increased substantially in the 2<sup>nd</sup> and 3<sup>rd</sup> versions.

With the persisting constrains and small budget, keeping in mind the demand and necessity of young research students, the organizers arranged two courses on the *electron microscopic characterization of materials* and *nano-medicine and their future perspectives* delivered by two experts in the fields, 3 keynote lectures and 9 invited talks by eminent scientists and nanomaterial specialists of Mexico, United States, Spain and India, 26 oral presentations and 136 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 of Nano Materials (Trans Tech Publication, Switzerland) 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 April 30, 2013.

We wish to express our sincere thanks to the sponsors of the workshop for their valuable support. 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, March 15, 2013.

**Umapada Pal** (Chairman)

**Velumani Subramaniam** (Co-chairman)

**Alejandro Escobedo-Morales** (Co-chairman)

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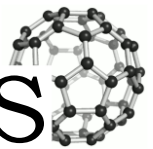
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# SHORT COURSES



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## **Understanding Nanomedicine: Introduction and Perspectives**

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This short course will be focused in the basis of nanoscience and nanotechnology for biological and medical applications. The part 1 of the course will cover some of the biological fundamentals applied in the area, the present proposals and promises of nanotechnology in medicine. The second part will be a discussion related with the principal topics and current applications of nanomedicine. Finally we present the biomaterials and biosensors research work carried out in the Laboratory of Nanobiotechnology at MICRONA-UV.

### **CONTENT**

#### ***Part I***

- 1.1. Fundamentals of Nanomedicine
- 1.2. Nanomedicine history: Proposals and promise

#### ***Part II***

- 2.1. Nanomolecular Diagnostics
- 2.2. Nanodivices for Medicine and Surgery
- 2.3. Nanoparticles for drug delivery
- 2.4. Nanomaterials and Tissue Engineering
- 2.5. Worldwide development and commercialization of nanomedicine
- 2.6. Some ethical considerations
- 2.7. MICRONA's contribution to Nanomedicine

## **Caracterización de Materiales por Métodos de Microscopía Electrónica y Técnicas Afines**

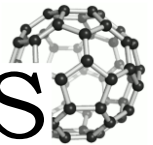
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La ciencia y tecnología actuales se están desarrollando a nivel micrométrico o aun nanométrico, por lo que las técnicas de caracterización fina son un requisito indispensable. Para este propósito, los microscopios electrónicos y sus técnicas afines como espectroscopia de dispersión de energía (EDS, por sus siglas en inglés), espectroscopia de pérdidas de energía (EELS, por sus siglas en inglés), contraste “Z”, etc., son una excelente combinación para lograr este cometido. Con dichas técnicas se puede saber la morfología de las partículas en 3 dimensiones así como la presencia o ausencia de defectos en los materiales. Asimismo se puede saber el contenido químico de las mismas y la distribución de los elementos en el espacio. El curso incluirá funcionamiento y aplicaciones de microscopia electrónica de barrido, microscopia electrónica de transmisión y EELS.

# KEYNOTE LECTURES



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## Infrared Plasmonics via ZnO

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Plasmon polaritons are the quasi-particles formed from resonant interactions of light with the collective motions of conduction electrons in materials. Most of the plasmonics studied so far involve metals, but metal-based plasmonic resonances are mainly limited to  $\lambda_{\text{res}} < 1 \mu\text{m}$ , and thus metals interact effectively only with light in the UV and visible ranges. We have recently shown that highly doped ZnO can exhibit  $\lambda_{\text{res}} \geq 1 \mu\text{m}$ , thus moving plasmonics into the IR range. We illustrate this capability with a set of thin ( $d = 25 - 147 \text{ nm}$ ) Al-doped ZnO (AZO) layers grown by RF sputtering on quartz glass. These samples employ a unique, 20-nm-thick, ZnO:N buffer layer, which minimizes the usual strong thickness dependence of mobility  $\mu$  on thickness  $d$ . Plots of the sheet concentration  $n_s$  vs  $d$  for buffered (B) and unbuffered (UB) samples give straight lines of similar slope,  $n = 8.36 \times 10^{20}$  and  $8.32 \times 10^{20} \text{ cm}^{-3}$ , but different  $x$ -axis intercepts,  $\delta d = -4$  and  $+13 \text{ nm}$ , respectively, where a positive  $\delta d$  denotes a depletion region. Plots of  $\mu$  vs  $d$  can be well fitted with the equation  $\mu(d) = \mu(\infty)/[1 + d^*/(d - \delta d)]$ , where  $d^*$  is the thickness for which  $\mu(\infty)$  is reduced by a factor 2. For the B and UB samples,  $d^* = 7$  and  $23 \text{ nm}$ , respectively, showing the efficacy of the ZnO:N buffer. Finally, from  $n$  and  $\mu(\infty)$  we can use degenerate electron scattering theory to calculate bulk donor and acceptor concentrations of  $1.23 \times 10^{21} \text{ cm}^{-3}$  and  $1.95 \times 10^{20} \text{ cm}^{-3}$ , respectively, and Drude theory to predict a plasmonic resonance at  $1.34 \mu\text{m}$ , confirmed by reflectance measurements. These layers are useful as wave guides for surface plasmons. Simulations with COMSOL Multiphysics over a mid-IR wavelength range of  $4 - 10 \mu\text{m}$  allow a study of propagation loss and Plasmon confinement dimension  $L_{\text{plas}}$ . In many cases,  $L_{\text{plas}} < \lambda_{\text{light}}$ , thus showing that IR light can be manipulated in semiconductor materials at dimensions below the diffraction limit.

## Graphene and Beyond: From N-Doped Graphene to WS<sub>2</sub> Monolayers

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Large-area, high-quality monolayer nitrogen-doped graphene sheets have been synthesized on copper foils using ambient-pressure CVD. Scanning tunneling microscopy (STM) and spectroscopy (STS) reveal that the defects in the doped graphene samples arrange in different geometrical configurations exhibiting different electronic properties. Interestingly, these doped layers could be used as efficient molecular sensors and electronic devices. In addition, the synthesis of hybrid carbon materials consisting of sandwich layers of graphene layers and carbon nanotubes have been synthesized by a self assembly route. These films are novel, energetically stable and could well find important applications as field emission sources, catalytic supports, gas adsorption materials and super capacitors.

Regarding transition metal dichalcogenides we will describe various approaches to synthesize WS<sub>2</sub> and MoS<sub>2</sub> triangular monolayers, as well as large area films using a high temperature sulfurization of WO<sub>x</sub> clusters deposited on insulating substrates. We will show that depending on the substrate and the sizes of the oxide clusters, various morphologies of layered WS<sub>2</sub> could be obtained. In addition, photocurrent measurements on these materials were performed using five different laser photon wavelengths ranging between 457-647 nm. Our results indicate that the electrical response strongly depends on the laser photon energy. The excellent response observed to detect different photon wavelengths in WS<sub>2</sub> materials, suggest these materials could be used in the fabrication of novel optoelectronic devices. The structural and spectroscopic characterization of these materials will also be presented.

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## The Nanostructured Catalysts Based on Au for Environmental Chemistry

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It is well known that gold being supported on different supports is active in the several practice reactions: low temperature CO oxidation, water gas shift reaction and hydrogen peroxide production. The catalytic performance depends on the Au nanoparticles size, method of gold deposition, nature of supports used and conditions of catalysts pretreatment. For example, easiness of red-ox transformation of ceria results in the high activity of gold supported on ceria. The redox properties of ceria being controlled by the structural defects could be tuned through the diminishing of ceria particle size or the partial replacement of Ce atoms with Zr atoms. The present work is dedicated to the characterization of gold species supported on nanostructured ceria, ceria-alumina and ceria-zirconia-alumina mixed oxides in the DeNO<sub>x</sub> and CO oxidation. The Ce-Al-O and Ce-Zr-Al-O supports with different content of ceria and ceria-zirconia mixed oxides (10 and 30%) were prepared by sol-gel technique using organo-metallic precursors. Gold (3%) was supported by deposition-precipitation method using H<sub>2</sub>AuCl<sub>4</sub> as a gold precursor and urea as a precipitation agent. The obtained catalysts were characterized with TPR, TPD, XPS, UV-Vis, EXAFS and TEM techniques.

Prepared catalysts had a high surface area and nanosized ceria and alumina particles. Partial replacement of cerium atoms with zirconium atom led to the drastic decrease of ceria particle size and the improvement of oxygen-storage-capacity of ceria based supports. The gold catalysts based on nanostructured supports were characterized with a high content of gold species none detectable with TEM with extremely high activity in CO oxidation and NO reduction.

The authors acknowledge the support of CONACyT and DGAPA-PAPIIT (Mexico) through grants IN 179619 and 203813, respectively.

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INVITED TALKS 

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**Plasmonic Biosensors**

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## All-plasmonic Fano Resonances in Metallic Nanostructures

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Fano resonances (FRs) are typical spectral features caused by the coupling of a discrete state with a continuum [1]. This phenomenon has been known for many years in atomic physics but only recently it has been achieved in all-plasmonic systems [2]. This phenomenon has a great potential for the fabrication of sub-wavelength waveguides, low-loss metamaterials and chemical sensors [3]. Symmetry-breaking is the most common approach for producing FRs in plasmonic nanoparticles (NPs). This modification allows coupling between dipolar and higher-order modes, which are forbidden in symmetric systems by orthogonality reasons [4]. Heterodimer structures [2,5], non-concentric multilayered nanoshells [6] and ring-disk nanocavities [7] and nanoparticle clusters [8] are examples of this approach.

Unfortunately, this systematic and controlled symmetry-breaking is very complicated to attain experimentally and requires complex and expensive methods, which severely reduces their application potentials. This limitation has attracted some interest for FRs in symmetric systems but so far they have been reported only in a few cases: bimetallic NPs [9], simple [10] and multilayered [11] nanoshells and gold@dielectric core-shell structures [12]. In this talk we will discuss the state of the art in the field of plasmonic FRs, exemplifying the advantages and disadvantages of both approaches.

OPR thanks Moncloa Campus of International Excellence (UCM-UPM) for offering a PICATA postdoctoral fellowship.

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## **Solar Energy Conversion Systems Based on Nanomaterials: Dye-sensitized Solar Cells & Direct Water Splitting**

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The dye-sensitized solar cell (DSC) is a third generation photovoltaic device based on nanomaterials that holds promise for the low-cost conversion of solar energy to electricity. The light absorbing electrode consists of a mesoporous, nanostructured metal oxide film, sensitized to visible light by an adsorbed molecular dye, which absorbs sunlight. The current record efficiencies are above 12% [1]. On the other hand, the conversion of solar energy directly into clean fuels such as hydrogen is an important goal to be achieved in the near future. Currently, there is strong interest in the use of nanomaterials with specific optical and electronic properties for the direct splitting of water into oxygen and hydrogen [2]. In this presentation, examples will be given of research and progress in both fields in our group at CINVESTAV-Mérida.

We acknowledge partial financial support from CONACyT and FOMIX-Yucatán, Mexico, through the grants No.178510 and No.170120, respectively.

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## **AG, TL and OSL Dosimetry Assessment of Doped and Undoped CVD Nanodiamond**

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High quality CVD diamond has been recently investigated in clinical dosimetry applications due to its near tissue equivalence effective atomic number, being chemically inert and reusable. The dosimetric properties reside on the existence of deep and stable trapping levels inside the wide band gap of diamond (5.5 eV). Impurities and doping materials may significantly change the number of defects in CVD diamond and consequently the trapping and radiative recombination properties of diamond, previously exposed to ionizing radiation, followed by thermal or optical stimulation. We report on the afterglow (AG), thermoluminescence (TL) and optically stimulated luminescence (OSL) in B and N doped CVD nanodiamond films and its performance as ionizing radiation dosimeters. The TL glow curve is highly reproducible up to high doses of several kGy without any special treatment. The integrated TL as a function of dose is linear for doses below to 500 Gy and sublinear for higher doses with no apparent dose saturation effects. The observed AG is mainly due to charge carriers freed from shallow trapping levels around room temperature. The optically stimulated luminescence, excited with an IR diode laser (870 nm, 145 mW/cm<sup>2</sup>), showed typical time decays with stronger signal for undoped diamond films. The samples presented a good and reproducible OSL dose response behavior in the range from 0 to 1.8 kGy. These preliminary results indicate that CVD nanodiamond may be suitable for dosimetric application; however more investigation is required in order to optimize its TL/OSL performance and to reach sensitivity levels as those compared to commercial dosimeters.

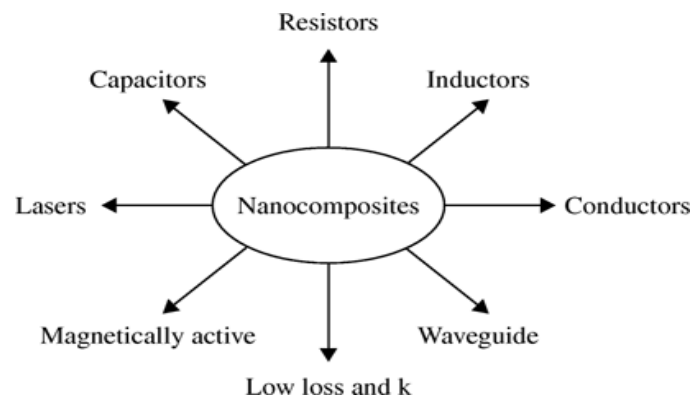
## Multifunctionality at Nanoscale

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Nanocrystalline materials have attracted much attention during last two decades, and it is well known that all the physical and chemical properties changes drastically when size goes down to nanometer range. Materials at nanoscale offer new and largely unexplored opportunities. Nanoscale multifunctional materials provide a multidisciplinary review of the diverse properties, functions, and applications of nanomaterial. A major barrier in the development of new applications and uses of materials at the nanoscale is the ability to synthesize nanoparticles, nanostructures with precisely controlled size, composition and shape in a way that is economically and ecologically sustainable. Therefore, processing of the nanoscale building blocks into the real materials suitable for applications is of essential importance in view of revealing the high performance and new properties. This presentation involves different synthesis method and proper characterization of various nanostructured materials (ZnO, BFO etc) which demonstrate new functionality. Effort will be made to develop a structure property correlation to understand the fundamental aspect of materials at nanoscale, paving the way for wider application of high performance nanocomposites.



## **Carbon Nanotubes: Advances and Perspectives**

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Carbon nanotubes are one of the most important materials in basic science, with applications in materials science, physics and chemistry. Since the publication of Iijima's paper [1], there have been more than eighty thousand research articles published involving the topic "carbon nanotube". From these, only 47,937 papers include in its title the phrase "carbon nanotube". From these data, the present work discusses and analyzes the development and impact of carbon nanotubes on several research areas, journals, specific papers and emerging research areas. Considering the production of papers in this area from 1997 to 2012, The People's Republic of China is emerging as the more powerful country in the developing of research in carbon nanotubes over passing The United States of America to the first place. Currently, Mexico is in the 22th position below Brazil (17th) and above Portugal (37th). However; during the last 4 years this situation is changing negatively affecting the evolution of the research in this subject in Mexico. Some ideas are exposed to improve the progress and to revert this unfavorable situation.

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## Nanostructured Metamaterials

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The existing homogenization theories for calculating effective parameters of both photonic and phononic metamaterials will be revisited. This kind of artificial materials is characterized by extraordinary physical properties which could be totally different from those of the components because of their complicated structure. Thus, for example, metal-dielectric photonic crystals, having a negative index of refraction belong to such a class of materials. This unusual property has been achieved in double negative metamaterials with simultaneously-negative effective permittivity and permeability. Several forms for the metallic inclusion in the unit cell of such negative-index materials (NIM) have been proposed: split-ring resonators, dual-bar rods, fish-net structures, double crosses, etc. In order to apply NIM in the optical range, it is necessary to fabricate periodic metal-dielectric nanostructures. However, the damping effects in nanostructures with metallic components are important and, hence, the fabrication of low-losses photonic metamaterials is a great challenge.

On the other hand, phononic metamaterials can also possess negative effective parameters such as dynamic mass density, bulk and shear moduli. In the talk, new forms of elastic metamaterials, based on distinct solid nanostructures, will be presented. Besides, the physical origin of the negative effective elastic parameters for nanostructured metamaterials will be discussed.

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**Behavior of Silver Nanoparticles in Natural and Synthetic Zeolites**

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A simple, low-temperature, hydrothermal method for the synthesis of silver nanoparticles supported on the surfaces of the natural zeolite chabazite and synthetic zeolite Na-A has been developed. The synthesis method includes two ion exchange processes: the first is a conditioning process to exchange the natural cations included in the zeolites with  $\text{NH}_4$  ions, and the second exchanges the latter ions with silver ones. The precipitation of silver nanoparticles is achieved by thermal annealing of the silver-exchanged zeolites at 300-400°C depending on the type of zeolite. The samples were studied with X-ray diffraction, Fourier-transform infrared spectroscopy, energy dispersive X-ray spectroscopy, transmission electron microscopy and diffuse reflectance spectroscopy. The results show the presence of both silver cations and nanoparticles in the zeolite matrix, the silver nanoparticles being located at the surface of the zeolite microcrystals. The silver nanoparticles are crystalline with an average size of 5-10 nm and show cube-truncated shapes. The absorption spectra of the silver nanoparticles display several plasmon resonance transitions due to their geometry. The silver-supporting chabazite powders have bactericide properties against several types of bacteria as was shown by the inhibition of bacteria growth on conventional agar medium. The silver-supported zeolite A powders show thermochromic and photochromic properties.

## Bismuth Nanostructured Derivatives and Some Potential Applications

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The first part of this contribution outlines the synthesis of zero-valent bismuth nanoparticles (ZV-Bi NPs) colloidal dispersions, in dimethyl sulfoxide (DMSO) [1]. This reaction pathway yields small and well faceted rhombohedral particles, with an average size of 3.3 nm, SD of 1.0 nm, determined by HR-TEM. These are the smallest ZV-Bi NPs, synthesized by a fast, and straightforward colloidal method, found in the literature. The obtained ZV-Bi NPs are stable and free of oxide traces. In this work, early evidence of the inhibitory antimicrobial effect of bismuth nanoparticles against growth of *S. mutans* and its capability to form a biofilm, also will be disclosed. The biocidal activity of bismuth nanoparticles was very similar to that obtained with chlorhexidine, a commonly used oral antiseptic [2].

Next, we will disclose the synthesis, characterization and stabilization of colloidal dispersions of particles of  $\text{Bi}_2\text{O}_3$ , in DMSO and water. Subsequently, we analyze the fungicidal activity of bismuth oxide nanoparticles against *Candida albicans* and their anti-biofilm capabilities. Our results show that aqueous colloidal bismuth oxide nanoparticles display 85% of antimicrobial activity against *C. albicans* growth and a complete inhibition of biofilm formation. These results are better than the obtained with the most effective oral antiseptic and commercial antifungal agents [3].

Finally, we will summarize the synthesis and the comprehensive characterization of high-purity  $\text{BiFeO}_3$  nanoparticles, prepared using tartaric acid or glycine, as promoter agents, in the combustion reaction. The obtained  $\text{BiFeO}_3$  NPs are crystalline of average sizes of 23, 26 and 67 nm. We found an easy method to obtain high purity  $\text{BiFeO}_3$  nanocrystals at relatively low temperatures. This process is straight forward, simple, energy-saving and cost effective [4].

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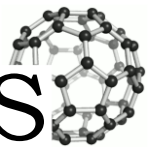
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# CONTRIBUTED TALKS



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**Synthesis and Characterization of Polyhedral Stacked Microcolumns  
and Microparticles of Zinc by Thermal Evaporation  
and Condensation Technique**

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Metallic zinc microcolumns and microparticles with oblate spherical shape have been synthesized by thermal evaporation and condensation technique using zinc powder at 650 °C for 60 minutes and nitrogen gas as carrier at atmospheric pressure. The material was characterized in structure, morphology and composition by X-ray diffraction (XRD), scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS). Zinc microcolumns consisted of stacked polyhedral microparticles and they seem formed by hexagonal platestacks with size of several microns and about 50 nm in width. Polyhedral stacked microcolumns had 40 μm in width and up to 10<sup>4</sup> μm in length. On the other hand, the oblate spherical particles had 40 μm in diameter and also formed by hexagonal platestacks. The X-ray diffraction patterns revealed peaks, on both types of structures, corresponding to hexagonal zinc with lattice parameters of  $a = b = 0.272$  nm and  $c = 0.4954$  nm, nearly equals to their bulk values of  $a = b = 0.2667$  and  $c = 0.4947$  nm. This indicates that the structures underwent no obvious lattice change. No peak corresponding to other impurities or catalytic particles was detected according to those obtained by EDS measurements. The last fact leads us to assume that the vapor-solid (VS) mechanism is the route for growth and formation of those zinc structures.

## Epitope Peptide from HA H1N1 Conjugated to Gold Nanoparticles

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In the last years gold nanoparticles (AuNPs) have been extensively used in biological applications because of their biocompatibility, dimension and ease of characterization [1]. These features make these structures easily exploitable to meet the requirements of biomedical applications [3]. Surface modifications of AuNPs are often used to increase the functionality of nanoconjugates. These nanoparticle modifiers/conjugants include various peptides which can specifically recognize a target, thus improving cell type uptake and ensuring that the AuNPs reach the desired target. Peptides attached to a single nanoparticle make the individual targeting signals more accessible to cell receptors, thus allowing them to participate in ligand-receptor interactions. In particular epitopes from HA H1N1 virus has been used for applications in immunology research and epitope vaccine development. Some reports describe the conjugation from defectuous proteins peptides like targets for diagnostic or therapeutic use.

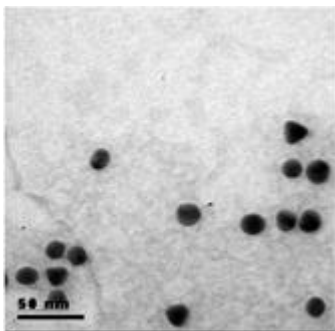


Figure 1. Typical TEM micrograph of gold nanoparticles employed for conjugation with epitopepeptide.

In this work we have conjugated the epitope peptide from HA H1N1 virus to AuNPs whose typical appearance can be observed in the TEM micrograph of Fig.1. The average particle size used in this experiment was near 20 nm. Also, the procedure of conjugation was characterized by UV/VIS spectroscopy through the monitoring of the surface plasmon resonance (SPR) at 520 nm, which suffers a shift to low energies due to the effect of peptide which acts as dimmer diminishing the optical absorption frequency of SPR. This kind of nano structured design can be used for biomedical applications through of the recognizing of specific targets as HA H1N1 virus.

We acknowledge the partial financial supports of SIP-IPN, Mexico.

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## **Enhanced Transmission through Subwavelength Slits**

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We present FDTD calculations for transmission of electromagnetic waves through periodic arrays of nano-slits in a metallic screen. The results show resonant, frequency dependent, transmittance peaks for subwavelength widths of the slits which can be up to a factor of ten with respect to those out of resonance. Although our conclusions agree with previous work by Lezec and Thio as regards both the magnitude of the enhancement and the lack of contribution of surface Plasmon polaritons of the metal surface to this effect, we derive an interpretation from a theory that deals with emerging Fabry-Perot resonances of the perforated screen considered as an effective medium and with the topological charge of phase singularities.

## The Influence of Mo Doping on the Physical Properties of Nanostructured WO<sub>3</sub> Films Deposited by Pulsed Spray Pyrolysis

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The effects of Molybdenum (Mo) doping on tungsten trioxide [WO<sub>3</sub>] thin films deposited on FTO/Glass substrates have been studied. The pneumatic pulsed spray pyrolysis technique was used to fabricate pure and doped WO<sub>3</sub> thin films. The nominal content of Mo was varied from 2 to 10 at.% by adding different amounts of molybdenum (VI) oxychloride into the precursor solution.

The incorporation of different amounts of Mo respectively modifies in a noticeable fashion the morphology of the WO<sub>3</sub> nanostructures and influences the optical and electrical properties of the materials. The structure and morphology evolution as the Mo content is risen was followed with X-rays diffraction, transmission and scanning electron microscopy together with atomic force microscopy. The opto-electronic properties were derived from UV and Visible spectroscopy observations and the electrical parameters were obtained from Hall and van der Pauw methods measurements. Also the electrochromic behavior of Mo: WO<sub>3</sub> thin films were followed using polarization curves and cyclic voltammetry methods.

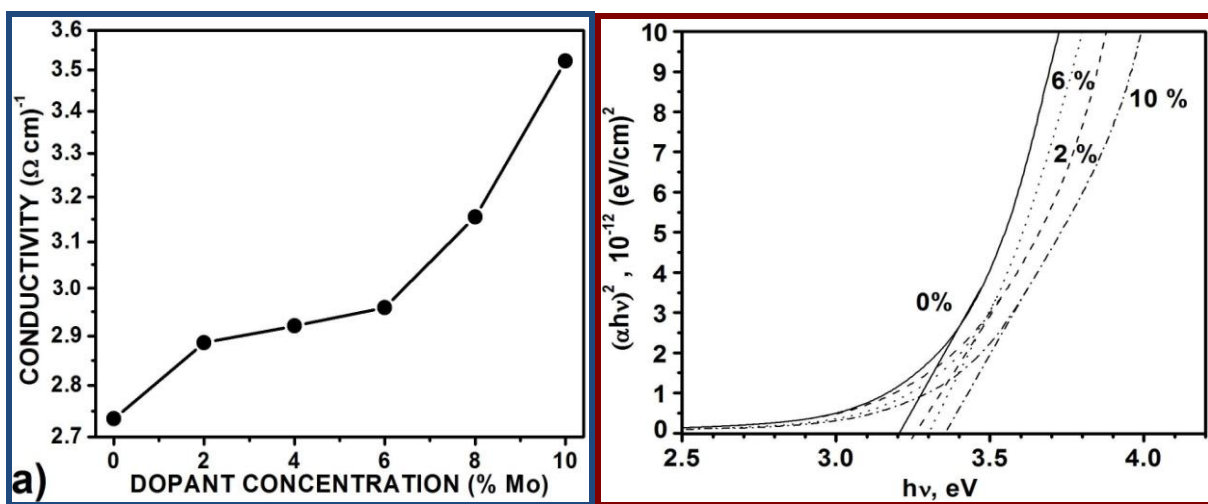


Figure 1. The variation of electrical conductivity with the Mo content in the starting solution.

Figure 2. The band gap shift under Mo doping are displayed in this graphic

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## Effect of Symmetry-breaking on the Optical Properties of Metallic Nanoshells

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Recently a considerable amount of research has been devoted to study the optical properties of metallic nanoparticles. Of special interest is the controlled variation of the nanoparticle's geometry since this allows obtaining tunable optical properties that are not present in solid metallic particles. A good example of such strategy is metallic nanoshells (a dielectric core surrounded by a metallic shell), for which the structural tunability of the plasmon frequencies has been shown both experimentally and theoretically. Tunability of plasmon position makes these nanoparticles particularly attractive for applications such as resonant photo-oxidation inhibitors, optical triggers for opto-mechanical materials, drug delivery implants, environmental sensors, and Raman sensors. Moreover, symmetry breaking of these structures provides an additional mean to further tailor the optical response. In spite of so much interest, there are few works in the literature on the systematic study of the optical properties of metal nanoshells on their geometries. In this work, we have studied the dependence of the Surface Plasmon Resonance (SPR) on the geometry for different metal nanoshells. For this, we performed calculations using either Mie theory or the Discrete Dipole Approximation. It is observed for the symmetric nanoshells that the SPR position linearly red shifts on increasing the core-radius to shell-thickness ratio. On the other hand, new SPR modes appear when the symmetry of the system is broken. We show using the plasmon hybridization model that they arise due to the excitation of the antibonding plasmons.

## Controlling the Movement of Plasmonic Nanoparticles with Swift Electrons: Electron Tweezers?

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We have recently showed that it is possible to induce forces on a small metallic nanoparticle (1-5 nanometers in radius) [1,2] with the use of swift electron beams, like those typically used in electron microscopy, opening the possibility of moving plasmonic nanoparticles in a controllable way and suggesting a manipulating technique for such nanoparticles called *Electron Tweezers*. Depending on the impact parameter, it is possible to move the nanoparticle towards the electron beam or away of it. Thus, it is possible to induce coalescence between pair of particles, as has been observed and studied experimentally [3], or avoid that two nanoparticles approach each other, by simply controlling the impact parameter of the electron beam to the nanoparticles.

We study the dependence of the momentum transfer from the fast electron to the nanoparticle as a function of different parameters such as the velocity of the electron, the order of the modes excited, or the influence of retardation in the interaction. We present results of the momentum transfer from an electron to a Drude-like plasmonic nanoparticle, where the electromagnetic (EM) properties of the excitations are determined by the plasma frequency and the damping. We show that for ultra-relativistic electrons ( $\sim 0.95-0.99c$ , with  $c$  the speed of light in vacuum) there is practically no coupling between the EM fields generated by the swift electron with the nanoparticle, yielding to a very small repulsive momentum transfer to the nanoparticle. In the other extreme case, for slow enough electrons, there is strong coupling between the plasmon modes with the EM field generated from the electron, attracting the nanoparticle towards the electron beam. Under this scenario, there is a specific electron velocity in which a transition between attractive to repulsive behaviour occurs for a given particle radius and impact parameter. This information is tremendously important to design nanoscale particle motion induced by electron beams.

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## **Síntesis de Nano-hidroxiapatita Mediante Precipitación Asistida por Sonicación**

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En los últimos años la búsqueda de tecnologías hacia la manipulación de los materiales a una escala atómica, molecular y macromolecular ha llevado a buscar alternativas en la síntesis de los materiales. La radiación ultrasónica o sonicación es una técnica que ha sido usada para fabricar compuestos de tamaño nanométrico. En el presente estudio se desarrolla una hidroxiapatita mediante un método de síntesis húmeda siendo asistida por sonicación como método alternativo para reducir el tamaño de cristal y se presenta la comparación con un método de síntesis convencional. La síntesis de la hidroxiapatita se llevo a cabo a partir de soluciones de nitrato de calcio y fosfato acido de amonio ajustando el pH entre 8.5-9, con una relación Ca/P de 3 a 1. La caracterización química y estructural se realizo mediante técnicas de Difracción de rayos X (DRX) y espectroscopia de infrarrojo (FT-IR), la caracterización morfológica mediante Microscopia Electrónica de Barrido (MEB). Los resultados indican una variación en el tamaño de los cristales obteniendo nano-hidroxiapatita con el uso de sonicación demostrando la ventaja del método contra un método convencional.

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## Development of a Sensor to Detect Magnetic Field Using the Magnetoimpedance Effect

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In this work, we present the development of a sensor to detect small magnetic fields using the technique of magnetoimpedance (MI), which has a classical electromagnetic origin [1]. The material we have studied is an amorphous wire of CoFeSiB with 30  $\mu\text{m}$  in diameter, 3 mm long and a negative magnetostriction constant, where the domain structure is of bamboo type [2]. MI effect shows a sensitive change in ac impedance when the dc magnetic field is applied to the wire axis. At low frequencies (100-400 kHz), the impedance decreases  $\sim 9\%$  for a field of 2 Oe, with a sensibility of 5% per Oe; this behavior is due to inductive processes, and they are explained by field dependence with the circumferential permeability. For high frequencies (0.5-20 MHz), the impedance increases until to achieve 50% for 1-1.5 Oe, with a sensibility of 47% per Oe, and subsequently it decreases at a rate of 15% per 2 Oe. At these frequencies, the skin effect becomes very important and the skin penetration establishes the magnetization processes generated in the circumferential domains. As the best response exhibited by the material is in the frequency range of 5-10 MHz, we develop a prototype which consists of an oscilloscope connected in parallel with the amorphous wire, and it in turn is connected with a functions generator in series. We have also employed a coil of 250 turns, fed to a power source voltage of 8 V, which generate a magnetic field. The experimental curves of our prototype are in good agreement with MI measurements, the obtained result at 7.5 MHz is 0.15  $V_{PP}$  per 2  $V_S$ , where  $V_{PP}$  is peak-to-peak voltage in the oscilloscope and  $V_S$  is the source voltage.

We acknowledge the financial supports of CEP-UNAM, Mexico. We also thank the financial support of DGAPA-UNAM, through PAPIIT No. IN111111.

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## Characterization of Nano-Hybrid Compounds of Apatite-bisphosphonate Obtained by Mechanical Alloying

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Bisphosphonates (BPs) are characterized by two phosphonate groups sharing a common carbon atom. The bridge of carbon atoms are also linked to a hydroxyl group, responsible of the affinity for bone mineral, and a side chain responsible of their potency as inhibitors of osteoclastic bone resorption. Local delivery of bisphosphonates can reduce side effects and improve the efficiency of existing drugs. The addition of calcium phosphates together with BPs can reinforce this effect by providing calcium ions to the system. Reactive milling can be an effective and easy route to the preparation of hybrids bisphosphonate-hydroxyapatite granules that combines the advantages of both families of compounds.

Sodium alendronate trihydrate (Al, Sigma) and synthetic HAp obtained by a coprecipitation process were selected for the development of the method. Obtained specimens were characterized by thermogravimetric analysis TGA, vibrational spectroscopy ATR-IR, elemental analysis and scanning electron microscopy SEM.

Elemental analysis of the A and B are 1.45 % C, 0.92 % H, 0.28 % N, and 2.51 % C, 0.98 % H, 0.55 % N, respectively, which is compatible with the theoretical compositions of the hybrids. Thermal analysis shows that the compound HAp/Al is more instable than the HA powders. ATR-IR spectra shows bands that can be attributed to P-O, P=O (1150 to 1250 cm<sup>-1</sup>) and P-OH (930 cm<sup>-1</sup>) modes of the alendronate plus 960 cm<sup>-1</sup> of the HAp indicating that an effective bonding can be formed between OHAp and BPs using the method of reactive milling. An homogenous distribution can be observed by SEM.

In conclusion reactive milling is an effective method for the preparation of calcium phosphates/bisphosphonates hybrids that can be used as therapeutic agents on the treatment of diseases characterized by an excessive bone resorption.

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## Síntesis y Caracterización de Nanopartículas de TiO<sub>2</sub> sobre WO<sub>3</sub>-SiO<sub>2</sub> Mesoestructurado

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La obtención de materiales adsorbentes o catalíticos con una potencial aplicación en el combate de la contaminación ambiental es una de las áreas donde se registra mayor actividad en la investigación. En los procesos de oxidación avanzada el TiO<sub>2</sub> es ampliamente usado como fotocatalizador, debido a su marcada actividad, estabilidad química y propiedades no tóxicas, por lo que la fotodegradación con este material es uno de los procesos más efectivos para la remoción de contaminantes orgánicos presentes en el aire y en aguas de desecho [1]. No obstante, el uso de este material se ve limitado por el ancho de banda prohibida que es 3.4 eV [2].

Con el objetivo de mejorar el rendimiento de TiO<sub>2</sub> en reacciones de fotodegradación, primero se preparó un óxido mixto meso-estructurado de Si y W por calcinación de un gel precursor sintetizado por método de hidrotratamiento usando agente director de estructura. Posteriormente, se depositaron nanopartículas de TiO<sub>2</sub> incorporadas por método de sol-gel, buscando efecto promotor del WO<sub>3</sub> presente en el óxido mixto sobre las propiedades del TiO<sub>2</sub> soportado. La caracterización del sistema catalítico TiO<sub>2</sub>/WO<sub>3</sub>-SiO<sub>2</sub> incluye estudios de adsorción de N<sub>2</sub> para medir las propiedades texturales y de actividad fotocatalítica en la reacción de descomposición de naranja de metilo, seguida por espectroscopia UV-Vis.

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## **Vacuum-free Thin Film Deposition of Kesterite Absorber Layer by Using Paste of Binary Sulfides**

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Copper zinc tin sulfide ( $\text{Cu}_2\text{ZnSnS}_4$ , CZTS) is emerging as a promising absorber material for thin film solar cells. All the elements in CZTS are earth abundant, inexpensive and environmentally benign. In addition, CZTS has a band gap of  $\sim 1.5$  eV and high absorption coefficient ( $>10^4$   $\text{cm}^{-1}$  in the visible region of the electromagnetic spectrum) which are ideal for photovoltaic application. In this contribution, we present the fabrication of CZTS thin films by a simple paste-coating process using CuS, ZnS and SnS nanocrystals as precursors. The binary sulfides were synthesized in large-scale by a simple wet chemical route and thoroughly characterized using X-ray diffraction (XRD), Raman scattering, energy dispersive X-ray spectroscopy (EDS) and diffuse reflectance spectroscopy (DRS) to confirm their phase purity. Paste was made by dispersing appropriate stoichiometric quantities of CuS, ZnS and SnS powders in organic media. Obtained paste was deposited on FTO substrates using a simplified “Doctor blade” method by sliding a glass rod to form uniform and continuous layers. Kesterite CZTS layer was produced by annealing the deposited substrates at  $450$  °C in presence of elemental S under  $\text{N}_2$  atmosphere.

This work was partially supported by the project CONACyT 129169.

## **Control de Espesores y Propiedades de Películas Nanométricas de ZnS Obtenidas por RF Magnetron Sputtering**

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Controlar los espesores y la calidad estructural durante el depósito de películas de ZnS cambiando las condiciones de RF magnetron sputtering es importante por las aplicaciones en dispositivos electroluminiscentes y celdas solares.

En este trabajo se utilizó la técnica de RF magnetron sputtering durante los depósitos de películas de ZnS debido a que es posible obtener películas estequiométricas y uniformes. Además esta técnica es más económica comparada con otras técnicas de depósito como Epitaxia de Capas Atómicas (ALE), Deposición Química de Vapores Metal Orgánicos (MOCVD), Epitaxia con Haces Moleculares (MBE), entre otras.

Empleando esta técnica se obtuvieron películas nanométricas de ZnS variando las condiciones de potencia y tiempo durante la deposición por RF magnetron sputtering. Por medio de difracción de rayos-X en el modo de haz rasante Se determinó la estructura cristalina de las películas nanométricas de ZnS en la fase cubica con textura en la dirección [111]. Los espesores varían de 20 a 150 nm, los cuales fueron determinados con las técnicas de reflectometría de rayos-X y elipsometría espectroscópica. Mediante microscopia de fuerza atómica y microscopia confocal se evaluó la evolución de la superficie. Además se midió el espectro de fotoluminiscencia con microscopia confocal. Finalmente, se determinaron las condiciones adecuadas para poder controlar la calidad y el espesor de las películas nanométricas de ZnS.

## Interference Effects on Photoluminescence of AlGa<sub>N</sub>/Ga<sub>N</sub> Quantum Wells

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The III-nitride semiconductor materials have enabled the design of nanostructures that can operate optically from the infrared to the ultraviolet of the electromagnetic spectrum, which are highly suitable for making electroluminescent devices, sensors and high efficiency solar cells [1]. We have grown AlGa<sub>N</sub>/Ga<sub>N</sub> quantum wells (QWs) on Si(111) on sapphire substrates using a Ga<sub>N</sub> buffer layer by Plasma Assisted Molecular Beam Epitaxy (PAMBE). The nanostructures were characterized structurally by X-ray diffraction (XRD) and scanning electron microscopy (SEM), which show the interfaces of the QWs and the formation of wurtzite Ga<sub>N</sub> and AlGa<sub>N</sub>. Optical properties were characterized by photoluminescence (PL), cathodoluminescence (CT) and reflectance (R) spectroscopies. Reflectance spectra show interference oscillations of the different layers, which disappear at the band gap edges of the Ga<sub>N</sub> buffer layer (3.4 eV) and the AlGa<sub>N</sub> barrier layers (4.4 eV). The PL and CT spectra of the sample grown on sapphire show an emission centered at 2.92 eV, which is due to recombination of the carriers confined in the QWs. Furthermore, the sample grown on Si(111) presents a PL spectrum centered at 3 eV, which is modulated by the oscillations that match the reflectance spectrum. To understand the modulation of the photoluminescence spectrum, we measured PL and R spectra at different emission angles relative to the normal sample. The modulation has a red shift when the angle at which the spectrum is measured increases. We believe that the photoluminescence modulation is due to the Fabry-Pérot interference of light emitted in the QWs when this is reflected at the Ga<sub>N</sub>/Si(111) and AlGa<sub>N</sub>/air interfaces, which is not present in the sample grown on sapphire.

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## **Influence of Mg Concentration on Structural, Optical and Electrical Properties of Epitaxial-grown C<sub>60</sub> Thin Films**

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The structural and molecular changes caused by magnesium atoms in C<sub>60</sub> films were studied. Recently, it was reported that the conversion efficiency of C<sub>60</sub>/MEH-PPV organic cells was significantly improved by the automatically Mg-doping in a C<sub>60</sub> layer during the Mg electrode deposition [1]. On the other hand, R. P. Gupta *et al.* reported the energy band calculation of Mg<sub>2</sub>C<sub>60</sub> solids, and indicated that Mg<sub>2</sub>C<sub>60</sub> was semiconductor [2]. In this work it was found that entirely (111)-oriented epitaxial Mg-doped C<sub>60</sub> films can be grown on mica substrates at low deposition temperature in the region of low Mg concentrations by using a molecular beam epitaxy (MBE) system. The conductivity was controlled by the composition ratio of Mg/C<sub>60</sub>. An analysis of the X-ray diffraction patterns showed the presence of new peaks at high Mg concentrations [3]. On the other hand, the degeneracy of the active modes in Fourier transform infrared spectra showed that infrared modes that were initially inactive become active owing to the interaction of magnesium atoms with the C<sub>60</sub> molecule cage. These changes caused by magnesium atoms in C<sub>60</sub> films were due to the presence of triangular cyclic trimmers which suggests that rhombohedral and rhombohedral polymers are present in the C<sub>60</sub> films. These polymeric phases in the C<sub>60</sub> besides the deformation of isolated C<sub>60</sub> balls in a crystal films caused the crystal quality deterioration.

This work was supported by the Consejo Nacional de Ciencia y Tecnología (CONACYT), México; and by the MEXT as Grant-in-Aid for Scientific Research (C), 21560341, and as Support Program for Forming Strategic Research Infrastructure 2009-2013.

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## Nanostructured Silicon for Omnidirectional Antireflection Coating

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In this work we report the design and fabrication of a thin omnidirectional absorbing porous silicon multilayered (PS-ML) nanostructure within a wide frequency range, from ultraviolet to near infrared region of the electromagnetic spectra. The reflectivity spectrum of approximately 500 nm thick PS-ML structure was experimentally measured from 200 to 3000 nm. A reflectance of less than 4% is observed for different incidence angles between  $8^{\circ}$  -  $68^{\circ}$ . Theoretical simulations based on transfer matrix method confirmed this behavior for higher incidence angles. Such structures can have possible applications in increasing the efficiency of silicon solar cells.

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## Photonic Zener Tunneling in One Dimensional Dual-periodical Multilayer Structures Based on Porous Silicon

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Recently, one dimensional photonic superlattices made of porous silicon (PSi) have allowed the demonstration of optical analogues of electronic phenomena, such as photonic Bloch oscillations (PBOs) [1], Anderson localization and Zener tunneling (ZT) [2]. In the present work, Experimental evidence of photon Wannier-stark ladders (WSLs) and ZT in dual-periodical (DP) multilayer structures based on PSi, is presented. An introduction of linear gradient in physical layer thicknesses in DP structure, composed by stacking two different periodic substructures N times, resulted in the appearance of WSLs resonances. Depending on the values of gradient, Zener tunneling of the nearest resonances of two consecutive minibands can be observed. Theoretical time-resolved reflection spectrum shows photonic Bloch oscillations and Zener tunneling. Measured reflectivity spectrum verifies WSLs and ZT in the near infrared region.

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## Spinel and Perovskites of Iron Oxides Nanoparticles Obtained by Mechano-synthesis

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Transition metal oxides represent one of the most diverse types of materials with important structure-related properties. Many of them exhibit conductivity, superconductivity, ferroelectricity, magnetism, magnetoresistivity, or gas-sensing capabilities. It is evident that the synthesis of metallic oxides nanostructures will lead to important developments in the construction of new devices [1].

In this work, we present a variety of iron oxides nanoparticles with spinel or perovskite structure:  $\text{Fe}_3\text{O}_4$ ,  $\text{CoFe}_2\text{O}_4$ ,  $\text{YFeO}_3$  and  $\text{BiFeO}_3$ . These nanostructures have been successfully synthesized via an uncomplicated solvent-free method. The particle sizes were controlled by controlling the concentration of starting materials and calcination temperature. Their crystalline structures and average diameters (between 6 and 20 nm) were determined from XRD patterns and HR-TEM images. The UV-visible optical absorption and Raman spectra as well as their magnetic hysteresis loops show clear evidence of the quantum size effect. The synthesis method followed in this work presents an important advancement in the preparation of metallic oxides nanoparticles, specially, for the applications that require an easy and cheap procedure to obtain these materials.

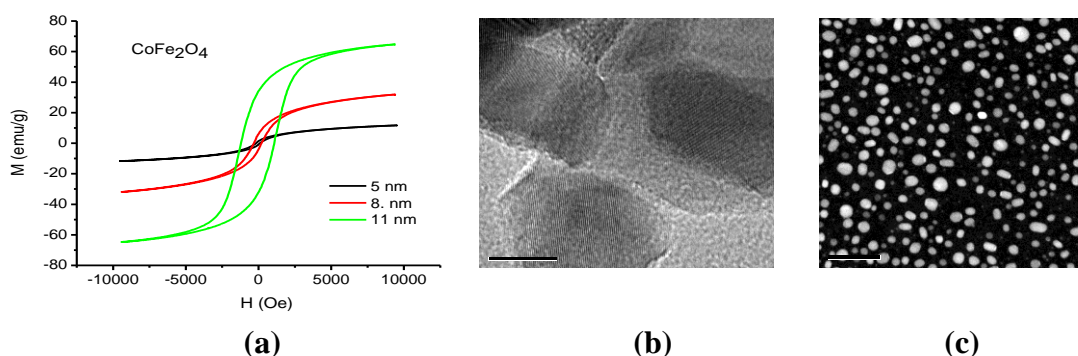


Figure 1. Magnetic hysteresis loops obtained at room temperature of  $\text{CoFe}_2\text{O}_4$  NPs. (a), selected HR-TEM image of  $\text{CoFe}_2\text{O}_4$  NPs (b), and Z contrast of  $\text{YFeO}_3$  NPs (c)

We acknowledge the financial support of CONACyT, Mexico, through the project 128460.

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## Estudio de Forma de Nanoclústeres Metálicos por Métodos Topológicos y Geométricos

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Se presenta un estudio de la morfología de nanoestructuras metálicas desde la perspectiva de la geometría y la topología algebraica. A través de un modelo matemático en dos dimensiones se representa la superficie de nanoestructuras metálicas. Por medio de medidas de curvatura se establecen las superficies más afines, y a través de un método topológico de transformación de superficies bidimensionales se establecen posibles caminos para la deformación de las mismas estudiando dos ejemplos específicos: del decaedro regular al decaedro de Ino y del cuboctaedro al icosaedro. El estudio es analizado y comparado con otros modelos teóricos y resultados experimentales.

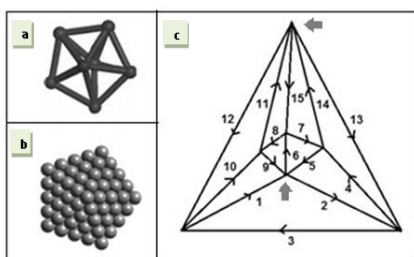


Figura 1. Sistema decaedro: a) y b) imágenes de la superficie decaedro, c) ejemplo de sistema poligonal decaedro ilustrado en un diagrama de Schlegel del decaedro.

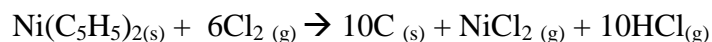


**Carbon Nanostructures Produced via Chlorination Reaction of Ni(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>**P.G. González<sup>1</sup>, E. Urones-Garrote<sup>2</sup>, D. Ávila-Brandé<sup>3</sup>, L.C. Otero-Díaz<sup>3</sup>

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Shaped carbon nanomaterials (SCNM) have reached high importance due to their characteristics yielding advanced materials for high gas storage capacity and high efficiency supercapacitors [1]. In the last years the chlorination method has been successfully applied on metallocenes, such as chromocene [2], as precursors of several carbon nanostructures. In this work, we present the synthesis and characterization of SCNM produced by chlorination of Ni(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub> (nickelocene) following the next possible reaction:



SEM micrographs, (JSM 6335 F at 10 kV and a working distance of 15 mm), have shown conglomerates made of spheres and foils. In the low magnification TEM images (JEOL 3000F (acceleration voltage of 300 kV) microscope equipped with an ENFINA spectrometer) we have found corrugated carbon foils and groups of hollow spheres (diameter from 85 to 240 nm and wall thickness from 6 to 40 nm) welded to solid spheres (diameter from 85 to 240 nm). After the scrutiny of the HRTEM images/diffraction we notice that these particles are formed by highly disordered graphene layers confirmed by the presence of the *hk0*-type reflections in the SAED patterns. Quantification of *sp*<sup>2</sup>/*sp*<sup>3</sup> ratio, obtained by EELS, indicates a high amount of *sp*<sup>2</sup> bonding (in the range of 89 – 100 %). Mass-density obtained from the low-loss region of the EEL spectra, is varied from 1.1 to 1.8 ± 0.1 g/cm<sup>3</sup> (almost 50% below graphite density = 2.2 g/cm<sup>3</sup>).

We acknowledge to CONACYT-México and to the projects with references number S-2009/PPQ-1626 and MAT2010-19460.

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**Birefringent Nanostructured Composite Materials**

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We use a very efficient recursive method to calculate the effective optical response of materials made up of arbitrarily shaped dielectric inclusions arranged in periodic 2D arrays within a metal matrix with a lattice constant much smaller than the wavelength of the incident light, so that we may neglect retardation. The starting point of the calculation is a digitized image of the system. The geometrical shape of the inclusions and their orientation in the 2D array induce a birefringent optical response of the whole metamaterial that can be tailored to specific needs.

## Ditiocarbamatos de Cadena Larga como Ligantes de Nanopartículas de Cobre

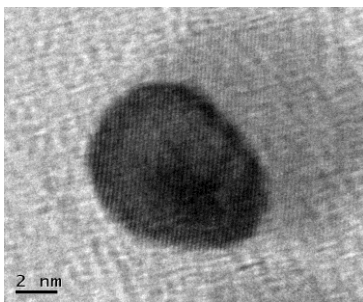
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Los materiales poliméricos tienen un amplio uso en nuestra vida diaria. Sus materiales compuestos tienen importantes aplicaciones en la ingeniería y a nivel industrial. Particularmente interesante resulta la búsqueda de propiedades antifúngicas y antibacterianas [1]. Para tal fin se han incorporado nanopartículas de Cu que hacen al material activo frente a microorganismos como *E. coli*. [2] Sin embargo las partículas metálicas forman aglomerados que reducen las propiedades de la matriz polimérica, así como su actividad. Una estrategia para evitarlo es un ligante que mejore su afinidad con el polímero y promueva una mejor dispersión. [3] Hasta el momento existen pocos trabajos relacionados a la modificación de nanopartículas de cobre con ligantes de cadena larga [4,5]. Por lo tanto se propone la obtención y caracterización estructural de nanopartículas de cobre modificadas con ligantes de tipo ditiocarbamato (DTC) de cadena larga.

Se realizó la síntesis de tres ligantes ditiocarbamato a partir de la amina correspondiente y



$\text{CS}_2$  en exceso. Posteriormente adicionando una sal de cobre y reduciendo con  $\text{NaBH}_4$ , se obtuvieron nanopartículas de cobre recubiertas con el ligante (Fig 1).

*Figura 1. Micrografía de TEM de nanopartícula de cobre con DTC.*

Agradecemos la beca CONACYT No. 258167 para estudios de posgrado.

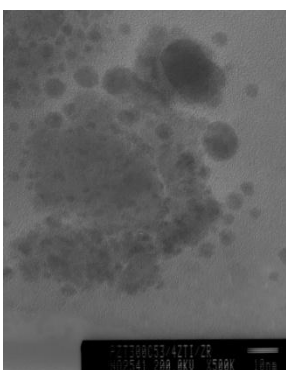
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**Obtaining of PZT Ferroelectric Ceramics Nanoparticles by Sol-gel Route**M.G. Garnica-Romo<sup>1</sup>, A Páez- Sánchez<sup>2</sup>, L García-González<sup>3</sup>,I. Domínguez-López<sup>4</sup>, L. Díaz-Flores<sup>5</sup>

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The sol-gel method has been widely used because it has the advantages of low temperature processing, high purity and composition control. The precursors synthesized by sol-gel can be used for the preparation of PZT thin films by spin or dip-coating. Also this technique can be used to obtain PZT powders, which in turns can be used for the preparation of bulk samples. In this work we present the synthesis of  $\text{Pb}(\text{Zr}_{12x}\text{Ti}_x)\text{O}_3$  powers by sol-gel route within compositions in the morphotropic phase boundary Zr/Ti: 53/47, 50/50, 45/55, and 40/50. The synthesized samples were calcined at 800 °C and sintered from 900 to 1150 °C. The structure and morphology of the obtained PZT samples were studied by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Raman spectroscopy, dilation, densification and pyroelectric response techniques. TEM microscopy (Fig. 1) reveals that the size of the



obtained PZT particles is less than 50 nm. On the other hand, the acquired X-ray patterns reveal the PZT phase, no pyrochlore phase was detected. It was found that the PZT ceramics with nominal composition of 53/47 showed the best pyroelectric response. The samples were used for high densification in order to be applied in pyroelectric sensors.

Figure 1. TEM micrograph of PZT nanoparticles obtained by sol-gel route.

## A Protected Annealing Process for the Production of Colloidal Iron Doped Zircon $\text{Fe-ZrSiO}_4$

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We have been investigating a post-synthesis process of “protected annealing”. The basic principle relies on thermal treatment of performed particles that have been previously dispersed into a sol-gel silica matrix. After annealing at temperatures up to 1000 °C, the dissolution of the host matrix allows recovery of a suspension of particles with similar size as the pristine particles [1, 2]. The present work consists in the preparation of non-aggregated particles of iron-zircon ( $\text{Fe}_x\text{-ZrSiO}_4$ ) with compositions  $0 \leq x \leq 0.15$  by colloidal route. The temperature of zircon formation (determined by differential thermal analysis, DTA) decreases with the use of iron, suggesting a catalytic effect of iron. Thermally annealed gels between 400 °C and 1600 °C were characterized by X-ray diffraction (XRD), infrared, ultraviolet-visible (FT-IR, UV-Vis) and Raman spectroscopies. These results confirmed the formation of tetragonal-zirconia ( $\text{Fe-t-ZrO}_2$ ) preceding the final zircon ( $\text{Fe-ZrSiO}_4$ ) formation. The comparison of refined XRD patterns using Rietveld method with foolproof; transmission electron micrographs (TEM) of non-agglomerated particles and half width half maximum (HWHM) analysis of Raman peaks, showed a uniform distribution of particle size and shape which varies from 40 to 60 nm. The lattice parameter variation and UV-Vis, suggest that the  $\text{Fe}^{3+}$  cations inside the zircon are distributed into tetrahedral sites replacing to  $\text{Si}^{4+}$ . This strategy is a way to join colloid chemistry and should lead the possibility to produce particles with optimized crystallinity while preserving their size, surface and dispersion state.

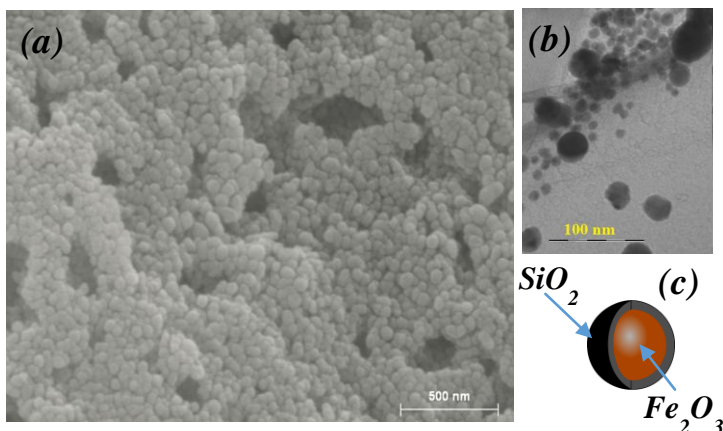


Figure 1. (a) SEM micrographs of  $\text{Fe}_{0.02}\text{-ZrSiO}_4$  at 1100 °C for 3 h; (b) TEM micrographs of  $\text{Fe}_{0.02}\text{-ZrSiO}_4$  at 1100 °C for 3 h; (c) representation of  $\text{Fe}_x\text{-ZrSiO}_4$  core-shell nanoparticles.

G. Herrera acknowledge the financial support of CONACyT, Mexico, through the postdoctoral fellowship grants # 129569 and # 172529.

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**AC Susceptibility Study of a Magnetite Magnetic Fluid** **$\text{Mn}_x\text{Fe}_{3-x}\text{O}_4$  ( $x = 0.1, 0.3$  and  $0.5$ )**

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Magnetic fluids of manganese ferrite  $\text{Mn}_x\text{Fe}_{3-x}\text{O}_4$  ( $x = 0.1, 0.3$  and  $0.5$ ) was synthesized from metal salts using a coprecipitation technique. The complex magnetic susceptibility  $\langle\chi\rangle = \langle\chi\rangle' + i \langle\chi\rangle''$  of magnetic fluids was measured as a function of temperature from 5 to 320 K and a weak ac field of 6 Oe for frequencies from  $f = 10$  to 10000 Hz. The saturation of ferrite manganese decreases in liquid state due to Brownian relaxation and in frozen state due to Neèl relaxation when the manganese content increase. In a magnetic fluid the real and imaginary components of the ac susceptibility show a prominent maximum at temperatures that increase with the measuring frequency which is attributed to a spin-glass-like behavior.

The susceptibility  $\langle\chi\rangle$  show a cusp as a function of temperature and the peak temperature obeys the Vogel-Fulcher law  $f = f_0 \exp\left[-\frac{E}{k_B(T_{p1} - T_0)}\right]$  where  $f_0$  and  $E$  are positive constants and  $T_0$  is a parameter related to particle interactions. There is another kind of peak in the loss factor  $\tan\delta = \frac{\chi''}{\chi'}$  as a function of  $T$ , which means the existence of a magnetic aftereffect, and the losses increase with the increase of content manganese.  $T_{p2}$  increase when the manganese content decrease, and Neèl relaxation is present.

## **Incorporación de Nano-sílices en Concretos Autoconsolidables**

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Investigaciones llevadas a cabo en el CTCC muestran que la incorporación de nano-sílice puede modificar significativamente las propiedades del concreto hidráulico premezclado. Más aún, la combinación de micro y nano partículas es esencial para la obtención de concretos de alto desempeño [1]. En los últimos años, los concretos autoconsolidables han sido cada vez más utilizados para facilitar la colocación del concreto sobre todo en elementos densamente armados con acero de refuerzo y con demandas de resistencias a edades tempranas. Dentro de las principales características que deben presentar estos concretos se encuentran una alta fluidez sin provocar la segregación de los materiales y un rápido desarrollo de resistencia. Se elaboraron mezclas de concretos autoconsolidables combinando tecnologías a micro y nano escala incorporando estos materiales en diferentes porcentajes para analizar propiedades fundamentales en el concreto como su flujo de revenimiento, el desarrollo de resistencia a la compresión, el módulo de ruptura y la permeabilidad del concreto. Los resultados demuestran que el empleo de nano-sílice en el concreto mejora las características en estado fresco y permite un mayor desarrollo de resistencia mecánica en comparación con concretos donde se utilizó micro-sílice. En cuanto a la disminución de la permeabilidad, la micro-sílice presenta un mejor desempeño en comparación con la nano sílice. Finalmente, la combinación de micro y nano partículas en el concreto permitió obtener los resultados más altos en las propiedades mecánicas de los concretos elaborados.



*Figura 1. Comparativa del aspecto de concretos autoconsolidables. A la derecha un concreto con una sustitución al 10% de micro sílice, a la izquierda un concreto elaborado con una sustitución de nano sílice al 1.5%. Se aprecia que la nano-sílice evita la segregación de los materiales.*

[1] Jeng-Ywan, S.; Ta-Peng, C. *Materials Science & Engineering A*. **2006**,424, 266-274.

**Columnar Nano-tracks in Silica and Quartz Induced by Electronic Excitation  
Mechanisms with Swift Ions; Fine Tuning of Optical Properties for  
Applications in Photonics**

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In this work we review our recent and extensive experimental and theoretical work on the ion high energy irradiations effects on both amorphous and crystalline SiO<sub>2</sub>. Particularly relevant has been our recent effort to perform simultaneous in-situ optical measurements of four phenomena: the optical reflectance (to obtain the refractive index), the transmittance (to obtain the absorption spectra in the range 1-6 eV), the Raman and the Ionoluminescence spectra. Additionally, comparison with standard RBS/C measurements and cathodoluminescence measurements has been done.

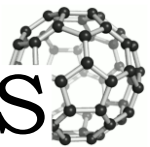
For low fluences most of the reflectance signal comes from the interface air-SiO<sub>2</sub>; i.e., we can follow the surface damage like in RBS/C but are not restricted to crystalline materials. Then, as the irradiation progresses, some light is also reflected in the damaged-pristine interface, producing interference that can be used to determine the thickness of the damaged layer. Somewhat surprisingly, interference is only produced for large fluences when the damaged layer is rather thick. This result indicates that the roughness of the damaged-pristine interface is very important for this effect. We will show that we can follow changes in the refractive index in both regimes, isolated nano-tracks and overlapping nano-tracks.

The growth kinetics of color centers approximately obeys a Poisson-type law, both, in silica and quartz. The saturation concentrations are similar for both phases but are about two orders of magnitude higher than those obtained by purely ionizing (gamma) irradiation. In the linear regime the energy needed to create one color center is about 5000 eV. No correlation of the kinetic parameters has been found with the deposition rates by elastic collisions. All the obtained results assess that new point defects are, indeed, generated by ion bombardment and that the responsible processes are associated to electronic excitation and not to elastic collisions.

We will discuss the experiments with the aid of phenomenological models as well as atomistic simulations to depict the underlying physical phenomena in terms of defect generation and annihilation. The combined use of sophisticated complementary experiments and the detailed simulations allow us to correlate the changes in the optical properties with the microscopic changes in the structures.



# POSTER CONTRIBUTIONS



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## Electronic Properties of Functionalized (5,5) BeO Nanotubes

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Using DFT theory we study the structural and electronic properties of functionalized single wall beryllium oxide nanotubes [1] with (5,5) chirality. The nanotube surface and ends are functionalized by the hydroxyl (OH) functional group the same way as we have worked with other tubular systems [2]. Our calculations consider the Hamprecht-Cohen-Tozer-Handy functional in the generalized gradient approximation to deal with the exchange-correlation energies, and the base function with double polarization DNP. The geometry optimization of both defects free and with defects nanotubes is done applying the criterion of minimum energy. Six configurations are considered with different functional group orientations. Simulation results show that the nanotube functionalization takes place at the nanotube ends with the Be-O bonds displaying hydrogen bridge bonds. Moreover the nanotube semiconductor behavior remains unchanged. The polarity is high (it shows a transition from covalent to ionic) favoring solvation. On the other hand, the work function value suggests this to be a good candidate for the device fabrication. When the nanotube contains surface defects the work function is reduced which provides excellent possibilities for the use of this material in the electronic industry.

This work was partially supported by projects: VIEP-BUAP (CHAE-ING13-G), Cuerpo Académico Ingeniería en Materiales (BUAP-CA-177), Cuerpo Académico Física Computacional de la Materia Condensada (BUAP-CA-194) and VIEP-BUAP-EXC11-G.

[1] Baumeier B, Krüger P, Pollmann J. *Phys. Rev. B* **2007**, 76, 085407.

[2] a) Chigo Anota E, Hernández Coccoletzi G. *J. Mol. Model.* (under review); b) Chigo Anota E, Hernández Coccoletzi G. *Mol. Simul.* (under review); c) Chigo Anota E, Escobedo Morales A, Hernández Coccoletzi H. *Appl. Surf. Sci.* (under review).

**Micro and Nanocontamination in Filters Used in Clean Rooms of the Electronics Industry Generates Corrosion in Microelectronic Devices**

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The deterioration of atmospheres in clean rooms of the electronic industry, where are manufactured microelectronic devices (MED), are generated by the some factors, being one of these, the contamination of electrical connections and connectors of specialized filters (SF), which avoid the introduction of air pollutants of the outdoor sources to the industrial plants. These SF form a barrier to not permit pass to finite particles as dust and gases as sulfurs, nitrogen oxides and carbon monoxide principally emitted by the traffic vehicle principally where are as Mexicali city. This city is located in the northwest of Mexico in an arid region, with some unpaved roads and the soil with very finite particles, that is typical of a desertic area. The excessive traffic vehicle in this city, with around 250,000 cars in a population of 900,000, generates concentration levels of air pollutants mentioned above. These micro chemical agents penetrate through holes and small crevices to indoor of industrial plants, and specially in the electronic industry where MED are manufactured, have SF and very isolated areas to avoid the generation of aggressive environments in these places of companies, avoiding the presence of corrosion in these type of micro components. If a process of corrosion is originated in the MED, then electrical failures are present and thereby economic losses that maintain very concerned the specialized people, managers and owners of the industrial plants. When SF function very well, the atmospheres of clean rooms not have any adverse effect in the fabrication of MED, but in change with dirty environments in these areas of the companies, and in periods of the year when the relative humidity and temperature levels are higher than 75% and 35 °C, respectively, this electrochemical process are promoted very easy and fast, damaging the micro electrical connections and connectors of the MED. This study made from 2010 to 2011, shows an evaluation of the operative yielding (OY) of SF and the causes of their low OY in some periods of the year with the Scanning Electron Microscopy (SEM) technique which indicates the principal air pollutants that reacted with the electrical connections and connectors of the SF and a proposal to avoid deterioration with a automatic control system to detect the low OY of SF.

## Encapsulamiento de Glucósidos a partir de Extracto de Llantén en Matrices de ZnO via Sol-gel

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En México, de acuerdo con la información publicada por el Sistema Nacional de Vigilancia Epidemiológica de la Secretaria de Salud, se establece a las quemaduras como una de las 20 principales causas de enfermedad con una alta incidencia, siendo el sexo masculino el más afectado con un 52% y el grupo de edad con mayor frecuencia fue de 1 – 4 años. Somos el país con más accidentes por quemaduras y representan un grave problema de salud pública, pues cada año se registran más de 115 mil casos y las personas con quemaduras más severas tenían que ser trasladadas a hospitales de Estados Unidos, ya que nuestro país carece de clínicas para su atención.[1]

Se sabe que un apósito (material de curación) no debe producir dolor durante su aplicación, ayudar a reducir el dolor, ser de costo efectivo y fácil de usar, así como ser accesible, con mínimos efectos colaterales, antimicrobiano y no-tóxico; por lo que es extremadamente importante realizar una elección adecuada. En primer instancia la extracción y caracterización de principios activos de plantas que tienen antecedentes farmacológicos sobre heridas y quemaduras, como es el caso de glucósidos como la aucubina y catapol, del llantén. [2] Por consiguiente sintetizamos nanoreservorios por el método sol-gel, para encapsular los glucósidos extraídos en matrices de óxido de zinc, por tres razones: la primera tener una alternativa que permita un aprovechamiento adecuado de los glucósidos, para ser aplicados con mayor eficacia y control; segunda utilizar las propiedades de las matrices como lo es, la liberación lenta del principio activo, la tercera aumentar el efecto terapéutico al utilizar el ZnO como material de las matrices, ya que este también es utilizado para cicatrización, causando un sinergismo. Parte importante de esta investigación es su caracterización a través de análisis espectrofotométricos utilizando UV-Visible, FTIR, DRX, EDS y SEM, mostrando que el ZnO presenta una forma cristalina tipo hexagonal, de tamaño promedio de partícula aproximadamente de 200 nm.

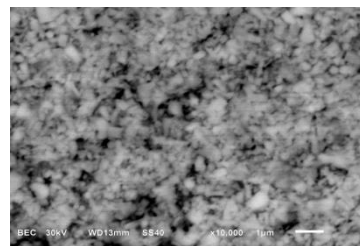


Figura 1. Microscopia de barrido de electrones (SEM) de matrices ZnO dopados con Glucósidos a 10000X.

[1] Asociación Mexicana para el Cuidado integral Y Cicatrización de Heridas A.C. Dir. Puente de Piedra

[2] [www.tec.ac.cr/sitios/Vicerrectoria/vie/editorial\\_tecnologica/Revista\\_Tecnologia\\_Marcha/pdf/tecnologia\\_marcha\\_21-2/21-2%2017-24.pdf](http://www.tec.ac.cr/sitios/Vicerrectoria/vie/editorial_tecnologica/Revista_Tecnologia_Marcha/pdf/tecnologia_marcha_21-2/21-2%2017-24.pdf)

## Silver Nanoparticles Obtained by Green Chemistry Using Common Plants in México

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M. Sánchez<sup>1</sup>

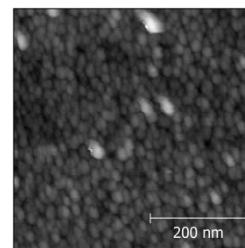
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The important antibacterial properties of silver nanoparticles (NP) are well known and its effectiveness at reducing the growth of various microorganisms has been widely reported [1]. Traditionally nanoparticles are produced by physical and chemical methods; some of these methods are ion sputtering, solvothermal synthesis and laser ablation which requires either expensive equipment or extreme conditions [2]. An environmental friendly method by using common plants in Mexico: *pelargonium graveolens*, *Opuntia*, *Aloe Vera* plants and *Cymbopogon citratus* leaves is proposed in order to obtain Silver Nanoparticles (NP). The plant phytochemicals with antioxidant or reducing properties are usually responsible for reduction of metal compounds into their respective nanoparticles [2]. The advantage of using plants for the synthesis of nanoparticles is that they are easily available, safe to handle and possess a broad variability of metabolites that may aid in the reduction.

Besides morphology characterization Atomic Force Microscopy (AFM) can be used as technique for nanoparticle sizing with statistical analysis (histograms) from sample micrographs. Chemical composition of all samples can be known by EDX analysis. The efficiency of the method at controlling the morphology and the chemical composition of Silver NP is studied.

Figure 1. SEM micrograph of silver NP obtained through Green Chemistry.



[1] Biomimetic Synthesis of Nanoparticles: Science, Technology & Applicability, Biomimetics Learning from Nature, Amitava Mukherjee (Ed.), ISBN: 978-953-307-025-4

[2] Biotechnology Advances 27 (2009) 76-83. Silver nanoparticles as a new generation of antimicrobials Mahendra Rai, Alka Yadav, Aniket Gade, Prathna T.C., Lazar Mathew, N. Chandrasekaran, Ashok M. Raichur and Amitava Mukherjee (2010).

## Synthesis of Nanostructured Bi<sub>2</sub>S<sub>3</sub> Films and their Photoconductive Response Characterization by EIS Technique

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To accelerate the processing of information and for reducing the size of the media where the processes take place, optical sensitive materials are investigated not only for promising to present important changes in their resulting physical properties induced by optical irradiations, but also, to implement systems that demand operations depending on more than one simple parameter for designing potential multi-functionalities with the same sample. The photoconduction is a property with potential applications to originate, simultaneously, changes in several photonic and electronic groups of data with the same signal employed for the stimulation. Besides, all the characteristics in the optical beams can be varied for the propagation through a photoconductive media for giving the possibility to change the conductivity and additionally for generating a photocurrent that can be a supplementary function that can be manipulated. A material with this nature is the Bismuth Sulfide. In this work, we report the characterization of photoconduction of Bi<sub>2</sub>S<sub>3</sub> thin solid films by using the separate optical excitation provided by five different semiconductor lasers at 405 nm, 445 nm, 488 nm, 532 nm and 650 nm wavelengths. Nanostructured films were obtained by using the spray pyrolysis technique as synthetic method. Electrical measurements in Bi<sub>2</sub>S<sub>3</sub> films were performed by the Electrochemical Impedance Spectroscopy (EIS) technique. The impedance spectrum was measured with amplitude of 10mV signal on a 5.0 mm<sup>2</sup> surface of the studied samples and with an integration time of 1 s. Photoconductive experiments performed with high intensity optical waves seem to confirm the possibility for generating multi-photon absorption processes in the thin films. We describe the optical control of the conductivity in the samples with potential applications for optoelectronic and filtering functionalities.

We kindly acknowledge the financial support from ICyT-DF through grant nos. PIUTE 10-129 and 10-82, and also from COFAA-IPN.

[1] J.P. Campos-López, et al., Optical absorptive response of platinum doped TiO<sub>2</sub> transparent thin films with Au nanoparticles, *Materials Science in Semiconductor Processing*, 15 (2012) 421-427.

## FTIR-CO Study of Natural Zeolitic Material

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B. Concepción-Rosabal<sup>2</sup>, G. Berlier<sup>5</sup>, V. Aguilar-García<sup>1</sup>, I. Hernández-Pérez<sup>6</sup>,  
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Powders of natural zeolite from Palmarito de Cauto, Cuba, with particle size  $-0.09 +0.05$  mm were separated by a gravimetric method and analyzed by XDR, UV-Vis-DR, EPR, magnetic susceptibility measurements, cyclic voltammetry and FTIR-CO spectroscopy (Figure 1). XRD pattern of zeolitic material before and after gravimetric separation shows mordenite and clinoptilolite zeolites as the main phases present in this material.

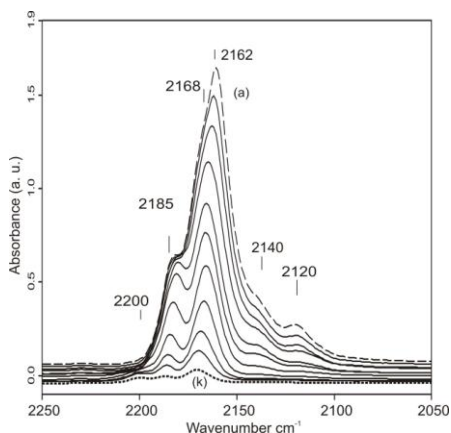


Figure 1. FTIR spectra of adsorbed CO over a zeolite sample from the middle part of column separation. Evolution of spectra as a function of equilibrium pressure of CO from 6 mBar (a) to a pressure of 0.003 mBar (k).

The use of spectroscopic techniques allows us to identify the presence of particles and nanoparticles of iron oxides [1]. Modified carbon paste electrodes with zeolites before and after gravimetric separation are electrochemically active in degrading a blue-AZO dye.

F. Chavez-Rivas and A. Manzo-Robledo acknowledge support of COFAA-IPN.

[1] Chávez-Rivas F., Rodríguez-Fuentes G., Berlier G., Rodríguez-Iznaga I., Petranovskii V., Zamorano-Ulloa R., Coluccia S., *Micropor. Mesopor. Mat.* **2013**, 167, 76.



## Synthesis of Carbon Nanofibers by Spray Pyrolysis

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The special properties of carbon nanostructures have attracted interest from researchers around the world, in both basic science and applications. Today, these nanomaterials represent one of the major research topics in nanotechnology. Carbon nanofibers (CNFs) are composed of stacked and curved graphene layers from a quasi-one-dimensional (1D)

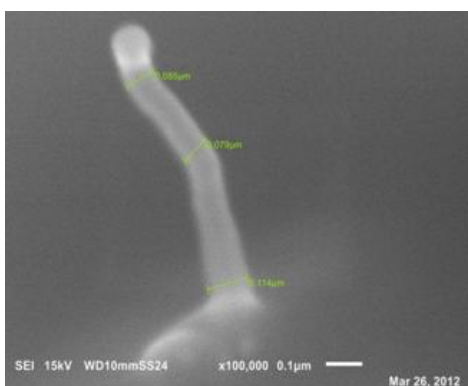


Figure 1. SEM image of a single CNF.

filament. CNFs have cylindrical or conical nanostructures; their diameters vary from a few to hundred nanometers, while lengths range from less than a micrometer to millimeters [1]. We synthesized CNFs by spray pyrolysis technique in an homemade reactor on silica substrates, hexane nebulized was the carbon source, nitrogen molecular ( $N_2$ ) flow was used as atmosphere, iron was used as catalyst and electrical furnace was the heat source. CNF was obtained in the range of 700 - 900 °C with ultrasonic nebulizer operating for 30 min. CNFs were characterized by X-ray diffraction and Scanning Electron Microscopy (SEM). Diffractograms indicate that the nanomaterial obtained with conditions mentioned previously correspond to carbon with some iron. SEM images confirm the synthesis of carbon nanofibers, in figure 1 it's possible to observe a curved nanofiber isolated with iron particle on the top, its thickness (114 nm bottom, 79 nm in the center and 85 nm on the top) represents the average diameter of the nanofibers obtained at 800 °C, at low temperature the nanofibers were thinner and shorter. Figure 2 shows a density cluster of CNFs, which is a homogeneous region with periodic interceptions in a grid.

It was possible to obtain CNF with high quality optimizing the synthesis parameters as nitrogen flow and temperature.

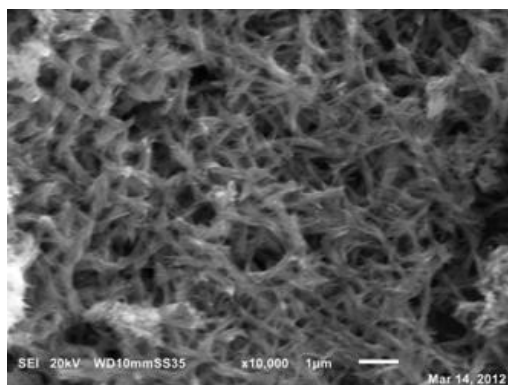


Figure 2. SEM image of CNFs cluster.

[1] Mostofizadeh, A.; Li, Y.; Song, B.; Huang, Y. *Journal of Nanomaterials*. 2011, 2011, ID 685081.

## **Dye-sensitized Solar Cell and the Relationship Between Anthocyanin and Electron Transfer**

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In the last years there have been attempts to develop Nano-crystalline solar cells based on the principles of the photosynthesis. In this sense one of the most interesting developments are the dye-sensitized solar cells (DSSC). This work describes the construction of a dye-sensitized solar cell constituted by two glasses that work as electrodes, in the surface of the glasses it is deposited a graphite-based thin film to make them conductors, as a conduction medium of electrons it is used the KI/I redox pair dissolved in ethylene-glycol, natural dyes are used as absorbent of solar energy and finally nanometric-TiO<sub>2</sub> is employed as medium where dyes are anchored. During the study it first were tested photosynthetic pigments based on a molecule called anthocyanin showed in some fruits as blackberries and blueberries and flowers as hibiscus, to find sensitizers showing performance in photocurrent and conversion efficiency. Then it was tried to introduce the principles of photosynthesis, such as electron transfer and absorption processes of solar light. Results show that the incorporation of dyes in the solar cell drastically modifies the morphology of the TiO<sub>2</sub> nanostructures in order to transfer electrons into the solar cell. Effect of dye concentration on sensitizers of the nanostructures is studied in this work.

## Zn Oxidation by Mechanical Alloying

S. Flores-Arroyo, A. Gusmán, M. Estrada-Flores, M. E. Manríquez-Ramírez,

C. Reza-San Germán

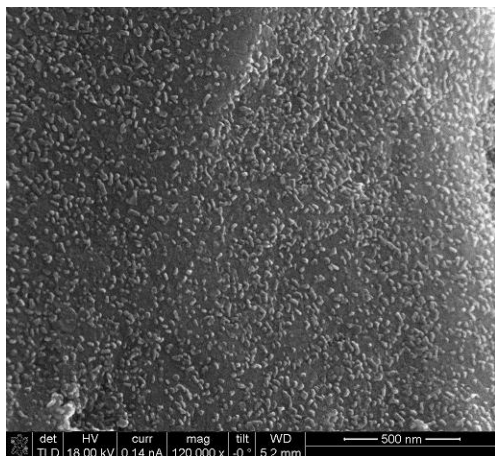
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In the last years there has been an increasing interest to synthesize nanostructures through low-cost chemical routes. Mechanical milling methods are an important means to obtain the structures with a small size. Given the current importance in obtaining zinc oxide powders with predetermined characteristics, appears the scientific and industrial interest reliably determine size distribution and particle morphology. To highlight its potential have been applied to the study of zinc oxide powders. This paper presents an analysis which system is under controlled synthesis.

Results are presented by X-ray diffraction and scanning electron microscopy which provides information on the state of the particles and their morphology.



*Figure 1. Typical SEM micrographs of ZnO nanostructures after 15 hr for milling.*

We acknowledge the partial financial supports of CONACyT and SIP, Mexico, through the grants # CB-82798 and # 20130604.

## Production and Characterization of Graphene Film Obtained by Microwave Synthesis Technique

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The synthesis of graphene thin film in a conventional microwave oven from the decomposition of camphor resin is reported. The crystalline structure of the sample was established by X-Ray Diffraction (XRD). By Scanning Electron Microscopy (SEM), we observed the sample is formed stacked carbon layers. Whereas in a High Resolution Transmission Electron Microscopy (HRTEM), we also observed that graphene main phase is the hexagonal. By Electron Energy Loss Spectroscopy (EELS) technique we were able to confirm the presence of graphene phase in good agreement with XRD observations. Sample is studied by RAMAN and X-Ray Photoelectron (XPS) Spectroscopies. By Raman the two typical peaks of graphitic structures: at  $1580\text{ cm}^{-1}$  (G band) and  $1350\text{ cm}^{-1}$  (D band) were observed. We also observed a 2D disorder band (D + G peaks) at  $2710$  and  $2940\text{ cm}^{-1}$ . Two small sharp peaks at  $2860$  and  $2890\text{ cm}^{-1}$  assigned to C–H stretching vibrations of remaining hydrocarbon in the sample are also present. By XPS is possible to prove that graphite and oxygen are present in sample because C1s and O1s were observed. The C1s peak was deconvoluted to observe its components: an asymmetric peak for  $\text{sp}^2$  centered at  $284.4\text{ eV}$  and four Gaussian peaks ( $\text{sp}^3$ :  $284.9\text{ eV}$ , C–O:  $286.25\text{ eV}$ , C=O:  $287.77\text{ eV}$  and \*:  $290.10\text{ eV}$ ). The obtained results indicate that graphene layers are composed of carbon (97.36% atomic) and oxygen (2.64% atomic).

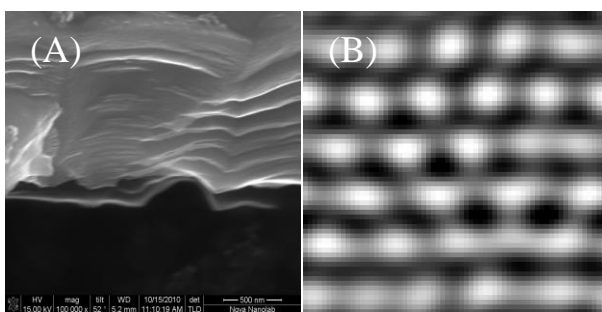


Figure 1. (A) Typical SEM micrographs of graphene layers (B) HRTEM Graphene structure.

## Synthesis of ZnO with Different Morphology by Chemical Bath Method Assisted by Microwave Radiation

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ZnO nanostructures of different morphologies were synthesized by a microwave assisted chemical bath deposition technique varying the pH of the precursor solution in between 9 and 11.14. It is known that the microwave radiation favors crystallization of nano materials. Structural characterizations of the samples were made by scanning electron microscopy (SEM), X-ray diffraction (XRD), and photoluminescence (PL) techniques. The nanostructures obtained at pH 9.2 present a growth along the c-axis in the form of spindle, whose prismatic planes (10 $\bar{1}$ 0) are not well defined. A higher pH of the reaction mixture leads to a better definition of prismatic planes, forming bar-shaped structures. For a pH 11.14, the growths along the polar directions reduced, favoring growths along nonpolar  $\pm [10\bar{1}0]$ ,  $\pm [0\bar{1}10]$ ,  $y \pm [\bar{1}100]$  directions forming sheets-like nano-structures. By varying the pH of the reaction solution the morphology of the ZnO nanostructures could be controlled.

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## ***In Silico* Study of Electro-Luminescence in SRO Thin Films due to $[\text{Si}_n\text{O}_n]^q$ Chemical Bonds**

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SRO thin films have been studied extensively due to their electro-optical properties. The low temperature emission of light from vibrational excited species is known as luminescence. When this emission is produced by an electric current passing through SRO thin films, Electroluminescence, (EL), is produced. Luminescence can provide significant information regarding the structure of a material; in the case of SRO thin films, electro-luminescence studies are particularly important, because SRO thin films can be used to fabricate luminescent devices. Even though the efforts made, no clear consensus has been reached regarding the origin of luminescence. Electro-luminescence phenomena is more complex than Photo-luminescence, because carriers are injected to the material; therefore electro-luminescence can be either due to relaxation of higher energy carrier's through radiative centers, by the recombination of excitons formed by impact ionization by the injected carriers [1], or by another unknown currently mechanism and EL could be inhibited by a charge-trapped mechanism. We employed DFT theory in order to evaluate theoretically electronic properties of a selected set of  $[\text{Si}_n\text{O}_n]^q$  nano-structures ( $q = \{+2, +1, 0, -1, -2\}$   $n = 5$  to 26), and their FTIR and luminescence spectra.

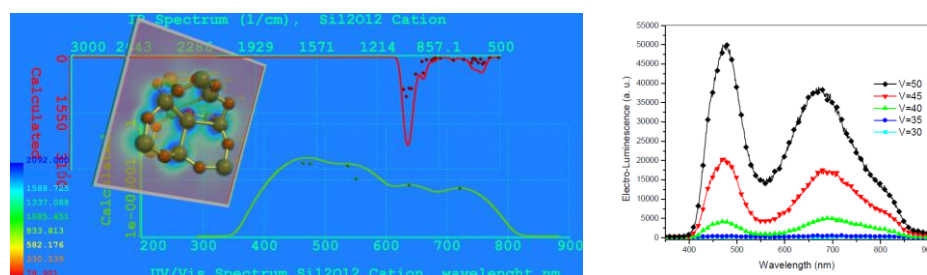


Figure 1. a) Calculated FTIR and Luminescence Spectra of  $[\text{Si}_{12}\text{O}_{12}]^{+1}$ .  
b) Experimental Electro-luminescence data of a SRO30 thin film [2].

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## Estudio Teórico y Caracterización por Espectroscopia UV-Vis-NIR de Nanopartículas de Cobre Sintetizadas por la Técnica de ALSL

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El interés por el estudio de nanopartículas de Cu (NPs Cu) proviene de la utilidad de sus propiedades, tales como la buena conductividad térmica y eléctrica a un costo mucho menor que otros metales nobles. También desempeña un papel crucial en aplicaciones como lubricantes, catalizadores, nanofluidos de transferencia térmica, materiales electrónicos y dispositivos ópticos [1-4]. Para sintetizar nanopartículas de cobre se utilizan métodos químicos, biológicos y físicos. Dentro de los métodos físicos, el de ablación láser de sólidos en medios líquidos (ALSL) proporciona una forma sencilla y flexible para la síntesis de nanopartículas. Dentro de la flexibilidad, está el que varios medios líquidos arbitrarios pueden ser utilizados. De esta manera es conocido que las propiedades finales de las soluciones coloidales dependerán de las propiedades físicas del medio líquido utilizado [5, 6]. En el presente trabajo se presentan resultados experimentales sobre la síntesis y caracterización de nanopartículas de cobre por el método de ALSL. Para los experimentos de ablación se utilizaron discos de cobre puro de 2.5 cm de diámetro por 1 cm de espesor y como medios líquidos metanol y acetona. Se utilizó un láser pulsado de Nd-YAG con emisión en 1064 nm, duración de pulso de 7 ns y operado a 15 Hz para irradiar el disco y llevar a cabo el proceso de ablación. Se realizaron experimentos variando el tiempo de ablación y a una energía por pulso de 47 mJ. Para la caracterización de las soluciones con NPs Cu en metanol y en acetona se utilizó la técnica de espectroscopía de absorción en el intervalo UV-Vis-NIR (por sus siglas en inglés). Los resultados muestran que las propiedades de absorción de las soluciones de NPs Cu dependen del medio líquido utilizado. Se presentan estudios teóricos preliminares de NPs Cu de diferentes tamaños y en diferentes medios.

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## **Evaluación de la Biocompatibilidad de Nanopartículas Magnéticas de Magnetita Estabilizadas con un Agente de Recubrimiento Superficial sobre la Salud de Ratones Sanos**

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Evaluar la actividad biológica de nanopartículas magnéticas (NPMs) es indispensable para su posterior uso *in vivo* como agentes de imagenología de resonancia magnética, como sistemas de transporte y liberación de fármacos o como materiales para tratamiento hipertérmico. Evaluar la biocompatibilidad de NPMs, con y sin recubrimiento superficial (polietilenglicol, PEG; trietilenglicol, TREG; conjugado de ácido fólico- fluoresceína, AF-Fluo) sobre la salud de ratones sanos.

Las nanopartículas se sintetizaron por el método del poliol y/o de coprecipitación química. Se administraron 10 mg/kg y 100 mg/kg de nanopartículas estabilizadas con cada uno de las diferentes recubrimientos por vía intraperitoneal en ratones macho CD1 (2 por tratamiento) y se mantuvieron en observación por 12 horas; luego se sacrificaron, se obtuvieron muestras de sangre para citometría hemática y disectaron para extirpación de hígado, riñones y cerebro. El análisis histopatológico de cada uno de los órganos permitirá evaluar cambios morfológicos y/o bioacumulación de NPMs en éstos. Se obtuvieron NPMs de 8-11 nm de diámetro (promedio) estabilizadas con PEG, TREG o AF-Fluo y sin funcionalización superficial. No se observaron modificaciones visibles en comportamiento o salud de los individuos luego de 12 horas de aplicación de 10 mg/kg y 100 mg/kg de dichas nanopartículas. Los resultados de citometría hemática no muestran variaciones significativas, respecto a valores del control o de referencia. Un análisis histopatológico indicará si los nanomateriales se bioacumulan preferencialmente en hígado, riñones o cerebro. Las NPMs con o sin funcionalización superficial son aparentemente biocompatibles en el modelo de estudio, lo que es favorable para evaluar aplicaciones biomédicas de las mismas.

Este trabajo de investigación se realiza con el apoyo del Fondo de Investigación en Ciencia Básica SEP-CONACYT N°. 154602 (“Nanopartículas magnéticas para aplicaciones en terapia hipertérmica, imagenología y transporte de fármacos: Estudio de las condiciones fundamentales de control de morfología, tamaño y estabilización”) (2012-2015).



## **Evaluación del Efecto de Nanopartículas de Magnetita (Fe<sub>3</sub>O<sub>4</sub>) Estabilizadas con Tres Agentes de Recubrimiento Superficial sobre la Salud de Ratones Sanos**

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Evaluar la actividad biológica de nanopartículas magnéticas (NPMs) es indispensable para su posterior uso *in vivo* como agentes de imagenología de resonancia magnética, como sistemas de transporte y liberación de fármacos o como materiales para tratamiento hipertérmico. Evaluar la biocompatibilidad de NPMs, con y sin recubrimiento superficial (polietilenglicol, PEG; trietilenglicol, TREG; conjugado de ácido fólico- fluoresceína, AF-Fluo) sobre la salud de ratones sanos.

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Los resultados de citometría hemática no muestran variaciones significativas, respecto a valores del control o de referencia. Un análisis histopatológico indicará si los nanomateriales se bioacumulan preferencialmente en hígado, riñones o cerebro.

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## Biocompatibility of Adipose-derived Stem Cells into Electrospun Membranes of PCL

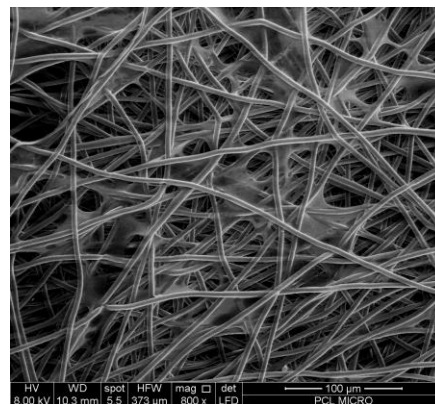
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Tissue engineering has been developed as a basic technology for regenerative medicine. Popular components used in tissue engineering approaches have generally included cells isolated from adult tissue or mesenchymal stem cells and biodegradable scaffolds 3-dimensional polymers as alternatives to mimic the native extracellular matrix which have been used for the reconstruction of tissues [1]. To understand this process, cell adhesion, cell-material interactions, proliferation and material information to the cellular environment is of great importance to the field of tissue engineering. In the first stage or cell adhesion is recently considered the most critical phase in the material surface, thus the understanding of how to perform this process is the process which greatly affects the subsequent step of the biological activity Cell as increasing proliferation, differentiation and maturation finally tissue [2].

*Figure.1 Typical SEM micrographs of electrospun membranes of PCL.*



For this reason, the synthesis and design as well as analysis and characterization of the influence of electrospun membranes substrates such as PCL on cell adhesion, cell material-interaction by using adipose-derived stem cells for application to periodontal ligament fibroblasts and odontoblasts may be useful in developing new design concepts for tissue engineering biomaterials based on biodegradable polymers with applications in dental tissue.

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## Effect of Nb Incorporation on the Structure and Optical Properties of ZnO Nanoparticles

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Recently, Nb has attracted much attention as a dopant of transparent conducting oxides (TCOs) due to its enhanced performance in electrical and optical properties of TCO thin films [1]. Reported results indicate that by Nb doping into ZnO nanoparticles [2], it is possible to achieve an equal amount of electrons with a lower cation substitution for Zn sites, which will result in lower disorder and lattice deformation. In this work, the morphology, structural and optical properties of Nb-doped ZnO nanoparticles were investigated for different Nb concentrations (0.0-5.0 mol % nominal). ZnO nanostructures with different Nb contents have been prepared by sonochemical technique, keeping all other parameters like pH value of the mixture solution, concentration of zinc precursor, sonication time, and temperature of reaction fixed. Zinc acetate dihydrate, EDTA, and ammonium hydroxide were used for preparing precursor solutions, and Niobium (V) Chloride in different amounts were added for Nb doping. Deionized (DI) water was used as the solvent for preparing the solution. The resulting solution was kept under ultrasonic irradiation for 3 h using a T-horn ultrasonic processor (UP400S, Hielscher, 400 Watt, 24 kHz) at 40 W dissipated power, under argon gas flow. It has been observed that Nb incorporation drastically modifies the structural properties of the ZnO nanostructures. Effect of Nb doping on the morphology, structural and optical properties of the nanostructures were studied using SEM, XRD, and DRS in UV-Vis spectral region.

The work was partially supported by VIEP-BUAP (VIEP/EXC/2013), and CONACyT (Grant # CB-2010/151767).

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## Use of *Trichoderma sp.* as Living Template for the Organization of Bio-synthesized Au Nanoparticles

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Use of bio-templates for the formation and manipulation of metallic nanostructures has been investigated recently [1,2]. Different biological entities, such as virus, fungi, bacteria, nucleic acids, and butterfly wings, have been utilized to profit from their natural morphological characteristics to organize inorganic structures. There exist also a few reports on the use of fungi as bio-template for the organization of gold (Au) nanoparticles to obtain monolayers, tubes and wires-like structures [3-5]. Use of bio-templates in nano- and microfabrication is advantageous due to their natural abundance and cheaper synthesis process.

In this work, we report on the fabrication of Au nanoparticles using soft organic reducer and their controlled organization over the cell walls of living fungus. Colloidal Au nanoparticles were bio-synthesized using D-glucose (DG) as a soft reducing agent, and water as solvent. Hyphae of *Trichoderma sp.* were cultivated in a prefabricated Au colloidal solution and utilized to immobilize the Au nanoparticles at their cell walls.

Formation of Au nanoparticle assembly at the cell walls of the hyphae could be observed after about 10 days of their cultivation. Formation and assembly of Au nanoparticles have been studied by UV-Vis optical spectroscopy, optical microscopy and scanning electron microscopy technique.

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## Growth of ZnO Nanostructures through Thermal Decomposition and their Photocatalytic Activity

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In the last years the level of environmental pollution has dramatically increased due to the human activities. It has motivated a fast development of new technologies which help to decrease its negative impact on the fragile balance of the ecosystems. A large number of these technologies are based in the catalysis phenomenon; however, their viability depends on the fabrication of novel materials exhibiting enhanced catalytic activity. In this regard, nanosized materials, with larger specific surface area than their bulk counterparts, have been recognized as potential catalytic materials, for example, nanosized ZnO, TiO<sub>2</sub>, and ZrO<sub>2</sub> have been successfully tried for the chemical removal of textile dyes from aqueous media [1]. Although significant progress to obtain efficient catalytic nanomaterials has been archived, development of alternative low-cost routes is still a challenge for scientist and materials engineers.

Here we report on the synthesis of ZnO nanostructures grown through thermal decomposition of ~20 nm diameter ZnO<sub>2</sub> nanoparticles. The ZnO<sub>2</sub> nanoparticles used as precursor were synthesized by a low-temperature hydrothermal method [2]. It was found that after thermal decomposition of ZnO<sub>2</sub> at 300 °C a pure wurtzite ZnO phase (*w*-ZnO) is obtained. Morphology, structural and optical properties of the *w*-ZnO nanopowder were studied by means of X-ray diffraction (XRD), scanning electron microscopy (SEM), low- and high-resolution transmission electron microscopy (TEM/HRTEM), and diffuse reflectance spectroscopy (DRS). The resulting nanostructures are round-shaped, with diameter about 150 nm and a sharp UV absorption edge. The analysis of XRD pattern suggests that the obtained nanostructures result from an agglomeration of smaller ZnO nuclei grown at the very early stages of the thermal decomposition of ZnO<sub>2</sub> nanoparticles. A proposed growth mechanism is presented. Finally, the photocatalytic activity of the obtained ZnO nanostructures to remove rhodamine B from aqueous media was evaluated and compared with the standard Degussa P-25.

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## **Influence of the pH on the Structural, Morphological and Compositional Characteristics of ZnSe Nanoparticles Obtained by Colloidal Method**

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We present a structural, morphological and compositional characterization of zinc selenide (ZnSe) nanoparticles (NPs), obtained by colloidal synthesis in aqueous solution at low temperature. We used zinc chloride (ZnCl<sub>2</sub>) to obtain zinc ions (Zn<sup>2+</sup>) and to obtain Selenium ions (Se<sup>2-</sup>) we used elemental selenium and sodium borohydride (NaBH<sub>4</sub>) as reductant agent. To protect the Zn<sup>+2</sup> ions we used a solution of sodium hydroxide (NaOH), penta sodium tripolyphosphate (Na<sub>5</sub>P<sub>3</sub>O<sub>10</sub>) and water (H<sub>2</sub>O) named Extran, also we used EXTRAN to vary the pH of the solution from 8 to 11 to observe its influence on the NPs size [1]. The Zn:Se molar concentration was of 1:1. A cleaning process was performed to eliminate the biproducts generated using hydrochloric acid (HCl). The ZnSe NPs size was estimated with powder x-ray diffraction (XRD), the morphology was studied by scanning electron microscopy (SEM) and the composition was determined by energy dispersive x-ray analysis (EDAX). XRD measurements show that ZnSe NPs exhibit a cubic zinc-blende phase structure. The size of the NPs obtained was estimated using the Debye-Scherrer equation [2]. The crystal size was found to be around 3.3 nm as calculated from the XRD patterns. We observed that the pH variation in the reaction does not significantly influence the size of the crystals.

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## Deposition of Size-selected TiN Nanoparticles on Different Substrates: Study of Their Size Quantum Confinement by Photoluminescence

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Size-selected TiN nanocluster ranging from 4 to 20 nm have been simultaneously deposited on Si(111), glass and stainless steel substrates by an ionized cluster beam (ICBD). This deposition system combines a glow-discharge sputtering with an inert gas condensation technique. The cluster size can be controlled by varying the principal parameters: the sputter power, flow of gasses, and the aggregate zone length. The nanoparticle diameter distribution is monitored in situ by a MesoQ mass filter before the deposition. After deposition, the size distribution of TiN nanoparticles was determined by AFM and HRTEM micrograph. The photoluminescence [PL] spectra of TiN nanoparticles at different sizes were also experimentally investigated. For the first time, it was reported the strong visible luminescence of TiN nanoparticles on Si (111) substrate due to the reduced size [1].

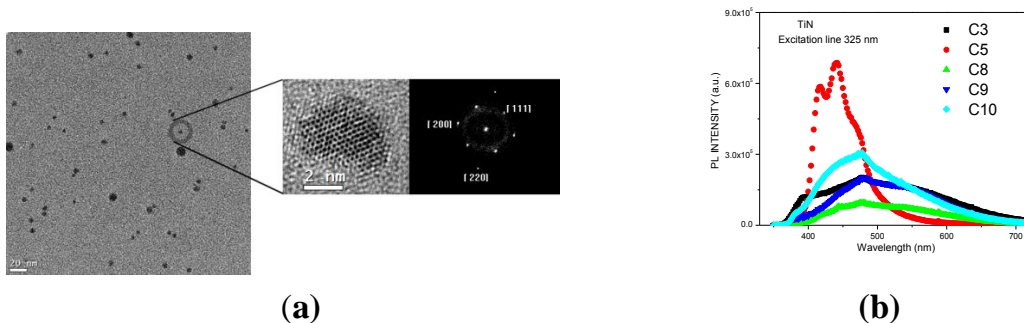


Figure 1. (a) TEM, HRTEM micrographs and the corresponding FFT of TiN nanoparticles grown by ICBD technique; (b) Photoluminescence spectra of TiN nanoparticles with different diameters.

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## **Fabrication of an Adjuvant Carrier Based on Biopolymers: PVP and Chitosan Structures**

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Nanoparticles of several materials have been extensively applied in biomedical field as biomarkers, drug carriers, biosensors and vaccines, among others. One particular application is nanopharmaceutics, which implies the development of new vaccine and specific drug carrier systems based on nanobiotechnology. In this work we present the synthesis of amphiphilic biopolymeric nanoparticles made of the biopolymers Chitosan (CS) and Polyvinylpyrrolidone (PVP) by using ionic gelation process under controlled speed dripping (15, 35, and 70 ml/hr). Also, the docking of E protein of dengue virus and linear chains of PVP and CS was carried out in order to study their possible function as adjuvant carriers. Our transmission electron microscopy, Fourier Transform Infrared spectroscopy and, Dynamic Light Scattering results shows the dependence between the nanoparticle size with the polymer molecular weight and/or surfactant aggregation velocity. In fact, the higher the molecular weight the higher the mean particle size, meanwhile if the surfactant aggregation velocity increases the mean particle size decreases. We confirmed that the ring-shaped molecules have shown affinity or preference for a place of vital importance in the virus's cycle of infection and replication. Then, theoretically PVP and CS biopolymers can fulfill the function of adjuvant carriers in the potential development of a chimeric dengue vaccine against the 4 serotypes of dengue virus.

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## Relaxometría de Nanopartículas de Óxido de Hierro como Medio de Contraste en imágenes de Resonancia Magnética

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En México no hay producción de nanopartículas que tengan las propiedades necesarias para poder usarse en la clínica como medio de contraste en la formación de imágenes por resonancia magnética, es por ello que hemos sintetizado y funcionalizado superficialmente con trietilenglicol (TREG) y Polietilenglicol (PEG), nanopartículas superparamagnéticas de óxido de hierro (SPIONs, por sus siglas en inglés). La preparación y funcionalización se realizó con la técnica de descomposición térmica de precursores inorgánicos de hierro en disolventes de alto punto de ebullición (técnica del poliol) [1, 2], probando diferentes condiciones en la síntesis, logrando así diferentes tamaños de partícula.

A partir de diluciones de concentración conocida de los dos tipos de SPIONs en medio Agar, se preparó un maniquí con el que se obtuvieron varias imágenes de resonancia magnética en un equipo Philips de 1.5 T en el Hospital Infantil de México 'Federico Gómez', en la ciudad de México. Para calcular la relaxometría a las imágenes obtenidas, se empleó un algoritmo en Matlab, donde en primer lugar se calcula el decaimiento de la intensidad de señal  $S$  y se ajusta a una curva monoexponencial  $S(TE) = S(0)e^{-R2 \cdot TE}$ . La magnitud de la señal *spin-echo* se puede utilizar para una medición precisa del tiempo de relajación T2 (tiempo de desaparición de la magnetización transversal después de una perturbación) o la tasa  $R2 = 1/T2$ . Algunos estudios *in vivo* [3], [4], así como *in vitro* [5] han demostrado que existe un alto grado de correlación entre la concentración de hierro en tejido y R2.

Los resultados muestran que los tiempos de relajación T2 cambian con el tamaño y concentración de las SPIONs, predominando la tendencia de que si disminuye la concentración, el tiempo T2 también lo hace. El estudio sentará las bases para poder utilizar las SPIONs como medio de contraste en la formación de imágenes clínicas empleando los equipos de 1.5 o 3 Teslas disponibles en hospitales de México.

Agradecemos el apoyo brindado por Jeff L. Coffey y Roberto González Rodríguez (Department of Chemistry, Texas Christian University, Fort Worth, Texas) por su apoyo para la caracterización por HRTEM. Este trabajo se realizó con financiamiento del Fondo Sectorial de Investigación en Ciencia Básica SEP-CONACYT, Proyecto N°154602 ("Nanopartículas magnéticas para aplicaciones en terapia hipertérmica, imagenología y transporte de fármacos: Estudio de las condiciones fundamentales de control de morfología, tamaño y estabilización", 2012-2015).

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## **|Synthesis of Carbon Nanotubes with Fe in its Interior by Microwave Irradiation**

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Carbon nanotubes can be synthesized with different techniques among which the most common ones are: electric arc discharge, laser ablation and chemical vapor deposition (CVD) [1]. These techniques, however, have their limitations; therefore it becomes necessary to explore alternative options. The importance of carbon nanotube synthesis via microwave irradiation stems from the fact that it allows improvement of aspects such as selective and homogeneous heating of the starting material, obtaining results in shorter times, efficient selection of carbon nanotubes and lower costs of production. In addition, the microwave technique appears to become an alternative method for the production of aligned carbon nanotubes and films as well as for the synthesis of carbon nanostructures that can result of interest for investigation. In this work we describe the synthesis and characterization of carbon nanotubes with Fe in its interior obtained from a mixture of graphite and iron acetate powders using a domestic microwave oven as energy source. The samples were prepared in sealed quartz ampoules under variation of the following experimental conditions: weight ratio of the graphite-iron acetate mixture; light grinding of the powders, and exposure time to microwaves. Samples were characterized with Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Raman Spectroscopy, and X-ray Diffraction (XRD). From this characterization we describe how experimental conditions affect nanotube diameter, nanotube content in the samples, and the presence of other carbon nanostructures. We also determined which experimental conditions produce the largest quantity of nanotubes.

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## Gold Nanoparticles Synthesized by *Neurospora Crassa* Extract and their SERS Properties

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Nanotechnology, the study of the controlling matter of an atomic and molecular scale, has emerged as an interesting and important scientific field and the controlled synthesis of nanostructures from different chemical composition as well as their shape, size, and dispersity are important areas of research. The so-called green chemistry, nanobiotechnology or bionanotechnology employs biological systems like microorganisms to fabricate nanostructures, having the benefit of improving the biocompatibility of nanomaterial. However, controlling average particle size and uniform particle morphology is still a challenge.

This work bases on the use of *Neurospora crassa*, a non-pathogenic filamentous fungus with rapid growth rate, for the biosynthesis of gold nanoparticles under different environmental conditions as well as the determination of their SERS properties. Briefly, the fungal extract was incubated with the gold precursor solution at different conditions of temperature, pH and time of reaction. Best results were obtained from incubations at 60°C. At pH 3, particles of different shapes (e.g. spheres, triangles, hexagons, pentagons, rhombs and bars) were formed while at pH 5.5 and pH 10 small quasi-spherical particles were formed with size ranges of 6 to 21 nm and 3 to 12 nm, respectively. High resolution transmission electron microscopy (HRTEM) using a FEI Tecnai F30 transmission electron microscope confirmed the crystalline and elemental character of gold nanoparticles. The synthesized gold nanoparticles of different shapes were shown to possess excellent surface-enhanced Raman scattering (SERS) enhancement ability relative to quasi-spherical gold nanoparticles. Small quasi-spherical nanoparticles of 3 to 12 nm enhances the Raman signals of methylene blue about 2 times, those of 6 to 23 nm enhance Raman signals about 25 times whereas nanoparticles of different shapes with a broad size range enhances Raman signals of methylene blue about 40 times. Results are promising and show that these gold nanoparticles might have potential applications for biological sensing and labeling systems.

**Biosynthesis of Gold Nanostructures Using Latex of *Jatropha curcas***

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Nanostructures have become significant in recent years and have created an impact in the areas of chemical, energy, electronic and biological science. The size, shape and surface morphology play a vital role in controlling the physical, chemical, optical and electronic properties of nanomaterials. The biosynthesis of nanostructures as an emerging highlight of the intersection of nanotechnology and biotechnology has received increasing attention

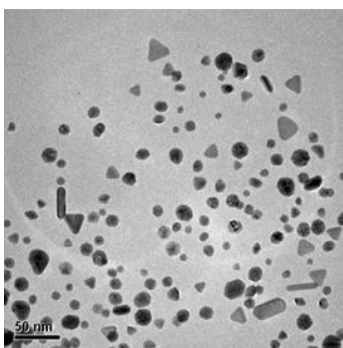


Figure 1. TEM images of gold Nanostructure by latex of *J. curcas*

due to growing need to develop environmentally-benign technology in material synthesis. Different microorganisms such bacteria, actinomycetes, fungi and plants have been investigated in metal nanoparticles synthesis. In recent years, plant mediated biological synthesis of nanoparticles is gaining importance due to its simplicity by eliminating the elaborate process of maintaining cell cultures and eco-friendliness. *Jatropha curcas* has emerged as an important reducing agent and stabilizer of metallic nanoparticles. Latex of *J. curcas* has been utilized in the synthesis of silver and lead nanoparticles [1,2]. We present biosynthesis of gold nanoparticles using latex of *Jatropha curcas* as reducing agent. The results demonstrate that the latex of *Jatropha curcas* can be utilized for the synthesis of gold nanostructures. Nanostructures of diverse morphologies such as nanorods, nanoprisms and nanoparticles could be synthesized.

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**NPt Nanoparticles for the Treatment of Adenocarcinoma: A Case Report**T. López<sup>1,2,3</sup>, S. León-Carballo<sup>4</sup>, M. Alvarez<sup>2</sup>

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Pt(acac)<sub>2</sub>-TiO<sub>2</sub> nanoparticles were prepared by the sol-gel process. Briefly, acetylacetone was dissolved Pt(acac)<sub>2</sub> in the proper amount to obtain 1% mol of platinum, then water was added (Rw=1:24) and mixed under continuous stirring at 60°C. Later, titanium butoxide was added drop-wise to the mixture and kept under reflux and stirring for 24 h. The sample was dried and milled until an ultrafine powder was obtained. The material was characterized and then tested in different in vivo cancer models where the particles demonstrated significant cytotoxic effect by decreasing the size of treated tumors. A clinical trial is currently undergoing to study bio-safety of these nanoparticles when administered in terminal cancer patients. Here we present a clinical case of a 49 years old male, with Adenocarcinoma of the esophagogastric junction diagnosed on March 2011. Endoscopic findings showed esophagus with a cylindrical mass with irregular and friable borders, from 37 cm to 41 cm in the lower third of the esophagus, stomach and retroflexion with tumor mass. The patient was classified as non surgical candidate and ELOXATIN y EPIRUBICINA chemotherapy was prescribed and despite of the treatment, the patient showed no improvement. On April 2012, a first dose of 1 g of nanoparticles was injected directly into the tumor by endoscopic surgery. Three additional applications have been carried out since then, one dose every two months. After second application, surgery tumor becomes softer and excision of 70% of visible tumor was done. General condition of the patient improves significantly, as he can swallow and is gaining weight. Although to date the tumor has not disappeared, its growth has been slowed allowing the patient a better quality of life.

## Incremento de la Actividad de Nanopartículas de CeO<sub>2</sub> por Agentes Surfactantes

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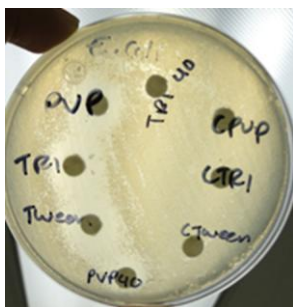
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En este trabajo, las nanopartículas (NPs) de CeO<sub>2</sub> fueron examinadas para evaluar su toxicidad utilizando *Escherichia coli* en presencia de surfactantes no iónicos. Las NPs fueron sonicadas a diferentes valores de pH y de tiempo, después se le agregaron los diferentes surfactantes (Triron X-100, Polivinil Pirrolidona (PVP) y Tween-80) al 0.002% v/v. Se encontró que el sonicado favoreció la dispersión coloidal y produce partículas con un tamaño promedio de 100 nm. El material fue toxico para *E. coli* a pH 7 cuando se utilizó solamente medio mínimo M9, no se observó una respuesta en un medio rico. El efecto tóxico en medio mínimo se mejoró cuando se le agregaron los surfactantes antes mencionados. Se observó que la concentración mínima inhibitoria (CMI) para *E. coli* se redujo al usar el CeO<sub>2</sub> más el surfactante. El mejor efecto se observó con Tween-80, siendo 0.15 mgmL<sup>-1</sup> la CMI comparado con 3 mgmL<sup>-1</sup> de CeO<sub>2</sub> solo (casi 20 veces). Estos hallazgos sugieren la importancia de las diferentes sustancias que pueden interactuar con



NPs, como surfactantes, usualmente presentes en sistemas de aguas residuales que pueden llevar características inesperadas no deseables de materiales tóxicos generalmente considerados como inocuos.

Figura 1. Prueba de disco resultante de la prueba de los tres diferentes surfactantes. Se observa la inhibición de un diámetro de 13 mm para PVP, 14 mm para Triton X100 y 15 mm para Tween-80.

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## Synthesis of Carbon Nanotubes from Metal Acetates

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This work presents the synthesis of carbon nanotubes (CNTs) from metal acetates using the technique of chemical vapor deposition (CVD) and using a solution of ethanol (70%) - Toluene (30%) as carbon source. CNTs were grown on porous alumina substrates incorporating metal acetates solutions (SOLN). The precursor solutions were prepared by adding metal acetate mixtures (Co Mo, Fe: Mo, Fe: Co) in ethanol and then deposited on the alumina. Subsequently, a heat treatment was applied to the substrates with deposits at 500 °C for 10 minutes to obtain their metal oxides prior to the synthesis of CNTs by conventional CVD. The CNTs were synthesized at temperatures of 800 °C and 830 °C for 20 minutes in both the cases [1, 2]. The substrates with and without metal acetate and metal oxide deposits were analyzed by Atomic Force Microscopy and Confocal Microscopy, while the nanotube samples were characterized using Scanning Electron Microscopy (SEM) and Raman spectroscopy. The study of the substrate with deposit of acetates and metal oxides allowed to us to verify if they were distributed homogeneously. The characterization of nanotube samples synthesized by the deposits of metal acetates revealed the CNTs are multiwalled nature, grown randomly on the substrate with average diameters in-between 20-70 nm; some of them with shorter lengths and others with longer lengths.

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## Microwave Synthesis of Graphene and Few-layer Graphite Flakes

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The recent boom of graphene and its wide spectrum of potential applications motivate the development of new, efficient and low-cost synthetic routes [1]. In this work we synthesize flakes of graphene and few-layer graphite using a domestic microwave oven. In this technique, graphite powder (99.9995%, 200 mesh) is exposed directly to microwave

radiation and then sonicated in dichloroethane. After irradiation, graphite particles are expanded and a small amount of flakes are exfoliated. HCP crystalline structure is maintained but c-parameter increases with irradiation time [2]. Sonication results in the increase of exfoliated flakes. Irradiation effects and exfoliation were monitored with SEM, AFM, Raman spectroscopy and X-ray diffraction.

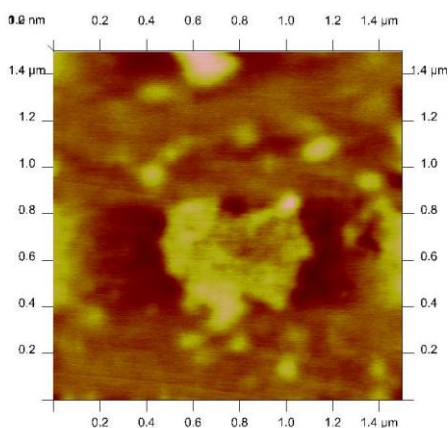


Figure 1. AFM image of a graphene flake.

\* COFAA-IPN fellow.

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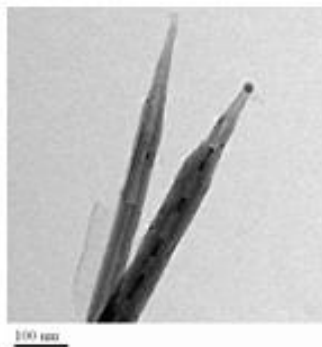
## Synthesis, Characterization, and Magnetic Properties of Defective Nitrogen-doped Multiwall Carbon Nanotubes Encapsulating Ferromagnetic Nanoparticles

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Nitrogen-doped multiwalled carbon nanotubes (CN<sub>x</sub>MWNTs) with multiple morphological defects were produced using a modified chemical vapor deposition (CVD) method. In a typical CN<sub>x</sub>MWNTs synthesis by CVD an acetone trap is used to catch organic by-products from the pyrolysis. In the present work a mixed solution of NaCl (26.82 wt%) and water (73.18 wt%) was used instead of acetone in the trap. Carbon nanotubes with sharp tips and lumps were found in the products. Scanning electron microscopy (SEM) showed the formation of several nanoparticles of different shapes inside the nanotubes. Powder X-ray diffraction analysis was used to characterize the crystal structure of the nanoparticles. Their electronic and magnetic properties were studied using a physical properties measurement Evercool system (PPMS). With this simple change in the CVD-trap it is possible to control the morphology of carbon nanotubes and encapsulated nanoparticles (see Fig. 1). The differences in gas flow are proposed as the possible mechanism to produce these changes in both the nanoparticles and CN<sub>x</sub>MWNTs.



*Fig. 1. TEM image of two different configurations of CN<sub>x</sub>MWNTs: 1) with small nanoparticles incrusting in the layers; and 2) with encapsulated cylindrical-like nanoparticles.*

## Thermal Effects on Nitrogen Doped Multiwalled Carbon Nanotubes (CN<sub>x</sub>MWNTs): From Nanotubes to Carbon Sheets

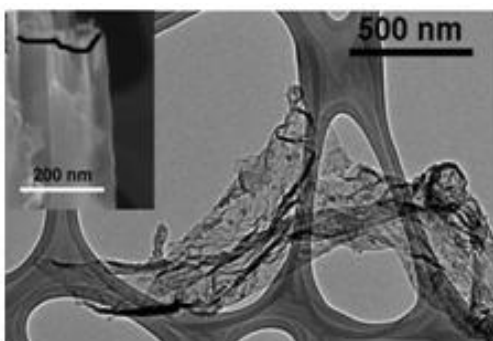
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N-doped multiwalled carbon nanotubes produced by chemical vapor deposition (CVD) using aerosols of benzylamine and ferrocene, were thermal treated during 26 hours at 1100 °C under a low flow (1 bubble per second) of Ar. Several morphologies were obtained after the heating treatment. Fig. 1 shows a TEM image of a carbon sheet (inset: SEM image of a CN<sub>x</sub>MWNT which starts to unroll). Other nanostructures, such as crystalline metallic nanoparticles, nanoribbons, junctions and coalesced nanotubes, were also observed. The N-doped nanocarbons may find applications in different fields as sensors, field effect transistors, and field emission sources. Ferromagnetic nanoparticles have importance in nanomedicine and magnetic storage. Possible mechanisms responsible for



the formation of these diverse nanostructures will be discussed.

Figure 1. TEM image of an unrolled CN<sub>x</sub>MWNT thermal treated during 26 h under an Ar atmosphere. Inset is a SEM image of a possible unrolled CN<sub>x</sub>MWNTs (see black line marking the edge).

## Effect of Particle Size on the Microwave Absorption in the Yttrium-iron Garnet

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Yttrium iron garnet,  $Y_3Fe_5O_{12}$  (YIG), belongs to a group of magnetic oxides, characterized by specific magnetic and magneto-optical properties. Also, YIG possesses the highest quality factor, in microwave regime, with the smallest linewidth in ferromagnetic resonance (FMR) among the magnetic materials [1]. A comparative study between YIG samples with different particle size (micro/nanopowders) is carried out, by means of FMR and a non-resonant microwave absorption technique. FMR spectra are illustrated in Fig. 1, for micro- and nanopowders at room temperature. We observe changes in the lineshape between both samples, and only in the nanopowders a more complex structure is observed, which can be due to spin waves.

A method to measure the non-resonant microwave absorption, as function of an applied magnetic field around zero field, known as the low-field microwave absorption (LFMA) is also employed. This technique provides valuable information about the nature of the magnetic ordering in materials [2,3]. LFMA technique is used to give a further knowledge on YIG samples, with different particle size, showing their main characteristics highlighted; where LFMA is a powerful tool for the research of magnetic materials at microwave frequencies.

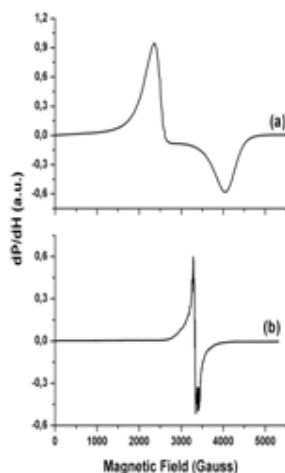


Figure 1. FMR spectra of ceramic YIG at room temperature in (a) micro- and (b) nanopowders.

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## Photoluminescent Characterization of Nanoparticles of $\text{HfO}_2\text{:Tb}^{3+}$ , Synthesized by Hydrothermal Route

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Nanoparticles (NPs) of hafnium oxide ( $\text{HfO}_2$ ) doped with Terbium ( $\text{Tb}^{3+}$ ), were synthesized by hydrothermal route in order to determinate their photoluminescent properties. The synthesis was carrying out at different hydrothermal treatment times and the acidity (pH) on the solution was change in the range of 4 to 12. The dopant concentration was 3% atomic of Terbium with respect to the amount of hafnium in the precursor solution, maintaining a hydrothermal treatment temperature at 200 °C. An important relationship between the hydrothermal treatment time, and therefore, the particle size with the intensity of the emission was observed. X-ray diffraction (XRD) showed a low degree of crystallinity at short times of hydrothermal treatment. When the reaction time increase, the material acquires a crystal structure, which corresponds to the monoclinic phase of  $\text{HfO}_2$ . The images obtained by field emission scanning electron microscopy (FESEM) show the increase in the particle size as a function of the hydrothermal treatment times. The photoluminescent emission spectrum, present peaks centered at 489nm, 543nm, 584nm and 622nm; associated to transitions  $^5\text{D}_4 \rightarrow ^7\text{F}_J (J=3-6)$  of Terbium trivalent ions.

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## Biosynthesis of Ag Nanoparticles with *Chenopodium ambrosioides* Extracts

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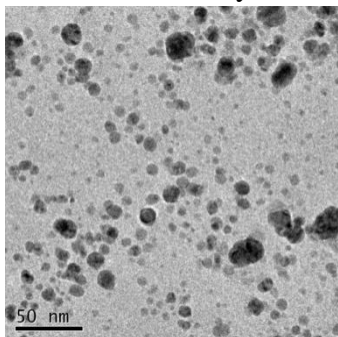
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The biosynthesis of nanoparticles with plant extracts is a promising technique and environmentally friendly, which has a potential not fully explored [1]. The aqueous extract of *Chenopodium ambrosioides* was used as bioreductor and capping in the synthesis of silver nanoparticles. Five volumes (0.5, 1, 2, 3 and 5 mL) of extract and two concentrations (1 mM and 10 mM) of AgNO<sub>3</sub> were tested. Formation of nanoparticles was determined by the volumes extract, being observed a direct relationship between volumes of extract and amount of particles formed. In contrast, the silver ion concentration was negatively related with particle size. The shapes of the obtained particles were considered quasi-spherical. Volumes higher to 5 mL do not produce nanoparticles, suggesting that high concentrations promote the aggregation in large clusters [2]. The nanoparticles obtained are polycrystalline and the structure corresponds to face-centered cubic (fcc) silver. With this system, the particles are stable for more than one year at 25 °C without



the addition of a stabilizer. The shape and size of silver nanoparticles can be controlled varying the bioreductor volume and silver nitrate concentration.

*Figure 1. Micrograph of nanoparticles of silver after the bioreduction. 3 mL of extract was exposed to 1 mM silver nitrate at 25 °C. Scale bar: 50 nm.*

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## Influence of Vanadium Tri-oxoalkoxides Precursors in V<sub>2</sub>O<sub>5</sub> Thin Films Morphology Obtained by Sol-gel

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The nature and features of V<sub>2</sub>O<sub>5</sub> thin films depend directly from the alkyl radical in vanadium tri-oxoalkoxides precursors [VO(OR)<sub>3</sub>] [1]. Prandlt and Hess [2] synthesized VO(OR)<sub>3</sub> precursors incorporating secondary alcohols, and vanadium acidic salts using an inert atmosphere with an excess of alcohol. In this work, it was synthesized two precursors implementing a linear and a secondary alcohol (ethanol & 2-propanol) in a 12:1 salt relation, while the azeotropic distillation avoided the usage of inert atmospheres. The purity of Precursors was corroborated by infrared spectroscopy. The precursor solutions were prepared by diluting 100:1 for VO(OEt)<sub>3</sub>/H<sub>2</sub>O and VO(Oi-Pr)<sub>3</sub> precursor was used directly, in order to fabricate thin films deposited onto Corning glass and Quartz by using sol-gel immersion technique at different withdrawal rates. All thin films were heat treated from 300 to 700 °C; likewise, V<sub>2</sub>O<sub>5</sub> gels were heated at temperatures of 300, 400 y 500 °C for each precursor. Results demonstrate grain sizes around 16 nm; as well as, V<sub>2</sub>O<sub>5</sub> phase formed at 500 °C for VO(Oi-Pr)<sub>3</sub> thin films, presenting a better V<sub>2</sub>O<sub>5</sub> crystallographic arrangement phase and homogeneity along the film than those obtained by VO(OEt)<sub>3</sub>. However, precursors influence is directly demonstrated by the morphology of the powders, going from multilayer distribution (VO(Oi-Pr)<sub>3</sub>) to nanorods (VO(OEt)<sub>3</sub>), having itself in both an orthorhombic structure.

We acknowledge the financial supports of CONACyT, Mexico, through the grants # 183355.

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## **Novel Information Criteria to Locate Electromagnetic Resonances in Nanostructured Materials**

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Novel information criteria based on the principle of minimum fisher information [1] are presented in order to locate electromagnetic resonant wavelengths at which field enhancement appears within symmetrical metallic nanostructured materials. A comparison with those results obtained with electromagnetic theory is done. Nevertheless both theories agree, we show the former method is numerically more efficient and reliable.

[1] B. Roy Frieden. Physics from Fisher Information Unification, Cambridge University Press, 1998.

## **Deposición de Nitruro de Aluminio en Compuestos de Carbono**

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En experimentos donde se sintetiza el nitruro de aluminio hexagonal, se hace uso de nanotubos de carbono (CNTs, por sus siglas en inglés) como semilla, además de alúmina como reactivo en una atmósfera controlada específica (1223K-1423K) bajo el flujo constante de gas nitrógeno. Lo que se observa al momento de realizar la caracterización haciendo uso del microscopio de tunelaje, es un ensanchamiento en la superficie externa de los nanotubos de carbono, así como cierto grado de quiralidad. Esta supuesta quiralidad y el aparente ensanchamiento en la superficie externa de los CNTs pueden asociarse a alguna forma de adsorción del dímero Al-N sobre los CNTs. Mediante un estudio computacional de primeros principios se ha encontrado la distancia interatómica de mínima energía del dímero Al-N, así como la distancia de mínima energía de los átomos de carbono en una malla de grafeno. Para poder explicar los resultados experimentales, se varió la distancia de manera discreta entre ambos átomos del dímero, así como también se usó la técnica de gradiente conjugado. Con base a lo anterior, se ha encontrado la posición de mínima energía del dímero de Al-N sobre la malla de grafeno. Esperamos extender este resultado a un nanotubo de carbono ya que dicha configuración nos permitirá describir la forma de adsorción y podría definir también el grado de quiralidad del arreglo superficial del cuerpo del cilindro.



## Electrochromic Properties of Nanoporous $\alpha$ and $\beta$ -nickel hydroxide Thin Films Obtained by Chemical Bath Deposition

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Nickel hydroxide thin films were deposited on ITO-coated glass substrates by the chemical bath deposition method employing two formulations. In the first one, deposition of films was achieved through forming an ammonium complex, producing the well crystallized phase  $\beta$ -Ni(OH)<sub>2</sub>, while the second one, obtained through urea decomposition, promotes the deposition of the turbostratic phase  $\alpha$ -Ni(OH)<sub>2</sub>. Both show complex nanoporous morphology, which consists of irregular interconnected nanosheets but with different size and disposition. After thermal annealing in air at 250 °C, electrochromic behavior of the films was tested by cyclic voltammetry, chronoamperometry and single wavelength transmittance. The optical contrast and structural transformations between colored and blanched states, were studied by ex-situ optical transmittance-reflectance, Raman, and infrared reflectance spectroscopies. It was found that the colored state of the  $\beta$  films corresponds to the  $\beta$ -NiOOH phase whilst for  $\alpha$ (II) films either the  $\beta$ (III) or Ni<sub>2</sub>O<sub>3</sub> · xH<sub>2</sub>O phase is obtained.

We acknowledge the partial financial support of CONACyT-México, through grants No. 103385 and No.156907.

**Near Field Topology in the Vicinity of a Nanometallic Slit**

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The phase of the near field produced by the interaction of electromagnetic beams with a nano metallic slit is analyzed as a function of several optogeometric parameters. The number, position and type of a phase singularity is considered as a function of the wavelength, width and thickness of the nano slit. It is shown that the topology of the near field spectrum presents remarkable changes when incident radiation is close to wavelengths where field enhancement occurs.

## Metal-oxide Catalyzers and their Influence in the Synthesis of Silver Nanorods

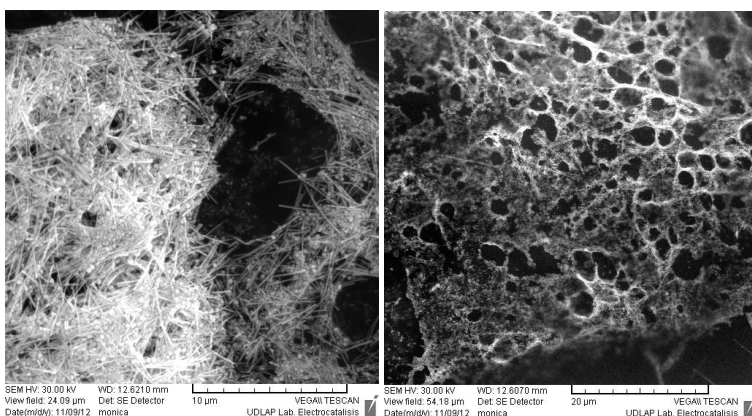
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Silver nanoparticles have received a lot of attention in the past years due to their special optical and electrical properties. These properties are mainly related to their size and shape. Therefore the precise control over different shapes and aspect ratios is important to be able to exploit these applications.

The process of synthesis of silver nanorods can be made through chemical or vapor phase methods. The most extended chemical method is the polyol process first described by Fievet, et al [1]. There have been different modifications of this method [2-5] by adding different ions as etching agents. We modified the polyol method by adding different metal-oxide nanoparticles as nucleation centers and etching agents to see its influence in the growth of anisotropic structures. We found that the size and concentration of the nanoparticles play a key roll in the precise control of the structures obtained.



*Figure 1. SEM micrographs of silver nanostructures obtained with our method.*

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## Optical and Structural Characterization of Antimony Doped Zinc Oxide Single Crystal

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We present the optical and structural analysis of zinc oxide (ZnO) antimony doped, performed by atomic diffusion. Diffusion is carried out at a temperature of 1000 °C for periods of 1, 2 and 4 hrs, from a solid source prepared by partial oxidation of antimony. Characterization of each step of the process was performed by photoluminescence (PL) and High Resolution X-Ray Diffraction (HRXRD). The photoluminescence shows the effect of doping with antimony in radiative transitions caused by the creation of impurity levels. Doped samples analyzed by high HRXRD and reciprocal space mapping, revealed the structural modification of the quality of the single crystal produced by the introduction of antimony. The results indicate that the antimony is introduced fully the volume of ZnO and does not modify the quality of the crystal.

We acknowledge the partial financial supports of CONACyT, Mexico, through a grant.

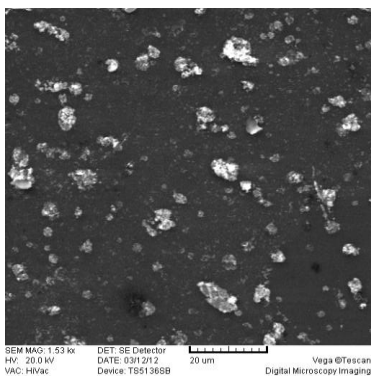
## Morphological Characterization of Gold Nanoparticles and their Aggregation by the Adsorption of the Pesticide Endosulfan

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Gold nanoparticles (AuNPs) have been used extensively during the last years to add on their surface several kinds of ligands, which serve as media to adsorb specific and chemically compatible compounds. In particular, endosulfan is one of the most stable pesticides known and it has been detected in the environment trough the world. Its presence has several repercussions on health. The adsorption of endosulfan on AuNPs has been reported previously [1], however there is few information on structural or morphological properties of the aggregates formed during the adsorption of endosulfan on



AuNPs. UV/VIS spectroscopy shows that the surface plasmon resonance (SPR) of the AuNPs at 520 nm suffers a shift to low energies.

**Figure 1.** Typical SEM micrograph of aggregates of AuNPs after adsorption of endosulfan.

After adsorption of endosulfan on the surface of AuNPs, a new SPR arises at 670 nm. This resonance suggests the formation of aggregates of micrometric size, as shown in Fig. 1. The size of these microstructures depends on the reaction time and on the concentration of endosulfan adsorbed.

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## **Fabrication of ZnO Thin Film Structure for Application as DNA Sensor to Detect Dengue Virus**

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Zinc Oxide sparked interests of scientists across the world due to its use in transparent conductive applications, especially in solar cells and biosensors. Due to its biocompatibility, it is also frequently used in impedance-type biosensors. The sensing apparatus consists of a ZnO thin film with a sequence-specific probe strand employed as recognition element. ZnO thin film deposition is carried out by Ultrasonic Spray Pyrolysis (USP) using an in-house designed equipment [1] at temperature of 450 °C with dry air as carrier gas with millimolar concentrations of Zinc Acetate as precursor to obtain transparent films of thickness around 250-300nm. X-Ray diffraction data shows the dominant peak corresponding to the (101) plane with the presence of other peaks corresponding to (102), (002), (100) and (103) planes indicating formation of the hexagonal phase of ZnO. Further, DNA immobilization is carried out electrostatically, taking advantage of distinct isoelectric points of ZnO (~4) and DNA (~9) [2] to make a biosensing apparatus with DNA as the recognition element. The biosensor is specific in diagnosis as the immobilized DNA is specific to each of the four serotype of dengue virus.

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**Mechano-chemical Synthesis and Characterization of Cu doped BiVO<sub>4</sub>**V. Ishrayelu<sup>1</sup>, S. Velumani<sup>1</sup>, R. Asomoza<sup>1</sup>, G. S. Miguel Angel<sup>2</sup>, A. Aldana<sup>1</sup>, G. Ignacio<sup>1</sup><sup>1</sup>*Department of Electrical Engineering- SEES, CINVESTAV – IPN, Zecatenco, D.F, C.P. 07360, Mexico;* <sup>2</sup>*Department of chemistry, UAM, Iztapalapa, C.P-28049 Madrid, Mexico.*

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Nowadays, Bismuth vanadate (BiVO<sub>4</sub>) has drawn many increasing attentions and has tendency to be a visible light driven photocatalyst for photo electrochemical water splitting and degradation of organic pollutants. Doping BiVO<sub>4</sub> photocatalysts with suitable metals, will enhance the absorption towards visible light region and increase the efficiency of photocatalytic degradation. Highly crystalline Cu doped BiVO<sub>4</sub> nano powders were prepared by mechano-chemical reaction between the bismuth oxide (Bi<sub>2</sub>O<sub>3</sub>) and vanadium oxide (V<sub>2</sub>O<sub>5</sub>) in a stoichiometric ratio of 1:1 by adding copper in the form of granules (<5mm) at different atomic percentages which are 1, 3, 5, 7, 10 and 15% for quantity of 8 grams by using high energy planetary ball mill setup. The following parameters for synthesis of Cu doped BiVO<sub>4</sub> catalyst were optimized by our group [1], the homogeneous mixture milled with speed of 400 RPM for continues 6 hours with 8:1 ball per powder ratio. BiVO<sub>4</sub> catalysts were annealed at 350 °C, 400 °C and 450 °C. X-ray diffraction (XRD) analysis confirmed 80% highly monoclinic scheelite structure for Cu doped BiVO<sub>4</sub> catalyst nanoparticles. Moreover, peaks at  $2\theta=34.52^\circ$ ,  $35.19^\circ$  and  $46.55^\circ$ ,  $47.34^\circ$  corresponding to (2 0 0), (0 0 2) and (2 4 0), (0 4 2) planes merged as single peaks at  $34.75^\circ$  (2 2 0) and  $46.96^\circ$  respectively, which affirms tetragonal structure with copper at % increment. From the Micro-Raman analysis observed a peak at  $344\text{ cm}^{-1}$ , corresponding to vibrational mode of CuO. Spherical shaped 50 nm sized particles were confirmed from FE-SEM micro graphs. Cu- BiVO<sub>4</sub> relative compositions were confirmed by Energy dispersive X-Ray Spectroscopy (EDAX). We observed increment of blue shift in absorption threshold edge in all the catalysts as the copper at % increment from Diffuse Reflectance Spectra (DRS) analysis. We confirmed the size 10 to 15 nm particles, which were agglomerated, and (011) orientation of monoclinic scheelite structure for Cu doped BiVO<sub>4</sub> catalysts from the HRTEM Bright field analysis.

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## Deposition of CIGS Thin Films by Radio Frequency (RF) Sputtering from a Single Quaternary Target

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Quaternary semiconductors of the type I-III-VI<sub>2</sub> have been extensively studied because of their potential applications in a variety of electro-optic devices. Among these materials CIGS thin films have received considerable attention as one of the most promising materials for thin film solar cells, due to their high absorption coefficient and potential for low cost manufacturing. In this study, CuIn<sub>(1-x)</sub>Ga<sub>x</sub>Se thin films were deposited on glass substrate by radio frequency magnetron sputtering process from powder target previously synthesised by uniaxial pressing of CIGS nanopowder. CIGS nanopowder was synthesised by mechanochemical alloying of elemental Cu, In, Ga and Se powder at a milling speed of 400 rpm for 2 hrs [1] and then pelleted out by applying 6 ton pressure for 30 minutes. During sputtering process argon gas flow rate was maintained as 20mT. We investigated the effect of deposition power on composition and structural properties of as deposited thin films. Thin films have been characterised by XRD, FEG-SEM, EDAX and Raman Spectroscopy in terms of deposition power from 50W to 150W with an increment of 50W. XRD study showed amorphous nature for all the deposited thin films in contrast to crystalline nature of synthesised CIGS nanopowder. The distinct peak in Raman spectra near 185 cm<sup>-1</sup> indicated presence of chalcopyrite phase in CIGS thin film deposited at 100W and 150W. EDAX analysis revealed that all the deposited CIGS thin films were copper poor and selenium rich. FESEM analysis showed dependence of surface morphology on sputtering power. The CIGS nanoparticles are packed densely over the glass substrate with increase in sputtering power. Results emphasize the necessity of selenization process to improve crystallinity, composition and homogeneity of as deposited CIGS thin film.

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**Síntesis Hidrotermal y Caracterización de Nanopartículas Luminiscentes**E. Navarro-Cerón<sup>1</sup>, J. Guzmán Mendoza<sup>1</sup>, G. Rodríguez Gattorno<sup>2</sup><sup>1</sup>*Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada del Instituto Politécnico Nacional, Legaria 694. Colonia Irrigación, 11500 México D. F.;* <sup>2</sup>*Centro de Investigación y Estudios Avanzados Unidad Mérida Km. 6 Antigua carretera a Progreso Apdo. Postal 73, Cordemex, 97310, Mérida, Yuc., Mex.*

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El tratamiento hidrotermal es uno de los métodos relativamente más eficientes en la síntesis de materiales de óxidos nanocristalinos [1]. Su uso es común en la preparación de soluciones para óxidos con valores de alto grado de saturación, que precipitan como un amorfo. La metodología hidrotermal permite el control de la composición de la fase y la morfología de los productos, variando parámetros como la temperatura, presión, tiempo, concentración y pH [2-4]. Es posible controlar el tamaño como resultado del proceso de *coarsening* involucrado en la redisolución-recristalización bajo condiciones hidrotermales (presión y temperatura alta).

En este trabajo se reporta la síntesis y la respuesta fotoluminiscente del HfO<sub>2</sub> impurificado con Eu<sup>3+</sup> (HfO<sub>2</sub>:Eu<sup>3+</sup>). La síntesis se llevó a cabo por la ruta hidrotermal a partir de HfCl<sub>4</sub> y EuCl<sub>3</sub>·6H<sub>2</sub>O con NH<sub>4</sub>OH en agua. Después de preparar la hidrólisis de los precursores, éstos se llevaron a tratamiento hidrotermal a 120 °C, bajo presión autógena a un tiempo de reacción de 24, 40, 52 y 72 horas. Las nanopartículas sintetizadas fueron caracterizadas por difracción de rayos X (XRD), microscopía electrónica de transmisión de alta resolución (HRTEM) y por espectroscopia dispersiva (EDS). Las muestras se excitaron con una radiación de 395nm, mostrando líneas de emisión correspondientes a las transiciones electrónicas <sup>5</sup>D<sub>0</sub> → <sup>7</sup>F<sub>J</sub> (J = 0 → 4), características del ion de Eu<sup>3+</sup>. La intensidad de la emisión fotoluminiscente se incrementa con respecto al tiempo de reacción, mostrando un máximo a 72 horas. El máximo del pico de excitación a 395 nm, hace de este material un excelente candidato para aplicaciones en lámparas blancas de estado sólido.

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## Electron-Energy-Loss Spectra of buckled Free-Standing Silicene

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Silicene, the silicon-based counterpart of graphene, is increasingly getting attention because it is a semi-metal material with Dirac cones and thus, in principle, has similar electronic properties [1, 2]. In this work we calculated the Electron Energy Loss Spectrum (EELS) of buckled free-standing silicene. Dielectric function is obtained by using a discretization method as has been suggested by Delerue *et al.* [3]. Tight-binding method is applied considering 2nd Nearest Neighbors with  $sp^2$  orbitals, the Slater-Koster parameterization [4] and the Harrison's rule. This has been done for plane and buckled silicon sheets. In the latter case with a structure based on DFT calculations [2]. The resulting dielectric function is compared to those of bulk silicon and graphene. Spectra of EELS are contrasted for plane and buckled silicene, particularly the plasmon frequency as a function of the  $z$  displacement of buckled silicone.

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## Synthesis and Characterization of Biocompatible Nanomaterials with Natural Active Ingredients for Potential Medical Applications

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The objective of this project is to synthesize different kind of nanomaterials modified with medicinal plant extracts to evaluate their *in vitro* biological activity. *Matricaria chamomilla* and *Catharanthus roseus* are being used to obtain their chloroform, hexane and methanol extracts, which are being purified by column chromatography and characterized by proton (<sup>1</sup>H) and carbon (<sup>13</sup>C) nuclear magnetic resonance (NMR) [1,2]. Iron oxide nanoparticles and calcium alginate nanocapsules were synthesized by coprecipitation of an iron sulfite precursor with ammonium hydroxide and by microemulsion method, respectively [3,4]. Iron oxide nanoparticles were characterized by transmission electron microscopy (TEM), infrared spectroscopy (FTIR) and Raman spectroscopy, while alginate nanocapsules were characterized by FTIR, dynamic light scattering (DLS) and confocal microscopy. The particle size ranges of iron oxide nanoparticles were between 6-10 nm with magnetite as the main crystalline phase. Regarding alginate nanocapsules, their particle size range was between 200-400 nm, but they show a high percent of aggregation. With these results, we continue with the biological activity evaluation of all the materials obtained employing bacterial models, which will be discussed later.

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## Optical and Structural Properties of Sol-gel ZnO Coatings

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In this work we have obtained thin film coatings of zinc oxide (ZnO) on glass substrates using the sol-gel process, and spin coating deposition technique with ZnO precursors and using water as solvent and acetic acid to adjust the pH. These solutions were initially synthesized as zinc oxide precursor using zinc acetate dehydrate ( $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ ).

The first solution was obtained by dissolving 3.731 g of zinc acetate in 50 ml of distilled water, then under constant stirring a solution of acetic acid 1 M was added dropwise to prevent the formation of colloids and precipitation [1]. The second zinc oxide solution was prepared diluting 3.1 g zinc acetate in a mixture of 15ml of isopropyl alcohol ( $i\text{-C}_3\text{H}_7\text{OH}$ ) and 0.86 ml of monoethanolamine ( $\text{HOCH}_2\text{CH}_2\text{NH}_2$ ) as complexing agent, which is used to control the solubility of the solutes [2]. Both solutions were maintained in constant agitation at 60 °C by one hour until a clear solution was obtained, and aged for 24 hours. After aging the coatings were deposited in 1, 2 and 3 layers with the spin coating in dry air conditions and 70 psi of pressure and 23.7 of vacuum, 3000 rpm of spin speed and running time of 1.3 minutes per sample using 1 ml of solution from each coating. The T% of the coatings was evaluated by UV-Vis spectroscopy, the surface morphology by SEM analysis and the structure was carried out by X-ray diffraction technique.

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## Structural, Morphological and Optical Properties of TiO<sub>2</sub>:V Coatings Obtained by Sol-gel Process

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Transparent oxide coatings of TiO<sub>2</sub>:V with high transmittance (>70%) in the visible region were successfully synthesized by the sol-gel process and deposited onto glass substrate using spin coating technique in dry air conditions. Titanium tetraisopropoxide, isopropanol ammonium *meta*-vanadate and deionized water were used as starting materials [1]. This precursor solution was deposited onto corning glass substrates by spinning at 6000 rpm and thermally annealed at 500 °C. These coatings were characterized using techniques such as scanning electron microscopy (SEM), for microstructure evolution as a function of sintering temperature. Through UV-Vis spectroscopy, we analyze adhesion and uniformity of the coating on the substrate, with values greater than 70% transmittance in the visible range. X-ray diffraction (XRD) results show us the degree of crystallinity of the anatase phase. With these results we found that the TiO<sub>2</sub> impurified with V causes that TiO<sub>2</sub>:V thin films have a high transparency in the visible range of light spectrum (about 70%), with particle size in nano range. UV-visible absorption studies show a blue shift in the visible range for TiO<sub>2</sub> films, which is a typical characteristic of nano-semiconductor [2].

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## **XRD and Raman Scattering Characterization of $\text{Cu}_2\text{ZnSnS}_4$ Nanocrystals**

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$\text{Cu}_2\text{ZnSnS}_4$  (CZTS) nanocrystals (NC's) were synthesized in oleylamine using the hot-injection technique for 24 h. This fast and uncomplicated preparation method delivers nanoparticles with a diameter of approximately 10–30 nm. The nanoparticles are characterized by powder-X-ray diffraction (XRD) and Raman scattering. The chemical composition of synthesized CZTS NC's was obtained by energy dispersive X-ray spectroscopy (EDX), which is in good accordance with the stoichiometric chemical composition.

**Raman Scattering and XRD Studies of SnS<sub>2</sub> Nanoparticles**

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Tin disulfide (SnS<sub>2</sub>) nanoparticles were successfully prepared by colloidal chemistry using the hot-injection approach, starting of tin(II) chloride, sulfur and oleylamine. The phase composition and morphology were analyzed by X-ray diffraction, Raman spectroscopy and scanning electron microscopy (SEM). The results show that the synthesis produces nearly-spherical SnS<sub>2</sub> nanoparticles around 20-50 nm in size, crystallizing in the hexagonal structure. The elemental analysis carried out by EDAX indicated that the obtained nanoparticles are nearly stoichiometric SnS<sub>2</sub>. A representative Raman spectrum reveals a sharp peak at 313 cm<sup>-1</sup>, which characterizes the hexagonal phase of SnS<sub>2</sub>.

## Synthesis and Characterization of SnO<sub>2</sub> Colloids by Sol-gel Method

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Tin dioxide (SnO<sub>2</sub>) colloidal suspensions were prepared by the sol-gel method using a mixture of tin tetrachloride pentahydrate (SnCl<sub>4</sub>·5H<sub>2</sub>O) and isopropyl alcohol solutions. Several concentrations of SnCl<sub>4</sub>·5H<sub>2</sub>O were used. The SnO<sub>2</sub> nanoparticles were precipitated by dropping ammonium hydroxide (NH<sub>4</sub>OH) into the tin salt solution under constant magnetic stirring. The obtained sol was dried at 80 °C, after this was calcined at 600 °C for 2 hours in air atmosphere. The structural and optical properties of the SnO<sub>2</sub> nanoparticles are investigated using X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FT-IR). The acquired XRD pattern shows that the obtained powders are SnO<sub>2</sub> with tetragonal crystalline structure. The calcined SnO<sub>2</sub> nanoparticles have an particle size from 8.2 to 19.61 nm. The evolution of the most important functional groups during the steps involved in this synthesis route is explained in view of the results obtained with FT-IR and XRD. FT-IR technique was employed to study the structural composition into of the SnO<sub>2</sub> lattice. The IR spectrum of the tin oxide nanoparticles exhibits a strong absorption around 615 cm<sup>-1</sup>. This shoulder was assigned to Sn–O bond vibration.

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**Simple Formation of ZnO Nanorods and Urchin-like Microclusters**

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Zn-ZnO nanorods and urchin-like structures were synthesized by the hot filament chemical vapor deposition at 825 and 1015 °C respectively. X-ray diffraction spectra showed a mixture of ZnO and Zn phases in both nanorods and urchin-like structures. The Zn-ZnO nanorods with diameter of about 100 nm showed dispersed morphology. The urchin-like structures of few micrometers in diameter exhibited porous and rough morphology with epitaxial formation of nanorods. Photoluminescence spectra showed a visible broad band centered at the wavelength corresponding to green emission. It was mainly associated with oxygen vacancies due to in-situ chemical reduction on the urchin structures.

## **Mechanical Properties of Iridium Nanostructures by Means of Molecular Dynamics Simulations**

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In order to study the mechanical properties of nanocrystals, we have performed molecular dynamics simulations using Cleri-Rosato potential for bulk and nanowires of iridium. For the nanowires and bulk models we used supercells and periodic boundary conditions, respectively. Uniaxial tensile strain is applied along the [001] direction and stretched at constant strain rate. Nanowires show a linear increase in stress until reaching to the maximum stress at a strain of 7.5%; after that the wires are collapsed by ductile fracture. The Young moduli for the nanowire are about 50 % compared to that of the bulk counterpart. On the other hand, the maximum stresses are 40 GPa and 15 GPa for bulk and wire, respectively.

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## Structural and Morphological Characterization of CdSe Nanoparticles Obtained by Colloidal Synthesis

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Structural and morphological characterization of cadmium selenide (CdSe) nanoparticles (NPs) is presented in this work. The CdSe NPs have been obtained by colloidal synthesis at low temperatures and atmospheric pressure, using Cadmium Chloride ( $\text{CdCl}_2 \cdot 2.5 \text{H}_2\text{O}$ ) and elemental selenium (Se) as precursors. The  $\text{Se}^{-2}$  ions were formed by using sodium borohydride ( $\text{NaBH}_4$ ) as a reducing agent. Also, in order to protect the  $\text{Cd}^{+2}$  ions, a solution of NaOH, penta-sodium tripolyphosphate and  $\text{H}_2\text{O}$  (“extran”) was used. The pH of the colloidal solution of extran protected  $\text{Cd}^{+2}$  was fixed at 8 and the Cd:Se molar concentration was varied from 3:1 to 1:3. X-ray diffraction (XRD) and high-resolution transmission electron microscopy (HRTEM) measurements show that the CdSe NPs have face-centered cubic structure and a grain size ranging between 3.3 and 4.4 nm depending on the molar concentration Cd:Se as estimated by the Debye-Scherrer equation [1].

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## Effect of pH Variation on the Synthesis of CdSe Nanoparticles Obtained with Different Precursors in Colloidal Solution

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A comparative study of the synthesis of CdSe nanoparticles (NPs) varying pH and the cadmium precursor is presented in this work. The pH of the colloidal solution was varied between 8 and 11. Cd<sup>+2</sup> ions were obtained at room temperature from different precursors (cadmium chloride, cadmium nitrate, cadmium acetate). The reducing agent used in the process was an aqueous solution of sodium hydroxide (NaOH), penta-sodium tripolyphosphate and H<sub>2</sub>O called "Extran". The Se<sup>-2</sup> ions were obtained using sodium borohydride (NaBH<sub>4</sub>) as reducing agent for the elemental selenium at 75°C. The byproducts of the reaction were removed through a cleaning process with hydrochloric acid (HCl) [1]. The samples were characterized by X-ray diffraction (XRD); it was found that the obtained NPs have a face-centered cubic structure. Grain sizes between 3.3 nm and 5.5 nm were estimated using the Debye-Scherrer equation [2], depending on the pH of the colloidal solution. A morphological study was performed with scanning electron microscopy (SEM), and compositional analysis was done by Energy Dispersive X-ray analysis (EDAX).

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## **Mechanical Strength of Aluminum Nanowires Doped with Magnesium: A Molecular Dynamics Study**

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The engineering stress-strain curves of aluminum nanowires doped with magnesium have been investigated by means of molecular dynamics. The nanowires were oriented along 001 direction and stretched at constant strain rate. For the aluminum we used the Cleri-Rosato potential [1] and for the interaction of Al-Mg and Mg-Mg we used a polynomial potential fitting from *ab initio* calculations. The effect of doping of magnesium in the aluminum nanowire is analyzed from stress-stress curves.

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## Density Functional Theory Studies of GaN Nanowires: Structural and Electronic Properties

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Gallium nitride (GaN), a wide gap semiconductor, has been extensively studied because of its technological applications [1]. It is well known that low dimensional systems exhibit novel structural and electronic properties. Particular attention has been paid on semiconductor wires with sizes in the regime of nanometer scale [2, 3] since they may be employed in the fabrication of optoelectronic devices such as field effect transistors. In this work we have performed first principles total energy calculations within the periodic density functional theory (DFT) to investigate structural and electronic properties of GaN nanowires. Calculations have been carried out within the generalized gradient approximation. We have studied GaN nanowires formation in the wurtzite fase with the growth axis along the [0001] direction. We have investigated different diameters for the nanowires. It is found that the outer Ga atoms move slightly towards the nanowire center while the surface N atoms move in the opposite direction. Band structure and density of states (DOS) show a band gap with the Fermi energy close to the conduction band. Formation energy studies reveal that structures with larger diameter are more stables than thinner ones.

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**Stability and Physicochemical Principles for  $Ti_9XO_{20}$** **(X = Ti, C, Si, Ge, Sn and Pb) Clusters:****A Prediction as Novel Catalytic Materials****D. Mora, M. Salazar-Villanueva, A. Bautista H.**

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The electronic and structural properties of  $Ti_9XO_{20}$  (X = Ti, C, Si, Ge, Sn and Pb) clusters have been obtained within density functional density (DFT) framework. The changes of bond length, binding energy, frontier orbitals and electric potential have been fully analyzed when one atom of titanium is replaced by elements with electrons four of valence inside of principal cluster. The atom which improves the properties mentioned, specially the catalytic, will be discussed very carefully.

## Raman Spectroscopy of Few Layers of Graphene on Curved Surfaces

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Chemical vapor deposition has proved to be an alternative method to produce high quality graphene films [1]. We used this technique to produce few layers of graphene on copper wire of 15 micrometers at 1000 °C and ambient pressure. At this temperature on the surface of copper wire, a partial fusion process is happened. When the system is cold, some spherical structures on the copper surface are formed. Finally, the layers of graphene acquire this spherical form. We found an effect in Raman spectrum of few layers of graphene on top of this spheres that is not observed in copper wire surface free of spherical structures. The most notable effect is observed in G\* band as is shown in Figure 1. This effect is probably due to the curvature of the spherical surface in which graphene is grown.

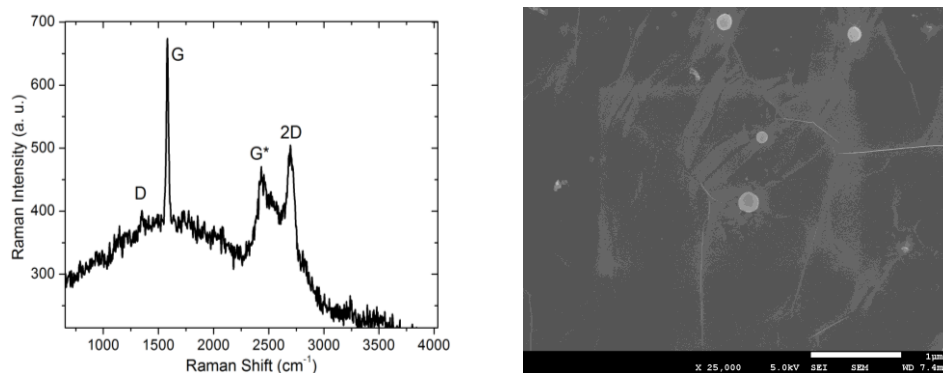


Figure 1. Raman spectrum and SEM images of few layers of graphene on spherical structures in copper wire after CVD process.

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## Modulation of the Optical Transmittance in Multilayer Graphene

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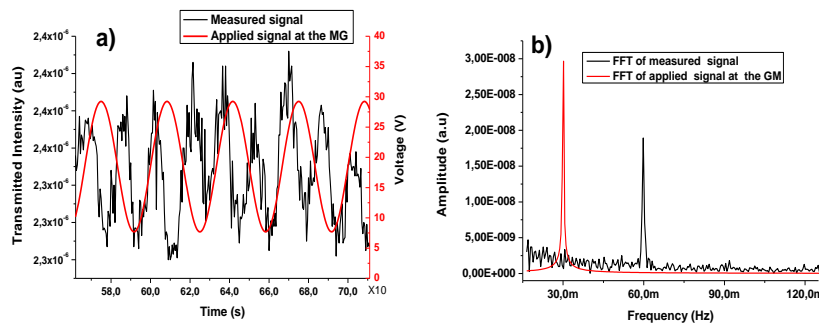
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The study of optical devices has increased in recent years for applications in data exchange, but the complexity and the bandwidth of the devices is also scaling (1). Graphene is a new material and due to its unique thermal and electronic properties it may revolutionize the field of photonics. Liu and coworkers reported that graphene function as an optical modulator which operates at frequencies up to 1 GHz (2).

This work presents the study of the modulation of the optical transmittance in Graphene Multilayers (GM). Modulation occurs when polarized light with constant intensity is passed through MG between two electrodes that are fed with an alternating current (AC) at frequency  $\omega$ . It is noted that the intensity of the transmitted light has an alternating component that oscillates at  $2\omega$ , which is twice the AC excitation frequency of the GM. This behavior is similar to that observed in the thermoacoustic effect (3). Figure 1 shows the results: a) oscillating component of the measured transmitted light intensity as well as the excitation AC signal applied to the GM, which was 30 mHz. Figure b) displays the FFT of the transmitted measured signal, which is centered precisely at twice the excitation frequency of the GM.

The simplicity of the implemented experimental device foresees potential applications of graphene as an optical modulator. It should be noted that to our knowledge this effect has not be reported in the scientific literature.



*Figure 1. a) Measured of Optical transmittance in GM (black), and signal applied GM between two electrodes (red), b) Frequencies obtained by FFT at signals of the Figure a).*

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## Estimación de la Dimensión Fractal de Superficie Mediante SEM y AFM

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En este trabajo, se determinó la dimensión fractal de la superficie de placas de FeCrAl oxidadas a 750, 800, 850 y 900 °C por 24 horas en atmósfera de aire, a partir de imágenes de SEM y AFM. Las imágenes de SEM pueden representarse como gráficas bidimensionales de intensidades contra posición, llamadas histograma de escala de grises las cuales en conjunto reconstruyen la topología superficial al asociar intensidades con alturas. Las imágenes de AFM dan directamente información 3D de la superficie, al graficar alturas relativas contra posición. A estas gráficas o “trazas” obtenidas por SEM y AFM, se les aplica el método de reajuste de escala (R/S) y mediante el programa BENOIT, se calcula la dimensión fractal (D) correspondiente. Así D representa la morfología superficial pues las trazas de donde fueron obtenidas representan las características locales de la superficie. Los valores de dimensión fractal obtenidos por SEM fueron, 1.402, 1.545, 1.557 y 1.583, mientras que por AFM fueron 1.494, 1.561, 1.573 y 1.593, para las temperaturas de 750, 800, 850 y 900 °C, respectivamente. Para ambas técnicas, la dimensión fractal aumenta con el incremento de la temperatura de oxidación, esto se interpreta como un aumento de la rugosidad al aumentar la temperatura, hecho que se observa directamente de las imágenes. El análisis fractal en este trabajo, se ubica en el intervalo  $1 \leq D \leq 2$ , pero puede extrapolarse a un comportamiento en 3D empleando el exponente de Hurst (H). En conclusión, la dimensión fractal aplicada a imágenes de SEM y AFM, plantea una alternativa para la cuantificación de la rugosidad de superficies micro y nanoestructuradas. También se puede hacer el seguimiento de los cambios superficiales con diferentes tratamientos, térmicos, mecánicos, ambientales, etc. Con esta metodología SEM deja de ser una técnica meramente cualitativa, en cuanto a textura superficial se refiere.

**Synthesis, Thermal and Structural Characterization of the  
Ba (Er<sub>0.5</sub>Nd<sub>0.5</sub>) (In<sub>0.3</sub>Sn<sub>0.3</sub>Pb<sub>0.3</sub>) CuO<sub>5-x</sub> Nanocomposition  
by Sol-gel Method Using Acrylamide**

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The sol-gel process is a wet-chemical technique widely used in the fields of materials science and ceramic engineering due to its capability to homogeneously distribute the crystals at nanometric scale and the quality provided by the purity of the used precursors.

Here we present preliminary results using sol-gel method to synthesize Ba(Er<sub>0.5</sub>Nd<sub>0.5</sub>)(In<sub>0.3</sub>Sn<sub>0.3</sub>Pb<sub>0.3</sub>)CuO<sub>4.55</sub> stoichiometric nanocomposition using acrylamide as gelating agent. The thermodynamic behavior of the nanocomposition was determined by DSC and TGA analysis, which showed the value of temperature in which the sample undergoes a phase change (the significant values were around 600 and 1000 °C). These results are the guide to determine the reaction temperatures of the sample. By XRD, SEM and EDX analysis we obtain an isostructural In<sub>2</sub>Cu<sub>2</sub>O<sub>5</sub> compound, organic material and reagents.

We acknowledge the support of the technicians of CUVyTT, Eric Reyes and Ricardo Serrano, and the technician of the Synthesis Lab, Roberto Alvarez.

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## Study of Silver Nanoparticles Obtained by AgNO<sub>2</sub> Reduction

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Metal nanostructures have been the focus of intensive research as a result of their electronic, optical, magnetic, thermal, catalytic, and other properties being distinctly different from their bulk counterparts, and considerable attention, in terms of both fundamental and applied research, has been paid to synthesizing and characterizing metal nanostructures [1]. It has also been demonstrated that the physical and chemical properties of the structures in the nanometer scale are closely related to their size and shape [2]. Silver nanoparticles (AgNps) are synthesized in both polar and nonpolar media and are employed toward an increasing number of applications in sensing, catalysis, therapeutics, labeling, diagnostics, and controlled release [3]. In this work, we are studying AgNPs for applications as dopant in other compounds. Thermal reduction of AgNO<sub>2</sub> in 2-methoxy-ethanol is the adopted process to produce AgNPs in the presence trisodium citrate and poly-(vinylpyrrolidone) to stabilize the solution. The formation of silver particles was manifested by the gradual appearance of a yellowish coloration in the solution. Transmission electron microscopy (TEM), UV-Vis spectroscopy and X-Ray diffraction (XRD) are used to know the AgNPs optical and structural characteristics.

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**Synthesis and Characterization of Superparamagnetic Nanomagnetite**

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In this work we present results about the synthesis, functionalization and characterization of magnetite superparamagnetic nanoparticles. Particles with size between 5-20 nm were synthesized by coprecipitation method in aqueous media, at the following temperatures: 20, 40, 60 y 80°C. The particles are dispersible on polar and non-polar media after their functionalization with oleic acid.

The objective of this work was to obtain nanomagnetite usable in biomedical applications. In this field, the instability of this material has been restricting their usage, and actually there is a great effort in stabilization. In this work we capped the nanoparticles with oleic acid.

The coprecipitation is a cheap and easy technic to obtain the nanomagnetite, it produces many size particles, and their applications are restricted. In this work we made experiments to size separation by a magnetic way and we demonstrate that with this technique we can obtain samples with 7.8% of polydispersity with superparamagnetic behavior.

The structural and magnetic properties were determined by X-ray diffraction, FTIR, HRTEM, MFM and magnetometry. The X-ray and FTIR analysis corroborated that in all cases we obtained magnetite. In agreement with the X-ray analysis the size of the particles was increased from 12 to 14 nm when the temperature rise from 20 to 80°C. After selection size the nanoparticles showed superparamagnetic behavior because their coercivity is zero. A sample with particle mean size of 5 nm and 7.8% of dispersion has a magnetic saturation of 55 emu/g. The magnetic domain distribution obtained by MFM is of 3.5 nm.

HRTEM characterization showed that the nanoparticles are crystalline individually. And we were able to measure the interplanar distance for the (111) direction of 4.9 Å. The nanoparticles functionalized with oleic acid, in the FTIR characterization the presence of the magnetite absorption bands in the range of (3000-2800cm<sup>-1</sup>) correspond to the C-H vibrations. This confirms the presence of oleic acid in the nanoparticles.

The X ray diffraction showed that nanoparticles synthesized at 20°C increased their size once they were capped with oleic acid from 12 to 14 nm, in the same way that 80°C capped nanoparticles which increased their size from 14-17 nm. Their saturation magnetization decreased from 52 to 36 emu/g in the 20° sample and from 65 to 63 in the 80°C one.

## A Model of Non-linear Chemical Kinetics of Gold and Silver Nanoparticles Synthesis

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The aim of this work is to propose a mathematical model of the fundamental chemical kinetics which take place through the synthesis of silver and gold nanoparticles (NPs) grown by chemical reduction [1, 2]. In this study  $\text{HAuCl}_4$  and  $\text{AgNO}_3$  were selected as precursors for the synthesis of gold and silver NPs, respectively; for both cases, the reducing agent was  $\text{NaBH}_4$ . The chemical kinetics were modeled using a non-linear mathematical analysis [3-5], in a similar way like those works based in the Gray-Scott model [6-9]. Here, we present two models of the chemical kinetics using reaction-diffusion equations. These models describe the spatial-time evolution of precursors and products concentrations in an inhomogeneous medium; however, at this stage, the effect of a polymer stabilizer has not been included [10-13]. While the time-dependent part of the proposed equations was solved by means of a numerical method (Euler), the spatial-dependent part was tackled using the discretization of the Laplacian. Our tri-dimensional simulations predict that under some specific conditions the synthesized metallic NPs are quasi-spherical in shape [14].

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## Synthesis and Characterization of TiO<sub>2</sub> Nano Reservoirs Supported with Platinum II and Sodium Bicarbonate Solution

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The TiO<sub>2</sub>-based nanoreservoirs have been the point for the development of new and better alternatives to the control and possible "elimination" of chronic degenerative diseases such as cancer, diabetes mellitus type II, Parkinson's, Alzheimer's and other to improve the living conditions and treatment of these diseases [1-5]. In this first phase have been synthesized, characterized and developed new nanoreservoirs of the titanium oxide (TiO<sub>2</sub>) doped with platinum II at a concentration of 0.1% (Pt-0.1/TiO<sub>2</sub>) and solution sodium bicarbonate to 15% (NaHCO<sub>3</sub>-15/TiO<sub>2</sub>) and "in situ" with platinum II and sodium bicarbonate (Pt-0.1-NaHCO<sub>3</sub>-15/TiO<sub>2</sub>) by the sol-gel method. Results from UV-VIS, FTIR and XRD showed that the TiO<sub>2</sub> and Pt-0.1/TiO<sub>2</sub> nanoreservoirs are amorphous, while Pt-0.1-NaHCO<sub>3</sub>-15/TiO<sub>2</sub> and NaHCO<sub>3</sub>-15/TiO<sub>2</sub> nanoreservoirs are crystalline due to the transformation of the acid salt (NaHCO<sub>3</sub>) to trona phase. It is established that the trona phase increases average particle size in the Pt-0.1-NaHCO<sub>3</sub>-15/TiO<sub>2</sub> nanoreservoirs of 130 nm to 180 nm and decreases markedly in the Pt-0.1/TiO<sub>2</sub> nanoreservoirs until 50 nm. Therefore, the trona phase encapsulates to TiO<sub>2</sub> particles as shown by SEM studies. Figure 1.

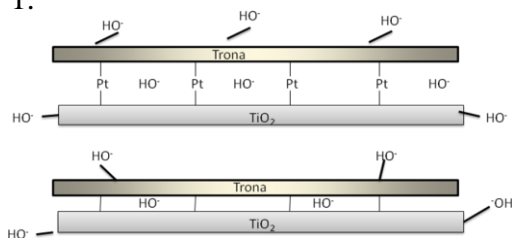


Figure 1. Schematic representation of the interaction of trona on TiO<sub>2</sub> surface.

We acknowledge the partial financial supports of M. C. José Guadalupe Quiroz, Faculty of Chemical Science

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## Estudio Fotocatalítico de Nanocatalizadores CuMn/ZrO<sub>2</sub> en la Degradación del Azul de Metileno en Función del pH

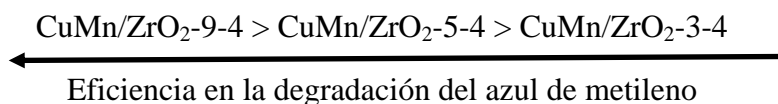
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 F. Hernández Aldana<sup>5</sup>, L.-A. Moreno Rodríguez<sup>6</sup>

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El óxido de circonio (ZrO<sub>2</sub>) ha demostrado ser un excelente soporte catalítico en diversas reacciones químicas, como: envenenamiento con Cu en la síntesis del metanol a partir de CO<sub>2</sub> e H<sub>2</sub>, con La-Cu en la reducción de NO con C, con Rh en la hidrogenación de CO y CO<sub>2</sub> a hidrocarburos, con Pt en la oxidación del propano a CO<sub>2</sub>, con Au en la oxidación de CO, con WS<sub>2</sub> en la hidrosulfuración de tiofeno y últimamente, en las reacciones de acoplamiento oxidativo del metano a través de dopantes metálicos básicos [1-3].

Las propiedades ácido-base de los óxidos metálicos pueden ser modificadas con tratamientos alcalinos tales como la adición de sodio o la adición de aniones como sulfatos, molibdatos, tungstano, etc. La importancia del ZrO<sub>2</sub> en todas las reacciones es la irradiación de la superficie de éste con radiación ultravioleta, produciendo reacciones del tipo redox y por consiguiente el proceso de fotoactividad catalítica. Para incrementar la eficiencia de la actividad fotocatalítica del nanocatalizador, en la síntesis por sol-gel del ZrO<sub>2</sub> se incorporaron iones bivalentes de transición interna como el Cu<sup>2+</sup> y Mn<sup>2+</sup> en medio básico (CuMn/ZrO<sub>2</sub>-9-4), neutro (CuMn/ZrO<sub>2</sub>-5-4) y ácido (CuMn/ZrO<sub>2</sub>-3-4). Todos los nanocatalizadores a base de circonio se calcinaron a 400°C. Se demuestra que el nanocatalizador CuMn/ZrO<sub>2</sub>-9-4 presenta mejor eficiencia en la degradación del azul de metileno que el nanocatalizador propuesto por Adela et. al; (CuMn/ZrO<sub>2</sub>-3-4) y por el propuesto por Isabel et. al. (CuMn/ZrO<sub>2</sub>-5-4).



Agradecimientos: José Guadalupe Quiroz Oropesa por el apoyo económico. Facultad de Ciencias Químicas BUAP.

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## Photocatalytic Degradation of Trimethoprim by Metallic Nanoparticles Supported on TiO<sub>2</sub>-P25

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The presence of pharmaceutical residues in wastewaters, as well as its effects on aquatic life and human health, has been widely reported as potentially harmful for living ecosystems [1]. Trimethoprim is an antibiotic used for treating various types of bacterial infections, when it is consumed by humans, about 40 to 60% of the dose is excreted in urine [2], causing water pollution. Advanced oxidation technologies, such as photocatalysis, have become an attractive alternative for water decontamination [3]; their mechanism, based on the absorption of light for the generation of active radicals, leads to the mineralization of organic matter [4]. The deposition of nanosized metal particles on TiO<sub>2</sub> has proved to provide important benefits for the efficiency of photocatalytic reactions involved in the degradation of organic compounds since these nanoparticles act as a sink of electrons. In this work, the photodegradation of trimethoprim is proposed by using TiO<sub>2</sub>-P25 modified with metallic nanoparticles supported. It is shown that the use of metallic nanoparticles brings important benefits to the activity of bare TiO<sub>2</sub>-P25. The photocatalysts were characterized by TPR, XRD, UV-Vis diffuse reflectance, TEM, ICP and EDS spectroscopy.

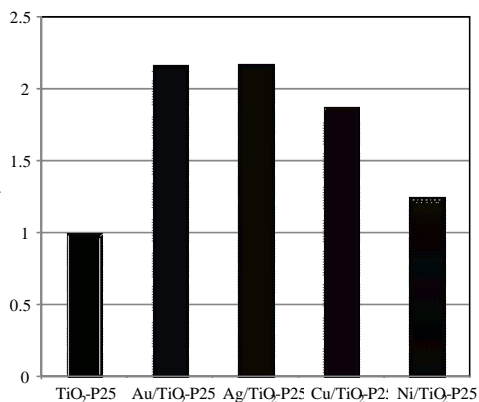


Figure 1. Comparative photocatalytic enhancements for the degradation of trimethoprim of TiO<sub>2</sub>-P25 modified with metal nanoparticles

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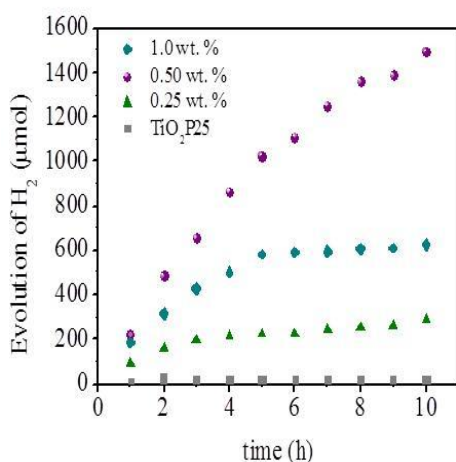
## Photocatalytic Water Splitting for Hydrogen Production by Gold Nanoparticles Supported on TiO<sub>2</sub>

S. Oros-Ruiz<sup>1</sup>, R. Zanella<sup>1</sup>, R. Gómez<sup>2</sup>, A. Hernández-Gordillo<sup>2</sup>, R. López<sup>2</sup>

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One of the most promising fuels is hydrogen since it may be produced from water, a renewable and a sustainable clean source, and its combustion is totally environmentally friendly [1]. At present, there are several techniques to produce hydrogen such as nuclear and fossil fuels [2], electrolysis, thermolysis and water splitting photocatalysis [3]. The ability of a photocatalyst such as TiO<sub>2</sub> to reduce aqueous protons can be improved by using co-catalysts. Recently, several studies on the deposition of gold nanoparticles have been reported for the improvement of the photoactivity of TiO<sub>2</sub> for water splitting, it has been proved that gold nanoparticles are relatively more reactive and suitable for the photocatalytic hydrogen evolution than the other investigated co-catalysts. In this work the



photocatalytic hydrogen production by water splitting was driven by gold nanoparticles. Several parameters such as gold content, thermal treatment of solids, mass of catalyst and gas atmosphere for treatment of solids were evaluated for an easy understanding of gold-titania systems in water splitting.

Figure 1. Effect of metal loading on the Au/TiO<sub>2</sub> photocatalysts for H<sub>2</sub> production.

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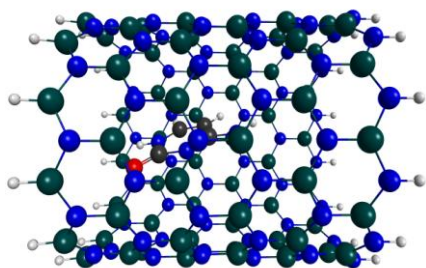
## First Principles Calculations of Organic Molecules Adsorption in Nanostructures

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We investigate the adsorption properties of three amino acids and five nitrogenous bases: glycine, serine, cysteine, adenine, guanine, uracil, thymine and cytosine on the inner surface of boron nitride nanotubes (BNNTs) by first-principles density functional theory calculations. The nanotube that encapsulates the molecules is a zigzag (12,0) BNNT  $B_{72}N_{72}H_{24}$ . Moreover, we study the behavior of the binding energy of these organic molecules with the inner walls of the BNNT, we also calculate the electronic Density of States (DOS) for each optimized structure, and we conclude that there is no bonding or adsorption between the molecules and the nanotube, according to the chemically inert nature of BNNT [1]. This suggest that organic molecules can safely pass through any cavity being protected by BNNTs, and can be useful in medical applications.



*Figure 1. Cytosine encapsulated inside a (12,0) BNNT. Colours for elements are grey (carbon), white (hydrogen), blue (nitrogen), red (oxygen), and green (boron).*

We thank partial support from CONACyT-Mexico (Grants 153930 and 263342).

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## **Effect of Poly(vinyl acetate) Concentration/Nanometric Silica over Mechanical Properties of Coating Hybrids**

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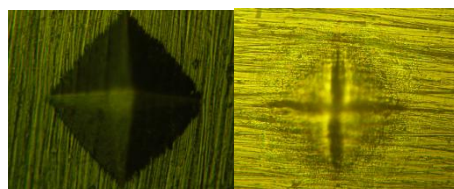
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In recent years, organic–inorganic polymer hybrids with a large variety of functionality have been studied intensively [1]. The combination of the two components at a molecular level would provide novel properties that are hardly obtained from conventional organic or inorganic materials, for instance an enhancement of the mechanical strength of organic polymers such as poly(dimethylsiloxane) with silica particles or a modification of the mechanical properties of silica by introduction of organic polymers into the silica phase [2].

Poly (vinyl acetate) (PVAc) was incorporated into silica gel using the sol-gel process involving tetraethoxysilane (TEOS) [3]. In order to prepare silica-gel nanohybrids, two different concentrations of PVAc were employed and applied to a piece of commercial copper. PVAc in concentrations of 25 and 50% w/w was added to the silica solution. The copper piece was dip coating into that solution and thermally treated at 373 K.

Properties of wear- and scratch resistance and the physical properties of the resulting two sets of nanohybrids were compared. The homogeneity of the polymer hybrids obtained was evaluated by SEM. Hardness properties were determined by using Vickers test at 1000g.

We have succeeded in preparing homogeneous organic–inorganic polymer hybrids by incorporating organic polymers. The effect of PVAc concentration on hardness is studied.



*Figure 1. a) Vickers test for commercial copper (98 HV) and b) Vickers test for copper coating with P50 hybrid (136.9HV).*

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## Microstructure of Alumina-Matrix Functional Graded Materials Reinforced with Nanometric Titanium and TiO<sub>2</sub>, TiC or TiN Dispersions

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The synthesis of alumina (Al<sub>2</sub>O<sub>3</sub>)-functional graded materials having nanometric titanium and TiO<sub>2</sub>, TiC or TiN reinforcement-particles has been explored. Two experimental steps have been set for the synthesis; the first step consisted of the pressureless-sintering of Al<sub>2</sub>O<sub>3</sub>-titanium powders which were thoroughly mixed under high energy planetary-milling and through the second step it was induced the formation of TiO<sub>2</sub>, TiC or TiN, through different thermochemical treatments such as: oxidizing in air, cementation packing process or nitriding in ammonia salts respectively. Scanning electron microscopy and Energy dispersive spectroscopy analysis of the microstructures obtained in both sintered and thermochemical treated bodies were performed in order to know the effect of the used as oxidant, cementing or nitriding agent on the titanium for each studied material. It was observed that a TiO<sub>2</sub>, TiC or TiN layer growth from the surface into the bulk of the sample and reaches different depth depending of the chemical product obtained by the reaction of titanium with oxygen, carbon or nitrogen.

Authors would like to thank to CONACyT, by the support offered for the accomplishment of the research work through Project 132406.

## Immobilization of Lipase Lip2 from *Yarrowia lipolytica* Using Nanoclay Bentonite as a Support

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Nanocatalysis has emerged as a promising area for enzyme technology [1], due to the variety of nanostructures such as nanoporous media, nanofibers, carbon nanotubes and nanoparticles and to their particular physicochemical characteristics resulting especially attractive for enzyme immobilization. Lipases are one of the most used enzymes in organic synthesis. They are one of the most versatile enzymes with applications in food, pharmaceutical, polymers and energy industries [2, 3]. Recently the immobilization of lipases on nanomaterials has been tested with some success [4-6]. In this work, we studied the immobilization of lipase 2 from *Yarrowia lipolytica* on one commercial available and unmodified nanoclay bentonite. Absorption kinetics and some of the properties of the immobilized lipase such as substrate preference and solvent resistance were evaluated. Finally XPS and microscopic characterization were also carried out.

To the Center of Nanosciences and Nanomaterials of the UNAM and the National Laboratory of Researches in Nanoscience and Nanotechnology (LINAN) of the IPICYT for their support to this research and the Project CB-2008-01-104429 for the given financial support.

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## Pd-doped TiO<sub>2</sub> Nanostructured Powders and the Photocatalytic Response on the Degradation of 4-chlorophenol

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In this work, Pd-doped TiO<sub>2</sub> nanostructured powders were obtained by sol gel method and characterized by XRD, Rietveld refinement, TEM, HRTEM, SEM, UV-Vis and RAMAN spectroscopy. Crystal structure, nature and different phases of TiO<sub>2</sub> were modified varying the temperature of the thermal treatment at 400, 500 and 600 °C during 1 h, as well as the concentration of the palladium (up to 5 wt%). The crystallinity of the powders was evaluated by XRD technique revealing the presence of β-TiO<sub>2</sub>, anatase and rutile phases as well as the co-existence of all of them on the different samples. The XRD data was refined by Rietveld analysis obtaining diverse percentages of the TiO<sub>2</sub> phases in each sample; in addition, the crystal sizes were calculated resulting in nanometric order. RAMAN spectroscopy revealed the characteristics bands of the different TiO<sub>2</sub> phases in the ceramics confirming the observed by XRD. TEM and HRTEM were helpful to determine crystal size in order of nanometers (~80 nm) in agreement with the calculated results obtained by Rietveld analysis. UV-Vis spectroscopy revealed a reduction on the band gap value attributed to the combination of phases in the samples. The photocatalytic response was tested on the degradation of 4-chlorophenol (4-CP) in aqueous phase under irradiation at 254 nm. In general, a good removal efficiency was obtained; the best result was using 1wt% Pd/TiO<sub>2</sub> at 400 °C.

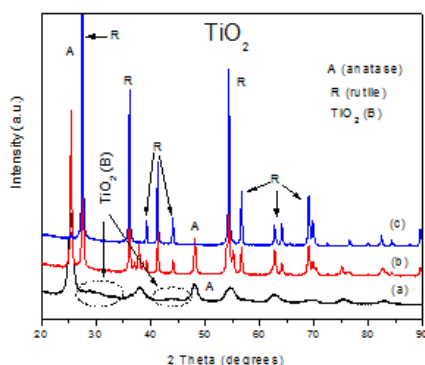


Figure 1. X-ray Diffraction spectra of TiO<sub>2</sub> nanostructured powders at (a) 400 °C (b) 500 °C and (c) 600 °C.

The authors are thankful to Dr. Javier Arturo Montes de Oca Valero (R.I.P.) for his unvalued support on the realization of this research. D. S. García-Zaleta is grateful for his postgraduate fellowship to CONACYT and SIP-IPN. We thank to JEOL and FEI for the support in high resolution microscopy. A special thank to Dr. Ricardo Gomez from UAM-Iztapalapa for his support on the photocatalytic evaluation.

## Nanostructured Materials Characterization of TiO<sub>2</sub>-SnO<sub>2</sub> Synthesized by Sol-gel

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Among a wide variety of nanostructured metal oxides the titanium dioxide (TiO<sub>2</sub>), in anatase phase, is the most widely used in the catalysis field. TiO<sub>2</sub> presents a slow electron-hole recombination, this is the reason why in recent years it has sought modify their properties by the union of other semiconductors or by ion incorporation [1].

In order to improve this property, in the present work were synthesized the TiO<sub>2</sub>-SnO<sub>2</sub> mixed oxides by sol-gel method with different tin content 1, 5, 10 and 15 mol% of TiO<sub>2</sub>. The samples were calcined at 500°C based on the results of thermogravimetric analysis.

X-ray diffraction patterns showed that rutile phase increases as the amount of tin dioxide augment, see Figure 1. BET surface areas of the mixed oxides were higher (73-93 m<sup>2</sup>/g) than pure TiO<sub>2</sub> (62 m<sup>2</sup>/g). As for the width values of bandgap (E<sub>g</sub>) are in the range 3.2-3.05 eV, of so that the tin incorporation affects the E<sub>g</sub> of the TiO<sub>2</sub>. The acidity, determined by FT-IR-pyridine adsorption, of the different TiO<sub>2</sub>-SnO<sub>2</sub> materials is modified by the presence of tin oxide, they are in the range of 154-217 μmol/g, only Lewis sites are present.

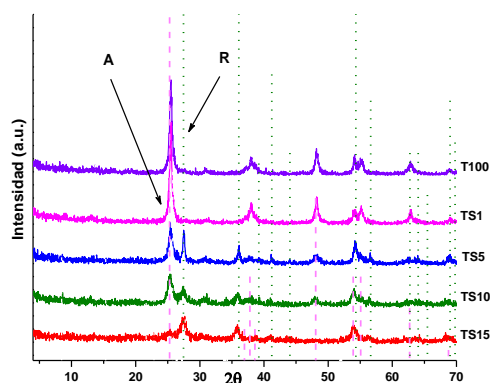


Figure 1. Diffraction patterns TiO<sub>2</sub>-SnO<sub>2</sub> materials, where A is the crystalline phase (anatase) and R (rutile).

Thanks to COMECYT for the scholarship.

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## Análisis por Micro-tomografía de Rayos-X de un Nano-cemento Geopolimérico

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En el presente trabajo se sintetizó un nano-cemento geopolimérico con una velocidad de fraguado y máxima resistencia a 24h [1], el cual al ser un material nuevo es importante conocer su microestructura interna, el acomodo de partículas minerales, grado de compactación, porosidad, entre otras; para determinar su comportamiento macro-estructural. Por lo tanto, utilizando la micro-tomografía de rayos X que es una técnica que proporciona un método no destructivo para analizar la microestructura interna de los materiales de manera tridimensional, la cual nos permite obtener una serie de radiografías de la muestra con una diferente posición angular y mediante la ayuda de un algoritmo matemático basado en el coeficiente de atenuación de los rayos X, es posible reconstruir una imagen 3D con la posición espacial de las diferentes fases que componen el material, [2]. El interés de este trabajo es examinar la microestructura interna de un nano-cemento geopolimérico estándar que está compuesto de 3 fases, nano-pasta geopolimérica, agregados cerámicos y porosidades, con el objetivo de determinar el porcentaje de cada una de ellas, su forma y distribución y por lo tanto determinar si esas características pueden ser mejores que las de un cemento portland típico.

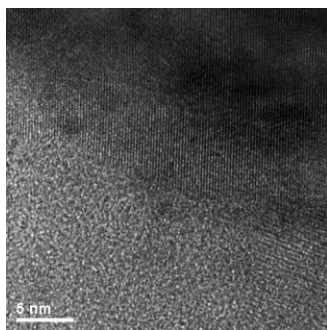


Figura 1. HRTEM de la nano-pasta analizada por microtomografía de rayos X.

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## Structural and Spectroscopic Studies of $\text{Lu}_2\text{O}_3:\text{Eu}^{3+}$ Embedded in $\text{SiO}_2$

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Recently, there is great interest to activate (doped) ceramic oxides with rare earth ions for the development of new optical devices. In this area, the development of new optical devices is closely related to the design, development and manufacture of high quality optical coatings. The  $\text{Lu}_2\text{O}_3$  doped with europium ion ( $\text{Eu}^{3+}$ ) is an excellent candidate due to the luminescent properties conferred by this rare earth. However, Nowadays the technology demands to maintain and/or to improve the properties of the materials in order to reduce the fabrication costs. An alternative has been to incorporate a portion of glass ceramic into the systems to enhance emissive properties as has been achieved with similar matrices ( $\text{Y}_2\text{O}_3:\text{Eu}^{3+}$ ) [1]. Specifically, for certain applications are required luminescent films with thicknesses greater than one micron which is difficult to obtain by conventional methods, for example by sol-gel route the thickness of one layer of the obtained films are commonly less than 50 nm, so that one solution has been incorporating rheological agents that increase them.

In this study, the effect of incorporation of polyvinylpyrrolidone (PVP) and silica ( $\text{SiO}_2$ ) to different precursor solutions for Lu-Si following molar ratios: 4:1, 6:1, 8: 1 and 10:1 were examined. Different systems synthesized by sol-gel and dip-coating technique, were used to produce glass-ceramic films of  $\text{Lu}_2\text{O}_3:\text{Eu}^{3+}$  (5 mol %) @  $\text{SiO}_2$ . For the preparation of glass-ceramic systems were employed as precursors: acetylacetonate lutetium, europium nitrate, tetraethylorthosilicate, methanol and hydrochloric acid. The obtained films had cubic phase, low roughness and homogeneous layers, these results were determined by means of RAMAN, XRD, SEM and AFM techniques. The system containing silica presented an important emission at 611 nm, the results were provided by photoluminescent spectroscopy.

The authors gratefully acknowledge the financial support of SEP-CONACYT (100764, 136269 & 178817) and SIP – IPN (20130665, 20130664) projects.

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## Synthesis of BaTiO<sub>3</sub>:Eu<sup>3+</sup>@SiO<sub>2</sub> Powders from Soft Chemistry Routes

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In recent years, lanthanide-doped ultrafine and nanocrystalline barium titanate materials have been widely investigated due to their interesting optical properties, which make them candidates in different advanced fields, such as phosphors for TV screens optical amplifiers and electroceramic applications. Recently there is an interest to produce rare earth ions doped perovskite base materials as barium titanate powders owing to its promising luminescent properties produced by soft chemical routes. The incorporation of a glassy component on the ceramic system has improved the luminescent properties in similar matrix as Y<sub>2</sub>O<sub>3</sub>:Eu<sup>3+</sup>. In this context, the solvothermal route was selected as promising option to prepare BaTiO<sub>3</sub>:Eu<sup>3+</sup> ceramic powders while the sol-gel method was chosen to elaborate the SiO<sub>2</sub> matrix. As well as, sol-gel method allow obtaining high purity and homogeneity in the synthesized materials. In the present work, the precursors employed for the synthesis of BaTiO<sub>3</sub>:Eu<sup>3+</sup> ceramic powders, were barium chloride (BaCl<sub>2</sub>, 99.9%, Aldrich), Europium (III) nitrate pent hydrate (Eu(NO<sub>3</sub>)<sub>3</sub>•5H<sub>2</sub>O, 99.9% Aldrich), titanium butoxide (Ti[O(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>]<sub>4</sub>, 97%, Fluka). Anhydrous methanol (CH<sub>4</sub>O, 99.8%, Sigma Aldrich) was used as solvent and metal potassium (K, 98%, Aldrich) as mineralizer. The alcoxide base precursors used for the elaboration of SiO<sub>2</sub> glassy sol, were tetraethyl orthosilicate (CH<sub>8</sub>H<sub>2</sub>OO<sub>4</sub>Si, 98%, Aldrich), ethanol (CH<sub>3</sub>CH<sub>2</sub>OH, 99.9% Fermont), hydrochloric acid (HCl, Fermont) and distilled water. In order to improve the luminescent properties of the BaTiO<sub>3</sub>:Eu<sup>3+</sup> ceramic powders, the synthesis of BaTiO<sub>3</sub>:Eu<sup>3+</sup>@SiO<sub>2</sub> glass ceramic powders are proposed in different Ba:Si molar ratio. The effect of SiO<sub>2</sub> (glassy sol-gel matrix) incorporation in BaTiO<sub>3</sub>:Eu<sup>3+</sup> (ceramic hydrothermal matrix) were chemically, structurally and morphologically analyzed by means of FT-IR spectroscopy, X-ray Diffraction and Scanning Electron Microscopy characterization techniques. Two glass BaTiO<sub>3</sub>:Eu<sup>3+</sup>@SiO<sub>2</sub> ceramic systems: Ba:Si=3:97 and 5:95 presented the major 611 nm red emission intensity as demonstrated by photoluminescent studies.

The authors gratefully acknowledge the financial support of SEP-CONACYT (100764, 136269 & 178817) and SIP – IPN (20130665, 20130664) projects.

## Stability Study of Magnetic Nanoparticle Suspensions in Solutions of Chitosan

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Organic-inorganic nanocomposites are of great interest for applications in biomedicine, environmental remediation and catalysis [1], especially when a material like chitosan -used for their properties of biocompatibility- and magnetite -with excellent magnetic properties- are combined [2-3]. This work is focused on the study of the stability of suspensions of ceramic nanoparticles of  $\text{Fe}_3\text{O}_4$  in acid suspensions of chitosan in aqueous medium for obtaining functionalized nanocomposite membranes of chitosan-magnetite. Mixtures of aqueous solutions of chitosan with nanoparticles, modifying the weight ratio chitosan: nanoparticle, 1:2, 1:3 and 1:4, incorporating different dispersants: Polyethylene glycol (PEG), polyethylene imine (PEI) and Pluronic F-127, and varying the ratio in the solution: 0.5, 1, 2, and 3% v/v, were studied by means of the zeta potential technique in order to evaluate the interaction between the particles in suspension. First the nanoparticles were characterized by scanning electron microscopy (SEM), laser diffraction, X-ray diffraction (XRD) and vibrating sample magnetometer (VSM). After that, the suspension was studied by means of potential z, in order to know the stability of the nanoparticles (magnetite) in the chitosan solution using dispersant agents. The results show that the best conditions for the suspension of nanoparticles chitosan solution is when Pluronic F-127 is used as a dispersing agent 1% v / v, with a ratio chitosan: nanoparticles 1:3. We present results of all types and concentration of dispersing agents employed.

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## Synthesis and Characterization of CeO<sub>2</sub>-ZrO<sub>2</sub> Ceramics by Sol-gel Method

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Cerium and zirconium have important mechanical and electrical properties to be applied as an electrolyte for solid oxide fuel cells (SOFC). Introducing zirconia to the cubic structure of ceria increases the ionic oxygen diffusion capacity, in addition many modifications in the defect structure of ceria are able to confer new properties to the material, such as better resistance to sintering at high temperature [2].

In this work some results of synthesis of CeO<sub>2</sub>/ZrO<sub>2</sub> system are presented for the following compositions: 10, 30, 50 and 90 %w of CeO<sub>2</sub> in ZrO<sub>2</sub> by using sol-gel method parting from two distinct precursors: oxide of cerium and zirconium propoxide into isopropanol solution and ammonium hydroxide to obtain pH=12 [1]. The selection of an appropriate precursor, the preparation method, composition, and textural properties, play an important role in the success of these materials in the field of fuel cell technology and catalysis.

After hydrolysis and condensation steps, ceramics were calcined at 1000°C for 2 hours. Structural results of final products are presented as XRD patterns, morphological characterization was made by SEM and the ionic conduction was measured using electrochemical impedance.

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## High Temperature Stability of Anatase in Titania-alumina Semiconductors with Enhanced Photocatalytic Properties

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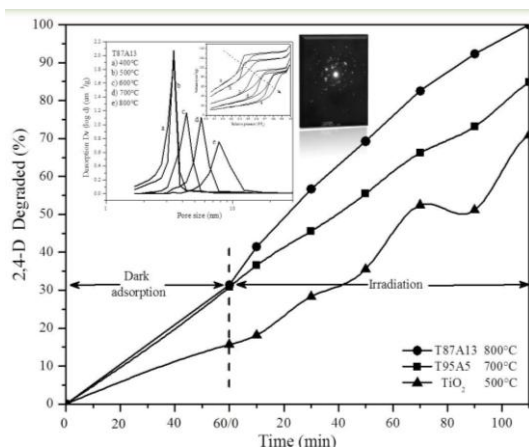
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The photocatalytic reaction efficiency depends on several factors and relation between them. The commonly analyzed parameters are: specific surface area, pore size, energy band gap, crystalline structure and crystallite size. Obtaining a high temperature anatase structure by modified sol-gel method incorporating aluminum acetylacetonate as alumina source allows a comparison of the aforementioned parameters. The incorporation of alumina prevents anatase crystals aggregation with the increase of temperature, reducing



the nucleation sites that form large rutile crystals. The photocatalytic degradation of harmful herbicide indicates that the pore and crystallite size are of principal relevance, indicating a beneficial relationship between the pore and crystallite size of 7 and 29 nm, respectively.

Figure 1. Photocatalytic behavior, pore size distribution and diffraction patterns of titania-alumina nanomaterials.

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## Chemical Functionalization of Carbon Nanotubes and its Effects on Electrical Conductivity

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Carbon nanotubes (CNT) are the focus of extensive research into the multifunctional composite materials science. CNT tend to form aggregates due to the presence of strong van der Waals interactions. This aggregation is not desirable for preparing polymer composites containing CNTs and surface modification of the CNTs is usually required in order to improve the compatibility between CNTs and the polymer matrix. In this work, the chemical surface modification of multiwalled carbon nanotubes (MWNTs) is presented. Three oxidation methods used to functionalize them were: (1) a mixture of concentrated H<sub>2</sub>SO<sub>4</sub> and HNO<sub>3</sub> (3:1, v/v) and ultrasonic agitation for 2 h, (2) the same mixture of H<sub>2</sub>SO<sub>4</sub> and HNO<sub>3</sub> (3:1, v/v) and mechanical agitation for 6 h, and (3) an aqueous HNO<sub>3</sub> (20%, v/v) solution in reflux and mechanical agitation for 6 h. MWNTs were analyzed by Raman spectroscopy showing an increase in the intensity of D band (defect band) as a result of the chemical modification. In addition, they had different grades of functionalization as evidenced by XPS. It was determined that the incorporated groups on the surface of CNT were mainly ether, carbonyl and carboxylic chemical groups in different percentages. Electronic conductivity was evaluated in order to know how far the functionalization affects that important property with respect to the pristine MWNTs. The resistance evaluations were made using a hydraulic press. 100 mg of powdery material was poured into a thick-walled nylon tube (inner diameter ¼") vertically fixed on a heavy support between copper electrodes which moves down in the cylinder, comes and closes the compression chamber. The electrical resistance was measured by LCR Meter Stanford SR720. A dial indicator was used to measure the displacement of the upper electrode. Thus, the length of the compression chamber and electrical conductivity are both determined for each material (oxidation conditions: 1, 2 and 3) and then plotted. The electrical conductivity shows an inverse behavior with the degree of functionalization. For oxidation condition 1 and 2, the electrical conductivity decreases 8.8 and 15.5%, respectively; whereas that oxidation condition 3 it decreases only 1%.

We acknowledge the partial financial support of CONACyT, Mexico, through the grants # 25496.

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## **Bond Strength of Self-etch Adhesive with Silver Nanoparticles to Fluorosed Enamel**

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Antibacterial activity of silver nanoparticles has received considerable attention for the development of new dental adhesives [1]. However, their performance on enamel fluorosed is still unknown. The aim of this study was to evaluate the shear bond strength of a self-etching adhesive with silver nanoparticles in different levels of fluorosis compare to a conventional total-etch adhesive.

The in vitro study was performed on 120 extracted non-cariou human premolars. The teeth were divided into 4 major groups according to severity of fluorosis, using the Tooth Surface Index of Fluorosis, TSIF 0 (n=30), TSIF 1-2 (n=30), TSIF 3-5 (n=30), TSIF 6-7 (n=30). The specimens in each TSIF group were divided into in 3 subgroups: Ex=Excite (n=10) with an etch-and-rinse technique (Ivoclar); Ap=Adper Prompt L-Pop (n=10) with a self-etching technique (3M); Ap-AgNps=Adper Prompt L-Pop with a self-etching technique plus silver nanoparticles (1:1 ratio). The silver nanoparticles were previously characterized.

Composite was bonded according to the manufacturer in acetate molds. The shear bond strength was measured using the Universal Machine at a crosshead speed of 1 mm/minute. The analysis of the failure mode was performed using an optical microscope (Olympus SZ-PT) and the images were analyzed with an image analyzer (Motic Images Plus2.0). The data obtained were analyzed with one-way ANOVA and Tukey test ( $\alpha=0.05$ ).

The higher values were in Ap-AgNps subgroup in the 4 major groups: 22.46±6.8 MPa in TSIF 0; 19.5±4.9 MPa in TSIF 1-2; 17.4±4.3 MPa in TSIF 3-5 and 17.5±6.0 in TSIF 6-7. Apparently the shear bond strength improves with the content of silver nanoparticles in TSIF 3-5 and TSIF 6-7 ( $p<0.05$ ). The predominant failure mode was cohesive.

We want to thank Mirna Ruiz Ramos and Victor Manuel Mendoza Nuñez from Unidad de Investigación en Gerontología FES-Z UNAM for the partial financial support.

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## **Entrapment of Pentoxifylline in Functionalized Solvent-free Sol-gel SiO<sub>2</sub> Nanostructured Matrix**

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Pentoxifylline (PTX), is a xanthine derivative with hemorrheologic properties, that has been useful in the treatment of several diseases. However, conventional routes of administration imply high doses, what is unnecessary to the organism, seriously increasing the risk of toxicity because of side effects. Pentoxifylline has physicochemical and pharmacological properties which make it as a potential candidate for encapsulation into vector systems. Due to its highly hydroxylated surface, sol-gel silica has been a useful material in matrix diffusion controlled systems. We prepared solvent-free SiO<sub>2</sub> material by the sol-gel process using acetic acid and an alkoxide/water ratio ( $R_w$ ) = 1/16. In order to determine surface functionalization, spectroscopic characterization was carried out by means of Infrared ATR and UV-Visible spectroscopies, and the effect of PTX inclusion on silica spectra was observed. SEM and EDS analyses were carried out to study the morphology and composition of the silica particles. Microporosity of the samples was confirmed by physisorption analysis and BET surface area values were 365 and 462 m<sup>2</sup>/g for silica and PTX-SiO<sub>2</sub>, respectively. Thermal studies showed the incorporation of the drug in SiO<sub>2</sub> due to the additional presence of an endothermic peak corresponding to drug decomposition. Finally, in vitro release was studied following the increase of the main UV absorption band of PTX at 274 nm. The silica matrix released about 40% of the drug during first 24 hours, and the release rate decreases later.

## Catalytic Activity of Cu, Ag and Au Nanoparticles for Diesel Soot Oxidation

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It is widely accepted that soot particles emitted by diesel engines act as carriers for a number of harmful soluble organic substances (SOF) adsorbed on the soot particles, and long term exposure to fine particulate matter is a proven risk factor for respiratory and cardiovascular diseases. Nowadays, soot emissions can be reduced by diesel particulate filters. The trapped soot in the filters has to be removed by combustion. A catalyzed soot oxidation is the way to decrease the soot burn-off temperature in a controlled fashion, increasing the overall fuel efficiency of the diesel engine [1]. The electron transfer from metal to O<sub>2</sub> is a key factor for the chemisorption of oxygen on a metal surface. In this study, we investigate the effect of the electron donating abilities of IB group metal nanoparticles like Cu, Ag, and Au, deposited over SiO<sub>2</sub> on the diesel soot oxidation process. UV-Vis absorption spectroscopy has been utilized to determine the oxidation state of the catalysts. The diesel soot oxidation on Ag/SiO<sub>2</sub> was shown to be strongly promoted by the presence of metallic silver probably due to the promotion of the formation and stabilization of the superoxide ion O<sub>2</sub><sup>-</sup>. Results showed that on Cu/SiO<sub>2</sub> catalysts, the lifetime of the superoxide species on metallic Cu may be too short to react with diesel soot, while on Au/SiO<sub>2</sub>, the superoxide species does not exist because molecular adsorption of O<sub>2</sub> does not occur due to the difficulty of the electron transfer from the metallic Au nanoparticles. The reaction mechanism for the complete diesel soot oxidation may be due to the interaction between the superoxide and the allylic C-H bond present in the organic soluble compounds (SOF) adsorbed on the diesel soot particles.

The authors are pleased to acknowledge valuable support for this research from Vicerrectoria de Investigación y Estudios de Posgrado (BUAP), Grant # 36/NAT/12.

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## ZnO/CuO/SiO<sub>2</sub> for Phenol Photodegradation Using Sunlight as Radiation Source and Air

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Application of the photocatalytic method for the destructive removal of aqueous pollutants has been extensively studied [1]. In this investigation, we have prepared a ZnO/CuO/SiO<sub>2</sub> catalyst, which is of semiconducting nature, having an intense absorption band in the UV-Vis region (200 - 800 nm), suggesting its utilization for photocatalytic degradation of aqueous phenol. The sunlight was utilized as UV-Vis radiation source to expose the reaction mixture (Figure 1). Ambient air from a compressor was fed into the reactor at the rate of 0.5 L·min<sup>-1</sup>. The oxygen in the air flow is used as oxidant for the phenol degradation. The reactors were exposed to solar irradiation from 9:00 h to 16:00 h during 30 days. On average, the intensity of the exposed solar radiation was about 1000 W·m<sup>-2</sup>. After these 30 days exposure. The photocatalytic process in the presence of our catalyst is shown to be quantitatively more efficient in the degradation of phenol than in the presence of ZnO/SiO<sub>2</sub> or CuO/SiO<sub>2</sub>.



Figure 1. Schematic layout of the photoreactor used for the photocatalytic phenol degradation. 1: Air compressor; 2: Mass flow controller; 3: Phenol, water, and catalyst mixture; 4: Thermometer; 5: Air outlet; 6: Solar radiation exposure.

The authors are pleased to acknowledge valuable support for this research from Vicerrectoria de Investigación y Estudios de Posgrado (BUAP), Grant # 36/NAT/12.

[1] C.S. Uyguner, M. Bekbolet. Water. Sci. Technol. 61 (2010)2581-2590.

**Negative Thermal Diffusivity Enhancement in Semiconductor Nanofluids**

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Colloidal suspensions of semiconductor InP@ZnS nanoparticles were prepared using single-step procedure without precursor injection. Thermal properties of toluene containing InP@ZnS semiconductor of different sizes (3.1, 4.2, and 4.6 nm) were measured by mode mismatched dual beam thermal lens technique. This was done in order to measure the effect of the presence of semiconductor nanoparticles and their sizes on the nanofluid's thermal diffusivity. The characteristic time constant of the transient thermal lens was estimated by fitting the experimental data to the theoretical expression for transient thermal lens. The thermal diffusivity of the nanofluids (toluene, containing InP@ZnS semiconductor nanoparticles) seems to be strongly dependent on the presence of semiconductor nanoparticles and their particles size. For the case of nanofluids consisting of InP@ZnS nanoparticles dispersed in toluene, it was observed a decrease in the thermal diffusivity. Such behavior differs from other nanofluids, in the sense that they had shown positive thermal diffusivity enhancement. The minimum diffusivity was achieved for the nanoparticles with smallest particle size. Plausible explanation for such low thermal diffusivity of the nanofluids with semiconductor nanoparticles is given. UV-Vis spectroscopy, TEM and high-resolution electron microscopy (HRTEM), and energy dispersive spectroscopy (EDS) techniques were used to characterize the InP@ZnS nanoparticles.

The authors are thankful to the Mexican Agencies, ICyTDF, CONACYT, COFAA-IPN, SIP-IPN for financial supports.

## Ferromagnetic Resonance Study and Magnetic Properties of Sputtered CoFeMoSiB/Au/CoFeMoSiB Trilayer

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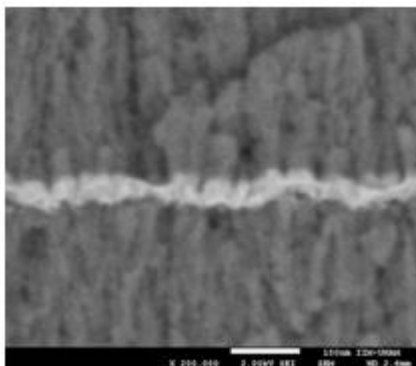
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In this work, the magnetic properties and the ferromagnetic resonance of CoFeMoSiB/Au/CoFeMoSiB trilayer are studied. The trilayers were constituted by two ferromagnetic layers separated by a nonmagnetic metal such as Au. The trilayers were deposited on a glass substrate by magnetron sputtering, using a target made up of amorphous ribbons of nominal composition  $\text{Co}_{67}\text{Fe}_4\text{B}_{11}\text{Si}_{17}\text{Mo}$ , with thicknesses of 300 nm and 130 nm for ferromagnetic layer and Au layer, respectively. As-deposited trilayer samples exhibit a perpendicular anisotropy, which can be ascribed to the preparation technique, the coupling of quenched-in internal stresses and the interface between both ferromagnetic and Au layers.

Structural measurements indicate an amorphous stage on ferromagnetic layer, as can be seen in the scanning electron micrograph of a trilayer presented in figure 1.

Magnetic properties have been investigated by employing a vibrating sample magnetometer (VSM). FMR spectra showed two distinct resonances absorptions, and



which are due to different contributions of magnetic anisotropy. The role of the magnetic anisotropy is thoroughly discussed with help of magnetic and ferromagnetic resonance measurements.

Figure 1: Typical SEM micrograph of a CoFeMoSiB/Au/CoFeMoSiB trilayer.

We acknowledge the financial supports of PAPIIT-UNAM No. IN111111.

## Characterization of Nanostructured TiSiNO Coatings Prepared by DC and RF Sputtering

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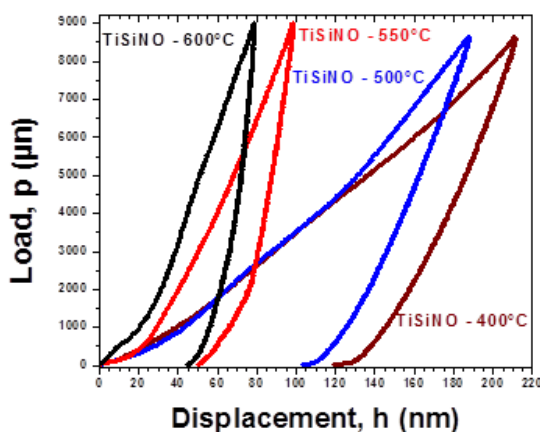
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The effects of substrate temperature on the mechanical properties, resistivity, structure and chemical composition of Nanostructured TiSiNO coatings prepared by DC and RF magnetron reactive sputtering have been investigated. The properties of the coatings have been analyzed through nanoindentation test (Figure 1), high resistivity measurement, X-ray diffraction, Raman measurements and EDS. The results showed that the increment in the substrate temperature favors hardness and Young modulus, and diminished the electrical resistivity. The TiN phase was identified showing (111), (200) and weak (220) textures and weak TiO phase is observed. According to these results, harder TiSiNO coatings (27.31 GPa) have smaller crystalline grain size (8.3 nm), minor value of electrical resistivity ( $1.06 \times 10^3 \mu\Omega\text{-cm}$ ) and the larger roughness (1.67 nm).



*Figure 1. Representative Load vs Depth curves obtained in the present study.*

This work was supported by CONACyT by means of project 58653.

## Novel Material Based on Sol-gel Al<sub>2</sub>O<sub>3</sub> Doped with Ce<sub>2</sub>O<sub>3</sub> as Photocatalyst for Phenol Photodegradation

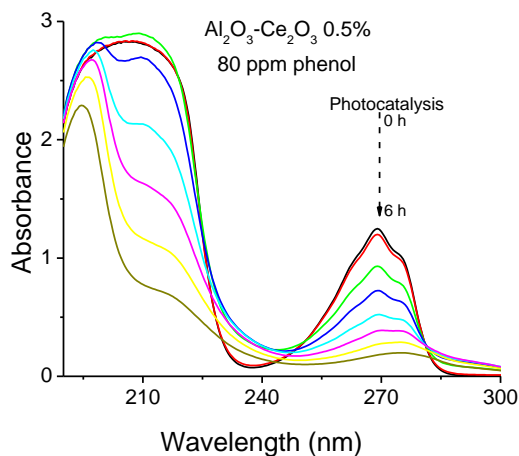
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Al<sub>2</sub>O<sub>3</sub> and Al<sub>2</sub>O<sub>3</sub>:Ce<sub>2</sub>O<sub>3</sub> (95.5:0.5, 99.0:1.0, 97.0:3.0 and 95:5.0 %w/w) nanomaterials were obtained by using sol-gel method. After calcination at 500°C/12h, the obtained materials were characterized by X-Ray diffraction (DRX), N<sub>2</sub> adsorption-desorption measurements, UV-Vis and IR spectroscopy techniques. The photocatalytic activity of these materials was evaluated in the photodegradation of phenol in aqueous phase. The results obtained show a total mineralization of phenol molecule measured by the Total Organic Carbon analysis (see Figure 1).



*Figure 1. Behavior during the photodegradation of phenol ( 80 ppm) with Al<sub>2</sub>O<sub>3</sub>-Ce<sub>2</sub>O<sub>3</sub> 0.5% catalyst*

The authors are grateful to CONACyT for the financial support to develop this research work (Projects 12411668). Guadalupe Mendoza thanks to CONACyT for the scholarship granted (Scholarship number: 252087).

**Gold Coated Magnetite Nanoparticles: Synthesis and Characterization**

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Magnetite nanoparticles (Fe<sub>3</sub>O<sub>4</sub>) are considered to be paradigm for Magnetic Hyperthermia and when conjugated with Gold nanoparticles (AuNP), exhibit Plasmonic therapeutic activity. This dual property of Hyperthermia and Photothermal therapy, can well be exploited for cancer therapeutics. Magnetite nanoparticles were initially prepared by chemical precipitation method using precursors such as FeCl<sub>2</sub> and FeCl<sub>3</sub> in the alkaline environment created by ammonia [1].



These particles were then used as nucleation centers for gold nanoparticle synthesis by dispersion of these particles in gold precursor (HAuCl<sub>4</sub>) and citrate reduction.



Such Gold-coated magnetic nanoparticles were characterized using Scanning Electron Microscope (SEM) and micrographs show monodisperse particles of size around 20nm. X-ray diffraction (XRD) was performed to confirm the crystallographic structures at 2θ values of 38.14°, 44.36° and 64.58° which correspond to the Au-Fe crystallographic planes of (111), (200) and (220) respectively [2]. FT-IR and Raman spectroscopy were also used to confirm the magnetite and Au coating on the Fe<sub>3</sub>O<sub>4</sub> nanoparticles. Transmission Electron Micrographs (TEM) appeared brighter due to gold coating on magnetite as compared with bare magnetite [3]. This core-shell formation is further staunchly proved with the aid of Magnetic Force Microscopy (MFM) and Scanning Transmission Electron Microscopy (STEM). We aim to extend the application of these nanoparticles for the diagnosis of cancer.

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## Synthesis of Europium(III)-doped Hydroxyapatite Nanostructures

### Prepared by Microwave Irradiation

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Hydroxyapatite (HAp),  $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ , is a bioceramic which conforms 65% of human bone. This material possess a hexagonal structure with unit cell parameters of  $a = b = 9.41 \text{ \AA}$  and  $c = 6.88 \text{ \AA}$  [1]. Several authors propose HAp for being used in maxillofacial and orthopedic prosthesis due to its biocompatibility, bioactivity, osteoconductivity, no toxicity and no immunogenicity [3]. Nevertheless, HAp presents fragility, low tensile strength and low impact resistance which limit its implementation in high performance applications [4]. Fortunately this undesirable mechanical properties can be enhanced with monodimensional (1D) nanomaterials such as nanorods [5].

This work reports the preparation of nano-HAp with  $\text{Eu}^{3+}$  impurities using microwave irradiation. The resultant white luminescent powders are characterized by SEM, FT-IR, AFM, XRD, Raman spectroscopy, UV-Vis and EDS to determine composition, cristallinity, optical properties and morphology. The acquired X-ray diffraction spectrum confirms high crystalline HAp in comparison with the untreated material. Furthermore, AFM and SEM studies show values about 30- 60 nm in the range of nanoscale diameters, corresponding to nanorod structure. On the same way, FT-IR spectroscopy ratified HAp typical composition and the  $\text{Eu}^{3+}$  presence is confirmed by EDS. At this moment, optical properties are being determined.

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## Effect of Substrate Treatment and Laser Irradiation on Formation Zinc Oxide Nanostructures on Porous Silicon Substrate

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In this work we report the laser induced structural modifications in zinc oxide and electrochemically etched nanostructured porous silicon composites. Effect of substrate and post deposition treatment has been studied. High power green laser was used to produce the laser-induced modifications. Depending on the substrate treatment, changes in the structural properties were seen in the form of different type of micromorphologies (Fig. 1) developed on the surface and were studied with the help of scanning electron microscope (SEM), atomic force microscopy (AFM) and X-ray diffraction. Optical characterization was performed to identify the luminescent properties of the composite.

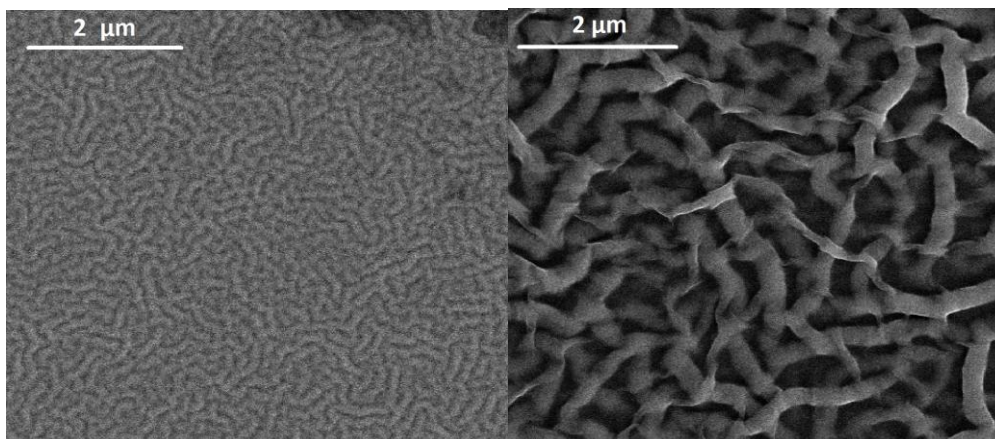


Figure 1. Labyrinth patterns formed on the nanostructured silicon (a) as etched (b) Oxidized substrate.

## **Influence of Cooling Rate Conditions on Mechanical Properties of Al-Mg-Si Alloy**

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The cooling rate effect is a combination key to modify the mechanical properties in an experimental trimetallic alloy. The Al-Mg-Si system solidified under various cooling conditions has been investigated. The material was made by as-cast technique, and was poured into a wedge shaped copper mold. The mold was cooled with liquid nitrogen, in order to get a higher cooling rate. The influence of high cooling rate was compared with a cooling rate from a silica-sand mold. The results showed an improvement in mechanical properties such as hardness; yield tension stress, and ultimate tension stress at high cooling rate.

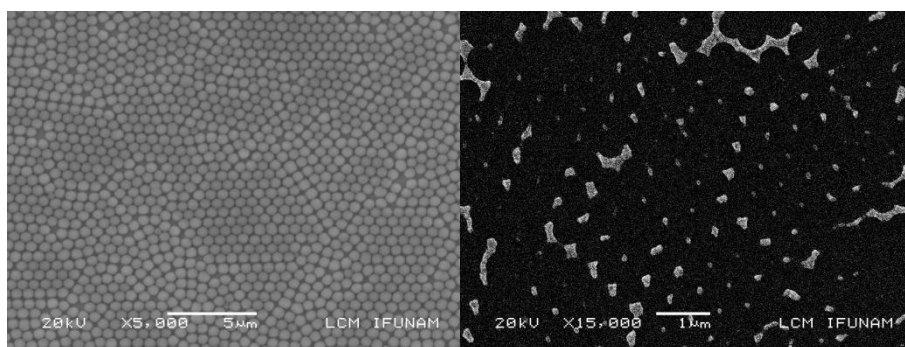
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## Characterization of Ordered Metallic Nanostructures Created through a Mask of Colloidal Silica Particles

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Colloidal silica particles are being intensively studied due to their potential applications in catalysis, intelligent materials, optoelectronic devices, photonic bandgap crystals, masks for lithographic nanopatterning, etc. Moreover, in nanoscale electronic and photonic devices, feature dimensions shrink towards a critical limit, and new experimental approaches have to be explored in lithographic patterning. For this work, spherical submicrometer-sized silica particles were prepared by the Stöber method and deposited as a monolayer onto SiO<sub>2</sub> wafers by means of a spin coater system. This sample is then used as a mask to create regular arrays of nanoscale surface features, such as Ag metallic deposits. After MeV irradiation with Si ions, the spherical silica particles turned into oblate particles, as a result of the increase of the particle dimension perpendicular to the ion beam and the decrease in the parallel direction. These ion beam modified masks were used to tailor the size and shape of the silica monolayer as a function of the ion fluence. By this way, the mask openings of the monolayer were modified and a subsequent evaporation of an Ag thin film allowed the formation of ordered arrays of Ag features, after removal of the silica particles. The same kind of silica mask can be used to create embedded Ag nanostructures by means of ion implantation using our Pelletron accelerator. The size, size distribution and shape of both the silica particles and the array of metallic deposits were determined by scanning electron microscopy and atomic force microscopy. Also, the surface plasmon resonance due to the ordered arrays of metallic nanostructures was studied by optical absorption.



Silica monolayer

Ordered Ag nanostructures

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## DFT Studies of the Phenol Adsorption on Boron Nitride Sheets

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We perform first principles total energy calculations to investigate the atomic structures of the adsorption of phenol (C<sub>6</sub>H<sub>5</sub>OH) on hexagonal boron nitride (BN) sheets. Calculations are done within the density functional theory as implemented in the DMOL code. Electron-ion interactions are modeled according to the local-spin-density-approximation (LSDA) method with the Perdew-Wang parametrization. Our studies take into account the hexagonal h-BN sheets and the modified d-BN sheets caused by the defects. The d-BN sheets are composed of one hexagon, three pentagons and three heptagons. Five different atomic structures are investigated: parallel to the sheet, perpendicular to the sheet at the B site, perpendicular to the sheet at the N site, perpendicular to the central hexagon and perpendicular to the B-N bond (bridge site). To determine the structural stability we apply the criteria of minimum energy and vibration frequency. After the structural relaxation, phenol molecules are adsorbed on both h-BN and d-BN sheets. Results of the binding energies indicate that phenol is chemisorbed. The polarity of the system increases as a consequence of the defects which induces transformation from an ionic to covalent bonding. The elastic properties on the BN structure present similar behavior to those reported in the literature for graphene.

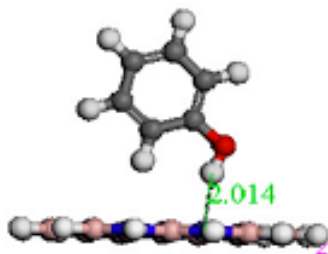


Figure 1. Adsorption of a phenol molecule on a boron nitride sheet.

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## **Análisis GGA-DFT de Nanohojas de Nitruro de Boro Funcionalizadas con Grupos Hidroxilo y Tiol**

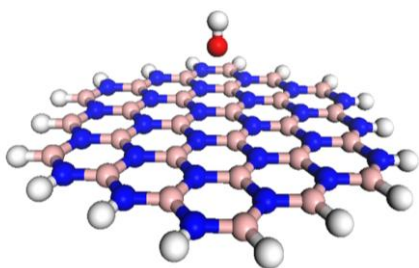
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Mediante la teoría del funcional de la densidad (DFT) se realiza un análisis de las propiedades estructurales y electrónicas de nanohojas de nitruro de boro hexagonal (hBN) debido a la interacción de su superficie y extremos con los grupos funcionales hidroxilo (-OH) y tiol (-SH). Para dicho análisis se usó una función de base con doble polarización y el funcional de intercambio-correlación de Hamprecht-Cohen-Tozer-Handy en la aproximación del gradiente generalizado (HCTH-GGA). Para la búsqueda de geometría óptima de los sistemas hBN-OH y hBN-SH se consideró el criterio de mínima energía analizando 14 posiciones geométricas posibles en cada sistema. Los resultados de la simulación indican que para ambos grupos el sitio preferencial de interacción se obtiene sobre la superficie, es decir, localizado arriba del hexágono central del sistema. Esto está en concordancia con lo ocurrido para nanotubos de BN interaccionando con los mismos grupos funcionales [1]. Además, se observa una disminución del gap HOMO-LUMO y se presenta alta polaridad, indicándonos su posible solubilidad. La función de trabajo sufre

una reducción para el caso hBN-SH indicando que el sistema pudiera ser un buen candidato para el diseño de dispositivos optoelectrónicos.



*Figura 1. Nanohoja de nitruro de boro funcionalizada con un grupo hidroxilo.*

Se agradece al proyecto VIEP-BUAP (CHAE-ING13-G) el apoyo otorgado para la realización del presente trabajo.

[1] E. Chigo Anota, Gregorio H. Cocolletzi, Accepted in J. Mol. Model. (2013)

## Nanopartículas Poliméricas Cargadas con Clorhexidina y su Evaluación Antimicrobiana

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La clorhexidina es un fármaco antiséptico derivado del clorofenilbiguanido, considerada como principal agente antimicrobiano oral. Su aplicación en el área Odontológica ha mostrado una deficiente sustentividad del fármaco en el área subgingival, reduciendo su acción antimicrobiana. Dentro de las modalidades de liberación sostenida de fármacos, las nanopartículas poliméricas (NPs) son sistemas coloidales constituidos por partículas con un tamaño alrededor de 150 nm, las cuales pueden actuar como agentes acarreadores de fármacos, potencializando su liberación en sitios de difícil acceso y permitiendo una mayor sustentividad del activo en el sitio blanco. El objetivo de presente trabajo es evaluar la incorporación de la clorhexidina en nanopartículas poliméricas y su liberación mostrando actividad antimicrobiana contra patógenos orales. Las NPs fueron preparadas a base de Eudragit<sup>®</sup> E 100 mediante la técnica de nanoprecipitación. Se desarrolló una formulación que se caracterizó en base a su tamaño y porcentaje de encapsulación de clorhexidina en las partículas, se purificó a presión reducida y se esterilizó mediante filtración. Posteriormente, se evaluó su actividad biológica contra *Streptococcus mutans*, por macrodilución empleándose NPs blanco y clorhexidina sin encapsularal 0.12% p/v, como controles. Se obtuvieron NPs con una distribución de tamaño promedio de 156 nm, con un índice de polidispersidad de 0.09, una eficiencia de encapsulación del 85% y un porcentaje de encapsulación del 25%. Las NPs con clorhexidina mostraron una actividad potencializadora sobre *S. mutans* al evaluarse de 24-72h. El presente trabajo muestra la incorporación de fármacos en nanopartículas poliméricas, pueden funcionar como potenciales acarreadores para su liberación prolongada y sustentividad del activo en el sitio de acción.

OERL agradece a CONACyT por el apoyo otorgado, a través de la beca 256972.

**Effect of Surface Electric Field on GaAs/AlGaAs Heterostructures with Double-2DEG Studied by Photoreflectance Spectroscopy**

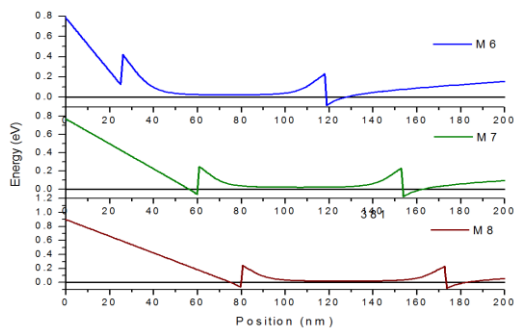
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In this work we report the characterization of GaAs/AlGaAs heterostructures with double two-dimensional electron gas (D-2DEG) by room temperature photoreflectance spectroscopy. In order to study the surface effects on the conduction band profile, GaAs/AlGaAs heterostructures were grown by molecular beam epitaxy with a GaAs cap layer of 25, 60 and 80 nm thickness. Two more samples with a cap layer of 1 and 2 silicon monolayers were grown. Photoreflectance spectra show Franz-Keldysh oscillations between 1.42 and 1.7 eV originated by the surface electric field. Analyzing these oscillations it was found that there is a surface charge density that varies from  $3.64 \times 10^{12}$  to  $8.68 \times 10^{11}$  e/cm<sup>2</sup> for the increment in the thickness of the cap layer, originated by the reduction of the depletion zone near to the surface. When the samples were capped with Si the surface electric field decreased from  $3.64$  to  $1.26 \times 10^{12}$  e/cm<sup>2</sup>. The calculated



conduction band profile show a D-2DEG system only for samples with cap layer of 60 and 80 nm.

Figure 1: Conduction band profile heterostructures with 25 nm (M6), 60 nm (M7) and 80nm (M8).

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## **Dependence of Porosity and Annealing Temperature on the Optical and Structural Properties of Tungsten Oxide Coated Nanostructured Silicon**

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In this work optical and structural properties of electrochromic tungsten oxide electrodeposited on porous silicon (PS) were investigated. Thin tungsten oxide films were obtained anodically on nanostructured mesoporous silicon substrate from a water/isopropanol solution containing peroxy-tungstates species. The characterization of WO<sub>3</sub>/PS structures was done as a function of annealing temperature and substrate porosity by using scanning electron microscopy (SEM), Fourier transformation infrared (FTIR), X-ray diffraction (XRD), and photoluminescence (PL) spectroscopy. With an increase in annealing temperature, evolution of PL peak corresponding to band edge emission (380 and 443nm) of WO<sub>3</sub> is observed. Apart from the emission corresponding to WO<sub>3</sub>, porosity of the silicon substrate and annealing temperature have been found useful for tuning emission of the composite structure within 300 nm of visible range. This opens a relatively economical route to produce composites for display applications.

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**Scandium Nitride Thin Film Formation on the GaN(000-1)-2x2 Surface**

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We have performed first principles total energy calculations to study structural and electronic properties of ScN thin film formation on the GaN(000-1)-2x2 surface. Calculations are based on the density functional theory (DFT), as implemented in the PWscf code of the Quantum ESPRESSO package. The electro-ion interactions are treated within the pseudopotential Vanderbilt method; exchange and correlation energies are modeled according to the generalized gradient approximation (GGA), with the Perdew-Burke-Ernzeroff (PBE) parameterization. The electron wave functions are expanded in plane waves with a kinetic-energy cutoff equal to 30 Ry, and for the charge density we have used  $E_{\text{cutoff}}=240$  Ry. A Monkhorst-Pack k-grid of 3x3x1 has been applied. To deal with the surface we have invoked the supercell method. The scandium absorption was studied at high symmetry sites: T4 (hcp), H3 (hollow), Top and B (bridge), considering different coverage. Results show that under N-rich conditions the formation of ScN bilayer on the ad-layer terminated GaN surface is energetically favorable, while in Ga-rich conditions the formation of ScN bilayer underneath of Ga monolayer is the most favorable structure. We present the density of states and projected density of states for the most stable reconstructions to explain the electronic structure.

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## **Análisis de la Capacidad de Adsorción de Compuestos Orgánicos Volátiles en Óxidos Mixtos de Al-Ce-Zr**

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El interés por mejorar la calidad del aire debido a la contaminación atmosférica por compuestos orgánicos volátiles ha llevado al uso exitoso del método de descontaminación por adsorción [1]. Trabajando con óxidos que presentan cualidades necesarias para este tipo de procesos, se utilizaron en esta investigación siete diferentes combinaciones de óxidos de Aluminio, Cerio y Zirconio para evaluar su adsorción mediante cromatografía de gases con benceno, tolueno y p-xileno, en un intervalo de temperaturas entre 200 y 250 °C. Las características de los siete óxidos fueron evaluadas por difracción de Rayos-X, microscopía electrónica de barrido y adsorción de nitrógeno a su temperatura de ebullición. Observándose que, los materiales obtenidos son amorfos, con áreas superficiales alrededor de 200 m<sup>2</sup>/g para las combinaciones de óxidos de Al-Ce-Zr, y menores a 40 m<sup>2</sup>/g para las que contienen sólo Ce-Zr. También es notable la distribución de tamaño de poro unimodal para las primeras y bi y tri-modal para las últimas. La adsorción de los BTX (benceno, tolueno, y xilenos) fue favorable para las combinaciones de óxidos de Al-Ce-Zr, y no favorable para las de Ce-Zr, mostrando una menor capacidad de adsorción y algunas de sus isotermas presentaron forma cóncava. En la mayoría de los casos la mejor temperatura de adsorción fue la de 200 °C.

El método para calcular los calores isotéricos de adsorción fue a partir de pares de isotermas de adsorción en un intervalo de temperaturas y la ecuación de Clausius-Clapeyron. Encontrándose superficies homogéneas y heterogéneas energéticamente hablando, dependiendo de la composición química de las muestras y del adsorbato.

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## Evaluation of the Fractal Dimension for the Quantification of Polyvinylpyrrolidone Fibers by Electrospinning

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The development of this new technology has fostered the creation and exploitation of materials with different properties known so far. One such material is nanofibers whose physical and chemical properties are most different from other forms of nanostructures and existing materials in bulk and atomic scale. The polymeric nanofibers are currently of great importance due to its great potential for applications in catalysis, biology and in industries such as pharmaceuticals, cosmetics, and textiles. The electrospinning technique is a unique method for making continuous fibers with nanoscale diameters and involves the application of high voltage between a container of polymer solution and a collector where the fibers are deposited. Although nanofibers of polyvinylpyrrolidone (PVP) have been produced by the electrospinning method, it is not easy to quantify the amount of spun fibers into a single fiber deposited by this technique. The estimation of the fractal dimension (D) for the quantification of fiber density analysis is an alternative, where fractality values indicate the abundance of fibers on a surface. SEM images of as-synthesized nanoscale fibers were analyzed by the method BCM (Box Counting Method) by acquiring the Hurst exponent (H), then its fractal dimension was determined by using Fractal 3e program. The fractal dimension values which range between 1.602 and 1.753, correspond to the images that have qualitatively lower and higher abundance respectively. In conclusion this methodology indicates that SEM is a new tool for the quantitative estimation of surfaces using fractal dimension, since images of SEM and D results are consistent.

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## Synthesis of Titanium Dioxide Nanotubes by Microwave Radiation Method

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We present the synthesis of Titania nanotubes by Hydrothermal method aid by microwaves, from a sodium hydroxide solution (10 molar concentration) combined with nanoparticles of commercial Titania from Sigma-Aldrich company (P25). To obtain the nanotubes, is necessary to irradiate at certain temperature, which can vary from 190 to 230 °C, and heating the sample with the use of a ramp between 20 to 60 minutes to achieve a maximum temperature and so avoid the destruction of the Titania's crystalline structure, and to prevent the formation of sodium titanate crystalline structure inside the nanotubes. After reaching the maximum temperature, the sample is heated for less than 120 minutes to avoid the destruction of the nanotubes. The obtained nanotubes had an average length from 100 nm to 1000 nm. Those nanotubes were characterized by SEM, EDS, XRD, AFM and UV-Vis.

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## CO<sub>2</sub> Adsorption on Nanoporous Na-erionite

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Adsorption processes are now a valuable option to remove certain types of fluid contaminants from gas streams [1]. In many industrial applications that have pores of solids near the molecular dimensions (pores with diameters less than 2 nm) are used as selective adsorbents because they display physicochemical specificity in contrast to most common mesoporous adsorbents. The zeolites may be used as selective adsorbents in gas separation processes, such as adsorption based on fluctuations of pressure and temperature, known processes such as PSA and TSA [2]. Various studies indicate that CO<sub>2</sub> is strongly adsorbed by a variety of zeolites, suggesting that these materials can play a crucial role in CO<sub>2</sub> capture technologies. In particular, recent studies have demonstrated the selective adsorption of CO<sub>2</sub> regard to H<sub>2</sub> and N<sub>2</sub> in 13X and 4A zeolites showing that these zeolites selectively adsorb CO<sub>2</sub> at room temperature [3]. However, natural zeolites from Mexico have been used as adsorbents for selectively adsorbing this potential gas under conditions similar to those reported when synthetic zeolites are used, specific cases are reported using ERI, HEU and MOR zeolites. The exchanged zeolites have better chemical properties and pore volume, excellent hydrothermal stability and good catalytic activity. The modifications of zeolites are performed by ion exchange to produce modified zeolites. Vacancies or pores created by the removal of the Al atoms are occupied by tetracoordinated Si atoms from other parts of the zeolite, and in some cases the structure may collapse. The goal of the present work is to study and compare the experimental results obtained from the CO<sub>2</sub> adsorption by Na-erionite zeolites using dynamic method to establish the order of selectivity of the zeolites to this gas under study.

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## Effect of Al Content on the Texture of Mixed Oxides Derived from Layered Double Hydroxides (LDH) and their CO<sub>2</sub> Sorption

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The use of fossil fuels supplies ~90% of world energy needs; however, the combustion of these contributes greatly to an increasing atmospheric concentration of CO<sub>2</sub>, which is considered one of the most responsible for the existence of global warming effect. CO<sub>2</sub> capture and storage (CCS) [1,2] is an alternative to reduce the vast amount of CO<sub>2</sub> released into the atmosphere. Layer double hydroxides (LDH) have lower sorption capacity than some other sorbents. However, the sorption capacity of these materials is significantly higher after thermal decomposition when they are transformed into their basic mixed oxides [3,4].

Magnesium - aluminum oxides derived from heat treatment of LDHs were tested on the sorption of CO<sub>2</sub>. In this work it is presented a detailed study of the synthesis of LDHs, their thermal decomposition and their effect on CO<sub>2</sub> capture. LDHs compounds were obtained by the coprecipitation method. The LDHs were characterized by XRD, FTIR, EDS-SEM, TGA and N<sub>2</sub> adsorption.

Pure phases of Hydrotalcite-like compounds were obtained with different Al content. The LDHs were calcined at 500 °C during 4h and it was observed that the surface area was higher in the mixed oxides. The surface area and the capture capacity of CO<sub>2</sub> increased as a function of Al concentration and temperature.

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**Deposition and Characterization of ZnO Thin Films by Evaporation**

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In the last decades has been increasing the interest in materials at nanoscale due the different potential applications and the present effects at this dimension. We present a new method to deposit ZnO thin films using as target nanoparticles, obtained from colloidal solution. The thin films were deposited from evaporation method at different times of deposition; these times of deposition were chosen in order to observe thicknesses from 75 nm to 135. By SEM was observed that the deposition of the thin films depends directly on time. Also de XRD pattern shows the intensity of the 002 plane is predominant and the others planes intensity starts to decrease. Also the UV-Vis results show when deposition time increases the porosity of the films decreases.



## **Annealing Effects on Different Atmospheres on Structural, Morphological and Electrical Properties of ZnO Thin Films**

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ZnO films were obtained by the sol-gel method utilizing zinc acetate dihydrate as the precursor of the Zn atom, monoethanolamine (MEA) as a stabilizing agent and 2-methoxyethanol as a solvent. The ZnO films were deposited on p-Si substrates via the spin-coating technique. The gel film was stabilized by pre-heating at 300 °C. This procedure was repeated 10 times. There after the films were crystallized by an annealing at 600 °C in Oxygen and Nitrogen atmospheres. The X-ray diffraction patterns have shown that all the films have (002) preferential orientation. The structural properties of the ZnO films depend on the annealing temperature and the atmosphere type. The surface morphology level of the films was examined by a scanning electron microscope (SEM). Carrier concentration, mobility and resistivity were obtained by means of the Hall effect measurements. Finally, all three techniques showed that the structural, morphology and electrical properties have correlation with the annealing atmosphere.

## Hydrothermal Synthesis and Characterization of Nanosize GaN Particles

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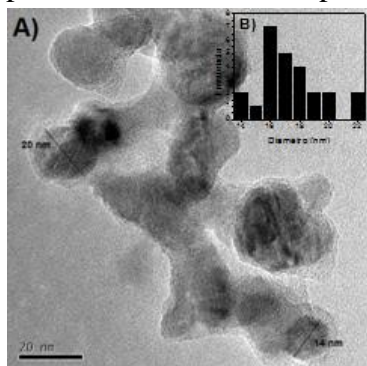
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Gallium nitride (GaN) has been successfully synthesized using a hydrothermal method at 240 °C during 72 h. In order to increase the cristallinity grade, solid was calcined at 900°C under nitrogen atmosphere. X-Ray powder diffraction (XRD) confirms the characteristic reflection of wurtzite phase [050-079]. The images by Screening Electron Microscopy showed agglomerated particles in the range of 0.5 micrometre, however Transmission Electron Microscopy (TEM) reveals that particles are composed by hexagonal nanoparticles with a size below 20 nanometers. The measured interplanar distance confirms that microstructure corresponds to wurzite phase. From the point of view of superficial properties GaN has showed 64 m<sup>2</sup>g<sup>-1</sup>, however after thermal treatment the specific surface area drop to 48 m<sup>2</sup>g<sup>-1</sup>. IR analysis only showed important signals form etallic bond for under waves below 1000 nm. These results promise interesting performance on hydrogen production by electrochemical and photogalvanic methods.



*Figure 1. Transmission Electron Microscopy of GaN prepared by hydrothermal method at 240°C. A) Image a 20 nm. B) Size distribution.*

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## **Optical and Structural Properties of ZnO Films Prepared by Sol-gel Spin Coating Method**

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Zinc oxide sol and films were prepared by sol-gel method. Zinc acetate dehydrate, 2-methoxyethanol and monoethanolamine (MEA) were used as a starting material, solvent and stabilizer, respectively. For film preparation, the solution was dropped onto silicon substrates; spinning rate was kept at 3000 rpm for 20 s. The wet films were dried at 300 °C after each coating, this procedure was repeated one, three, five and ten times for each deposition temperature and then films were subsequently annealed at 600 °C for 2 h under O<sub>2</sub> ambient. The structural properties of ZnO films were studied by X-ray diffraction measurements. X-ray diffraction pattern of the ZnO films obtained by sol-gel process shown a (002) preferred orientation. FTIR was used by obtained the chemical composition, the spectrum shows the vibration mode of ZnO in 410 cm<sup>-1</sup> and the vibration asymmetric stretching of Si-O bonds near 1080 cm<sup>-1</sup>. UV-Vis reflectance spectrum ZnO films were measured in a range of 220 to 800 nm. The ZnO films show a strong UV absorption below 387 nm. The optical band-gap obtained from the absorption spectrum was about 3.2 eV. The images obtained by (scanning electron microscope) SEM show a homogeneous surface of the films also, the average roughness values were measured by Atomic force microscopy (AFM) and are of 5 nm.

## **Analysis of Thermal Shock Resistant Cordierite-based Refractory Concretes**

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From the last decades studies on cordierite materials have been intensified, because they are used in applications that require low thermal expansion and high thermal shock resistance. Presence of mullite, alumina and liquid phases in cordierite matrices improve thermal shock resistance. We have determined the thermal shock resistance of refractory concretes, through essays comprising heating to 950 °C followed by immersion on water at 22 °C.

In the present work we present Scanning Electron Microscopy (SEM) and X-Ray Diffraction (XRD) results, obtained from refractory concrete probes after thermal shock. These results confirm that concretes with cordierite and liquid phases have better resistance to thermal shock.

**Characterization of ZnO Nanoplates Grown by SSCVD**

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In this work, we report the growth of ZnO nanoplates by SSCVD technique, on a glass substrate at a temperature of 400°C, using zinc acetate as a source of Zn and oxygen gas as the oxidizing agent. The optical and electrical properties of these nanoplates were investigated. The ZnO nanoplates have a hexagonal shape with area dimensions of 3-5  $\mu\text{m}$  and 50 nm in thickness approximately. Results of cathodoluminescence spectra suggested that the nanoplates contain more oxygen vacancies. The ZnO nanoplates showed a transmittance higher than 70% in the visible region. Electrical conductivity measurements were performed by C-AFM.

## Study of Surface Plasmons of Polyhedral Bimetallic Nanoparticles Using the DDA Method

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Bimetallic nanoparticles (BNs) are interesting because they offer the possibility to adjust their surface plasmon resonances through their component materials. Furthermore, their optical response depends on the size and morphology [1,2]. According to experimental reports [3-5], it is possible to synthesized BNs with different morphologies and with a core-shell distribution, i. e., a core made of one metal and a shell with another metal. In this work, we report the theoretical study of the optical properties of core-shell NBs of Au and Ag, with different shell thicknesses and also different morphologies, such as: sphere-cube, cube-cube, octahedron-cube, octahedron-octahedron and decahedron-decahedron. The theoretical spectra of the NBs were calculated using the discrete dipole approximation (DDA), which has been widely used in the study of polyhedral monometallic nanoparticles [6]. Our results show that the morphology of the shell, determines the number and position of the surface plasmons in the BN.

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## Thermal Characterization of $\alpha$ -Tocopherol Nanocapsules

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In the nutraceutical field nanotechnology has application in food industry considering that Food Drug Administration (FDA) accepts its application, which includes the use of virus detectors in meals and encapsulation of vitamins as well as other supplements. Many components of food are heat, light and oxygen sensible, carrying problems as lipid oxidation being this a critical factor in deterioration of foodstuff during storage time. Consequently the use of antioxidants to prevent this phenomenon is required. Antioxidants like carotenoids and other phenolic compounds are used as an excellent alternative for diminish these problems.

$\alpha$ -tocopherol is an essential vitamin, however this vitamin undergoes degradation reactions when is exposed to light and oxygen atmosphere. Therefore it is necessary to develop strategies to improve its stability and not affecting its biological activity. The objective of this work was to obtain nanocapsules by spray drying, using mesquite gum, maltodextrin and modified starch blends.

In this study were obtained nanocapsules of  $\alpha$ -tocopherol using three combination of mesquite gum, maltodextrins and modified starch C1 (33.33: 33.33: 33.33), C2 (50:25:25) C3 (25: 50:25) respectively. Compounds were dispersed in distilled water at 70°C.  $\alpha$ -tocopherol was added and later it was mixed with a homogenizer. Encapsulated samples were obtained using spray drying with airflow at 180°C. Moisture content, microscopic morphologic analysis and encapsulation efficiency of samples were determined.

Experimental results reported that nanocapsules contained moisture content of  $5.3 \pm 0.008$ ,  $6.1 \pm 0.05$ ,  $6.2 \pm 0.03$  expressed in wb for C1, C2 and C3 respectively. Nanocapsules morphology present a fractal dimension of surface (FDS) for C1 (FDS =  $2.48 \pm 0.04$ ), C2 (FDS =  $2.56 \pm 0.06$ ) and C3 (FDS =  $2.64 \pm 0.04$ ). Respect to encapsulation efficiency it oscillates between 71 and 79% for the three studied mixtures C1, C2 and C3. It is concluded that spray drying nanocapsules of  $\alpha$ -tocopherol, from mesquite gum, maltodextrin and modified starch blends, were successfully obtained.

Thermal analysis of encapsulated samples were obtained using a scanning calorimeter (TA Instrument Q500) with a heating rate of 2, 5 and 10°C/min of 30°C to 400°C. There were evident oxidation reactions of  $\alpha$ -tocopherol with an exothermic maximum temperature of the samples that varied upon heating rate and modified starch composition. Maximum temperatures varied near to 150°C up to 230°C, since the encapsulating material employed was constituted by hydrophilic and hydrophobic material in different concentrations. Respect to activation energy values and kinetic parameters of oxidation reactions the use of mesquite gum (C1 formulation) presented higher values (81.35-88.47KJ/mol) in comparison with the formulations C2 and C3 (60.26 and 68.53KJ/mol respectively) probable due to low oxygen permeability of encapsulating material. It is concluded that nanocapsules from mesquite gum are more suitable to be used to encapsulate  $\alpha$ -tocopherol.

## Aluminosilicate Condensations in Zeolite Pre-nucleation

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The reactions and clusters involved in the first stage of nucleation of aluminosilicate zeolites are studied using computational methods<sup>[1]</sup>. The role of the aluminosilicate monomers ( $\text{Si}(\text{OH})_4$  or  $\text{Al}(\text{OH})_4\text{Na}$ ) and dimers ( $\text{AlSiO}(\text{OH})_6\text{Na}$  or  $\text{Si}_2\text{O}(\text{OH})_6$ ) condensing with larger clusters is investigated. The aluminosilicate structures are modelled with a density functional method (DFT): BLYP/DNP//BLYP/DNP. A DFT simulated annealing is performed before the geometry optimisation, to avoid local minima. Solvation is modelled with a continuum dielectric method (COSMO)<sup>[2]</sup>, and in some cases with explicit water molecules<sup>[3]</sup>; the thermodynamical properties (including Zero Point Energy Correction) are calculated with standard statistical mechanical methods. A relevant role in the pre-nucleation of zeolites is found for the dimer  $\text{AlSiO}(\text{OH})_6\text{Na}$ , which produces structures following Loewenstein's rule, as observed in experimental synthesis.

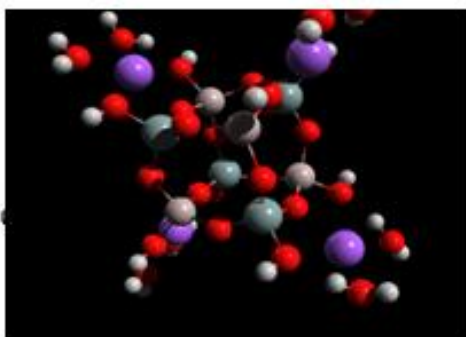


Figure 1. Doubled-four ring, aluminosilicate cluster involved in the prenucleation of zeolites.

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## One-step Synthesis of Ag, Pt and AgPt Nanoparticles on Graphene

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During the last years graphene and its composites have become one of the most important carbon-based materials due to their unique properties such as excellent electrical conductivity, charge carrier mobility and huge specific surface area ( $2600 \text{ m}^2/\text{g}$ ). Recently graphene has attracted much attention as the supporting material for dispersing noble metal nanoparticles in order to obtain composites of nanoparticles decorated graphene. Several reports have shown an improvement in electrocatalytic activity of monometallic and bimetallic nanoparticles due to the presence of graphene. In this work the synthesis and characterization of graphene-monometallic and graphene-bimetallic composites were studied. The composites were prepared by simultaneous deposition of metal nanoparticles (Ag, Pt and AgPt) on graphene sheets during the thermal reduction of graphene oxide (GO) mixed with metallic precursor. GO-based paper was prepared by drying a GO dispersion with the metal precursor; silver nitrate and/or chloroplatinic acid. The GO-based paper was thermally treated at  $400^\circ\text{C}$  under nitrogen atmosphere for 3 hr. resulting in Graphene composites. The morphology and crystalline structure of Np-Graphene composites were studied by scanning electron microscopy and transmission electron microscopy. Structural and chemical characteristics were analyzed by spectroscopy techniques such as UV-vis and infrared spectroscopy. The samples were also studied by X-ray diffraction.

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## Bioactivity and Degradability of Hybrid Nano-composites

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Hybrid materials with great application as biomaterials were synthesized. PDMS- modified CaO - P<sub>2</sub>O<sub>5</sub> - SiO<sub>2</sub> and PDMS – modified P<sub>2</sub>O<sub>5</sub> - SiO<sub>2</sub> hybrids materials, with different compositions, were prepared by *sol-gel* method. *In vitro* bioactivity and *in vitro* degradability tests were made in the materials. On the one hand, the hybrids were soaked for 1, 3, 7, 14, 21 and 28 days in simulated body fluid (SBF) to prove their apatite-forming ability. On the other hand, the materials were soaked for 1, 3, 7, 14, 21 and 28 days in phosphate buffer solution (PBS) to show their degradation process. In both *in vitro* tests, measurement of pH took place in order to have a control of the bioactivity and degradation process. The characterization of these materials was carried out to prove the growth of HA through X-Ray Diffraction, Infrared Spectroscopy, and Scan Electron Microscopy. The results showed that some samples have better bioactivity than others, especially the hybrid materials that contain CaO, which demonstrate HA growth since the beginning days. Moreover, during the degradation tests, all the samples presented weight loss, especially the ones that contain CaO.

A wide physical–chemical characterization of these materials was carried out to relate their microscopic structure and macroscopic properties. The effect of PDMS and the amounts of water used for the tetraethoxysilane (TEOS) hydrolysis on the mechanical properties of hybrid materials was investigated by three-point bending tests. For a given amount of water, as PDMS content in hybrids increased, the elastic modulus decreased. Furthermore, keeping the PDMS content constant, when the amount of H<sub>2</sub>O decreased, the elastic modulus increased. Regarding *in vitro* bioactivity and mechanical properties, the hybrid material obtained with molar ratios H<sub>2</sub>O/TEOS = 2 and TEOS/PDMS = 3.5 proved to be the best candidate for either soft tissue substitution or metallic implant coating since the hybrid material would promote the bonding with bone, and simultaneously dampening the mechanical.

## Characterization of Heat Treated HA-Al<sub>2</sub>O<sub>3</sub> Nanocomposite

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Hydroxyapatite (HA) is a calcium phosphate with a chemical composition similar to the human bone, making it biocompatible with living tissue. The biocompatibility allows use it in various medical applications. The alumina (Al<sub>2</sub>O<sub>3</sub>) is a ceramic with high strength and having features like bio-inert with no appreciable reactivity with implanting biological media.

In the present work, the hidroxyapatite was synthesized by precipitation method and the alumina by sol-gel method employing TSBAl as precursor. The HA was improved in addition 30 wt% of alumina. It was homogenized by high-energy ball mill during 20 min. and applying Spark plasma sintering process with a constant load of 12 N, at two different temperatures 900 and 1000 °C with a heating rate of 100 °C/min and annelling at room temperature inside the vacuum camera. The change of phases was studied by X-ray diffractometry, it was obtained a crystallin phase of alumina; the morphology and size of particle was analyzed by Scanning electron microscopy, the density was determined by Arquimides method, with a density of 3.04 g/cm<sup>3</sup> to 900 °C and 3.1 g/cm<sup>3</sup> to 1000 °C, the measurement of hardness was tested on both samples.

It was showed that the adition of alumina improve the mechanical properties of hardness addressing to new applications.

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## Localización en Células B16 de Híbridos a Base de Polvos Nanoestructurados de Gd<sub>2</sub>O<sub>3</sub> y MeTCPP

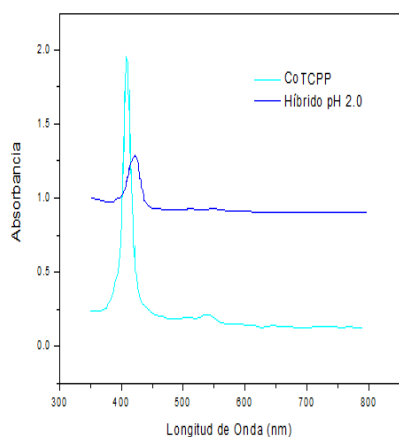
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La terapia fotodinámica (TFD) es una técnica alternativa para el tratamiento del cáncer que ya ha sido clínicamente aplicada desde hace varios años y aún permanece ubicada como una de las más prometedoras. En la TFD se usan fotosensibilizadores que actúan directamente sobre las células tumorales al generar especies reactivas de oxígeno, sin embargo, un inconveniente es su baja solubilidad. Por las ventajas que pueden presentar, en este trabajo se propone la obtención de metaloporfirinas (MeTCPP) unidas a nanopartículas de Gd<sub>2</sub>O<sub>3</sub>. Se estableció el protocolo de síntesis de las MeTCPP empleando como base la tetra (4-carboxifenil)porfirina (TCPP) y sales de níquel y de cobalto. Asimismo, mediante el proceso poliol se obtuvieron polvos nanoestructurados de Gd<sub>2</sub>O<sub>3</sub>. Se realizó la caracterización estructural de cada uno de los componentes de híbrido y de la forma híbrida mediante MEB, DRX. El Gd<sub>2</sub>O<sub>3</sub> presentó una estructura cristalina cúbica y agregados de tamaño comprendido entre 450 y 500 nm, conformados a su vez por partículas más pequeñas de 20 a 50 nm. Los híbridos Gd<sub>2</sub>O<sub>3</sub>-MeTCPP fueron igualmente caracterizados para comprobar la unión electrostática entre el cerámico y la molécula de TCPP al observarse desplazamiento en las bandas de absorción UV-Vis y en FT-IR.



Finalmente, se realizaron pruebas biológicas para comprobar el ingreso del híbrido a células B16, su localización celular y tiempo de permanencia.

*Figura 1. Espectro UV-Vis de un híbrido de Gd<sub>2</sub>O<sub>3</sub>-CoTCPP comparado con el de la TCPP.*

Los autores agradecen Dra. M.A. Hernández-Pérez por las observaciones MEB realizadas.

## Tuning Electronic and Energetic Properties of $\beta$ -silicon Carbide Nanowires by Chemical Control

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Silicon Carbide Nanowires (SiCNWs) are promising for wide applications such as light-emitting diodes, gas sensors, etc.; moreover they are suitable as potential electronic and optoelectronic devices operating at high temperature and high power. The use of SiCNW surface modification for band structure engineering does not have received attention despite its important potential. We report *first-principles* calculations of the electronic properties of [111]-oriented  $\beta$ -SiCNWs, we have studied systematically the modification of electronic structure for NWs of different widths and different surface coverage (H, F, NH<sub>2</sub>, CH<sub>3</sub>). The results indicate that the surface chemistry and the diameter have important effects on the band structure and the density of states; this allows a method for engineering of the electronic states of SiCNWs.

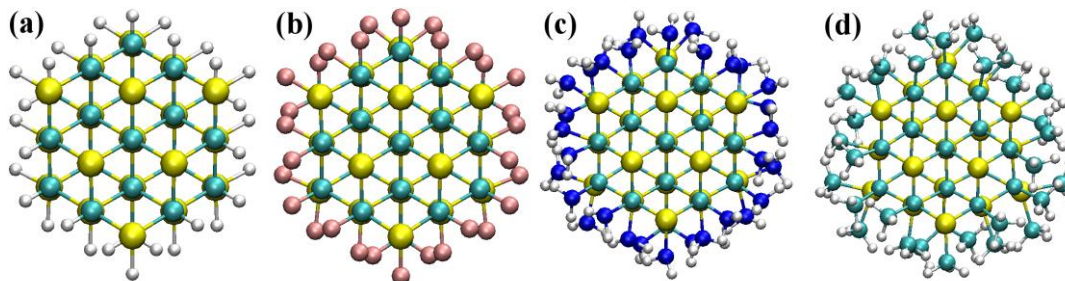


Figure 1. Optimized nanowires (a) H-, (b) F-, (c) NH<sub>2</sub>-, (d) CH<sub>3</sub>-terminated  $\beta$ -NWSiC.

We acknowledge the financial support Funding under Contract Nos. TEC2009-06986, FIS2009-12721-C04-03, and CSD2007-00041, project PICS012-085 from Secretaría de Ciencia, Tecnología e Innovación del Distrito Federal (SCTIDF) and Postdoctoral Abroad - CONACyT México.

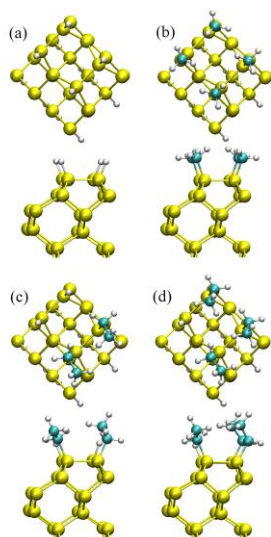
## First-principles Calculations of the Structural and Energetic Properties of Hydrogen, Methyl and Ethyl-terminated Silicon Nanowires

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Silicon nanowires (SiNWs) have been explored and studied both theoretically [1] and experimentally [2] for a long time, and they have emerged as a potential building material for a diverse variety of electronic devices, solar cells, chemical and biological sensors. The chemical properties of SiNWs are crucial to their stability and transport properties in nanoelectronic devices. We report *first-principles* calculations of the structural and energetic properties of hydrogen, methyl and ethyl-passivated Si surfaces, specifically



studying the energy required to form a dangling bond in the surfaces by removal of the corresponding passivating group. We have investigated a Si (100) surface as an approximation to a wide diameter SiNW facet, considering 50% and 75% coverage with C<sub>2</sub>H<sub>5</sub>, and 100% coverage with H and CH<sub>3</sub>. We show that, at 100% coverage, passivation with H requires more energy to form a DB than the case with 100% methyl coverage.

Figure 1. Optimized structures (a) H, (b) CH<sub>3</sub> (c,d) C<sub>2</sub>H<sub>5</sub>-terminated Si (100) surfaces.

We acknowledge the financial support Funding under Contract Nos. TEC2009-06986, FIS2009-12721-C04-03, and CSD2007-00041 and Postdoctoral Abroad - CONACyT Mexico.

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## Computational Study of the Effects of the Chemical Surface Passivation on the Electronic Properties on Porous $\beta$ -SiC

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Silicon carbide (SiC) is a binary semiconductor material, which has many interesting properties such as large electron mobility and wide band gap. On the other hand porous semiconductors have enormous surface area, which make them suitable for applications as fast response hydrogen sensors, in such applications the analysis of the surface passivation is of great importance. In this work we perform a computational study of the dependence of electronic structure and energetic stability on the chemical surface passivation and stoichiometry of cubic porous silicon carbide (pSiC) by means of the Density Functional Theory and the supercell technique [1]. The porous structures were modeled by removing atoms in the [001] direction to produce two different surface chemistries: one fully composed of silicon atoms and one composed of only carbon atoms. Changes in the electronic states of the porous structures were studied using different passivation schemes, one with Hydrogen (H) atoms, and other gradually replacing pairs of H atoms with: Oxygen (O) atoms, Fluorine (F) atoms and OH radicals. For the hydrogenated case, the calculation shows that the band gap is larger for the C configuration than for the Si case. The band gap behavior of the C phase depends on the number of passivation agents which is different from H per supercell by decreasing its band gap as the number of O or OH radicals increases, while the Si phase produces an irregular evolution in the band gap energy [1,2]. The results indicate the possibility of band gap engineering on nanostructures based on SiC by means of the surface passivation agents.

This work was partially supported by the multidisciplinary project 2012-1439 from SIP-Instituto Politécnico Nacional and PICS012-085 from Instituto de Ciencia y Tecnología del Distrito Federal (ICyTDF).

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## **Effect of Anisotropy on the Vibrational Properties of Si Nanowires: A First Principles Study**

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Silicon nanowires (SiNWs) are 1-D semiconductor nanostructures that have been extensively studied theoretical and experimentally in the recent years due to their potential applications. An important tool for characterization of nanowires are the phonon vibrational modes, since a variety of properties such as thermal transport, the Raman and IR responses of the material are understood by using the phonon theory. In this work we study the effect of anisotropy and quantum confinement on the frequency of the optical and acoustic vibrational modes and the thermodynamic properties of Silicon Nanowires, by means of first principles Density Functional Theory approach, using the generalized gradient approximation and the supercell scheme [1]. The nanowires are modeled by removing atoms outside a circumference in the desired growth direction. We compare the vibrational spectrum of SiNWs orientated in three different directions [001], [111], and [110]. Results show a clear dependence of the highest optical mode frequency with respect of the growth direction and diameter of the nanowires, since there is a shift of this mode to lower frequencies as the nanowire cross section decreases. These results could be useful for characterization of the nanowires through Raman spectroscopy techniques. Additionally we noticed changes in the sound velocity of the nanowires with respect to their growth directions, being a little bit higher in the [110] nanowires and also noticed a shift to lower frequencies of the acoustic branch maximums. For the thermodynamic properties of the nanowires we found that the heat capacity of the nanowires increases as the nanowire diameter increases.

This work was supported by project PICS012-085 from Instituto de Ciencia y Tecnología del Distrito Federal (SCTIDF) and multidisciplinary project SIP-IPN 2012-1439 from Instituto Politécnico Nacional.

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**Enzymatic Synthesis of Polyaniline-graphene Oxide Nanocomposites**

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Polyaniline (PANI) is a conductive polymer which has been studied with great interest in recent years due to its large number of applications. Recently, the formation of PANI composites with carbon-based materials like graphene oxide (GO) has been studied in order to obtain better electronic and mechanical properties. In this work, we studied the effect of GO on the enzymatic polymerization of PANI in aqueous dispersion and characterized the resulting composites. Enzymatic polymerization of aniline is an environmentally friendly method, whose oxidation is very different from chemical and electrochemical methods. Enzymatic oxidation occurs using hydrogen peroxide as oxidizer resulting in water as byproduct. The enzymatic polymerization of PANI was carried out in acidic medium using toluenesulfonic acid (TSA), horseradish peroxidase (HRP) and hydrogen peroxide. The polymerization reaction was studied using 1, 2.5 and 5 wt % of large GO sheets. No changes were observed in enzyme activity in the polymerization reaction of aniline in presence of GO. The morphology of resulting PANI-GO composites was studied by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and optical microscopy. Nanocomposites were also characterized by Raman spectroscopy and XRD diffraction, to study their structure.

The authors acknowledge the financial support by CONACYT-Mexico through the J-106365 project.

**Síntesis y Caracterización por HRTEM y Difracción de Electrones de  
Sistemas Unidimensionales Monocristalinos de  $V_2O_5$   
por Síntesis Solvotermal**

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Por síntesis solvotermal se sintetizaron nanoalambres de  $V_2O_5$  monocristalino usando 30 ml de agua destilada y 0.18 gr de  $V_2O_5$  de Aldrich grado reactivo. La solución fase precursora se obtuvo bajo agitación constante hasta obtener un pH de 4.7 y una solución de color naranja. En este punto se añadieron 2.5 ml de  $H_2O_2$  gota a gota para inhibir el crecimiento de algunas caras del cristal y favorecer el crecimiento unidireccional del cristal. La solución fase precursora se introduce en un sistema cerrado (bomba de digestión ácida) y es calentado en una mufla a 1800C por 48hr. Resultados de HRTEM muestran nanobarras de un ancho de 80nm en promedio y una longitud de varios micrómetros, los cuales son monocristalinos. Por difracción de electrones se están estudiando los ejes de crecimiento preferenciales. Difracción de rayos X muestra la presencia de una fase monocristalina de tipo ortorrómbico.

Se agradece a proyecto PAPIIT-DGAPA IN113411. Al laboratorio LAREC-IFUNAM por el estudio de difracción de rayos X.

## Ferromagnetic Resonance in Iron Yttrium Garnet (YIG) Films Obtained by Spin Coating Deposition

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Yttrium iron garnet ( $\text{Y}_3\text{Fe}_5\text{O}_{12}$ ) or YIG is a ferromagnetic oxide with applications in microwave devices for radar and telecommunication systems [1], and those applications are due to its magnetic properties at high frequencies in the range of 1-10 GHz. In this work, a ferromagnetic resonance (FMR) study is presented in YIG films obtained by spin coating deposition. Polymeric precursors of YIG synthesized by the Pechini method were spin-coated onto Si substrates at 2200 rpm, followed by thermal annealing at 900°C on air. X ray diffraction (XRD) and Raman spectroscopy confirmed the formation of single phase YIG in the deposited films. FMR studies were carried out at 9.4 GHz (X-band) in a JEOL JES-RES3X spectrometer. These studies showed a highly anisotropic response in the YIG films, where the angular variation of the applied magnetic field ( $H_{DC}$ ) on sample decouples

the different absorption modes; which are associated with the dynamic magnetic response of the YIG films. The contributions of film surface to the magnetic anisotropy of the system are discussed.

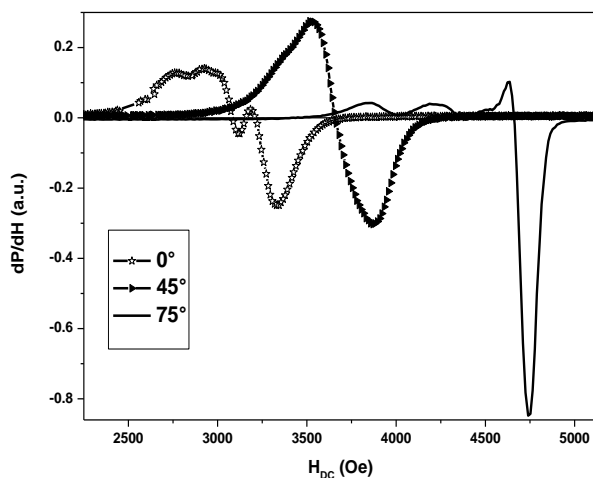


Figure 1. Angular dependence of FMR spectra measured with  $H_{DC}$  applied at 0°, 45° and 75° of the film axis.

We acknowledge the financial support of DGAPA-UNAM, through the grant PAPIIT IN111111. J.F. Barrón-López thanks to CONACyT-México for scholarship No.59119.

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## Growth and Optical Characterization of Inverse Opals Generated by Mixing $\text{SiO}_2$ – $\text{TiO}_2$

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The study of the electrical properties of materials technology revolutionized with the invention of devices such as transistors, diodes, etc., in recent decades the use of optical properties of materials has generated a significant technological advances, such as Examples include the fiber optic cables and waveguides, which have made a very significant contribution to the telecommunications industry, or lasers, high-speed computers, and other cases in spectroscopy, are some of the benefits from the knowledge of behavior of light in materials [1,2].

The design of optical devices with a great technological application are photonic crystals, they are periodic arrays of materials with different refractive indices. The possibility of generating inverse opals from PMMA base has opened possibilities opals grow various materials, and hence find their applications in this work, inverse opals grow from the variation of the mixed oxide metal  $\text{SiO}_2$  –  $\text{TiO}_2$ , that is, will generate combinations of these two compounds varying proportions, inverse opals grow initially be constructed of PMMA spheres (polystyrene and poly-methyl-methacrylate) in a FCC structure,  $\text{SiO}_2$  is then coated with either  $\text{TiO}_2$  and PMMA is removed, leaving the inverse opal, under these conditions it is possible to control the cell size, sphere size and width of the coating. Was characterized by SEM and reflection spectra are obtained, on the other hand through a theoretical model calculations will reflection spectra that serve as a basis for comparison with experimental results, in this paper we use the method transfer matrix, which is based on applying the continuity conditions of the tangential components of the electric and magnetic fields at the interfaces, and using a one-dimensional approach that has shown adequate results play an opal be modeled inverse [2,3]. From these comparisons it will be possible to model the inverse opals, that is, determining its size, mixture etc., Based on the expected properties also seeks to find if there is a linear relationship between the refractive indices to make a combination two different indices.

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## Study of Thermal Crystallization of Unhydrogenated Amorphous Silicon Films Deposited by RF Sputtering

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The amorphous silicon is a material which is deposited by means of RF sputtering technique. This system carried out deposits of thin films inside of an argon atmosphere. The thickness of the film can be controlled varying the deposit pressure, voltage bias that is reflected as RF power, and target-substratum distances. The amorphous *n*-type and *p*-type silicon films deposited by means of RF sputtering technique were prepared with the voltages bias 600 Volts, and the pressure into the camera was modified varying the argon flow to obtain a pressure of 40  $\mu$ Bar. An oil diffusion pump carried out the vacuum of the sputtering camera. The films obtained at 200°C, shown a better adherence on the substrate. We control the thickness of the amorphous silicon films through the deposit pressure and voltage bias. These parameters control the energy necessary for remove the atoms in the target, and deposit on the substrate surface. We observed that the uniformity of the film depends of the confined into of the plasma. The film thickness was determined when we evaluated the UV-Vis spectrum, which shows interference fringes. Those were analyzing by the Swanepoel method. The amorphous silicon films were annealing at 800°C to 1000°C to achieve a complete crystallization. This increase the conductivity and the size crystal grain to obtain a high mobility of energy to cross the films. Those parameters make possible application in solar cells. The crystallization evolution was observed in reflectance UV-vis, Raman spectroscopy, optical microscopy and X-ray diffraction.

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## Macroscopic Optical Response and Photonic Bands

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We develop a formalism for the calculation of the macroscopic dielectric response of structured systems made of particles of one material embedded periodically within a matrix of another material, each of which is characterized by a well defined isotropic dielectric function which could depend on frequency and could be complex as in dispersive and absorptive materials. The geometry of the particles and the Bravais lattice of the composite are also arbitrary. Our formalism incorporates retardation effects and goes beyond the long-wavelength approximation [1,2] and is very economical in memory and CPU usage compared with direct matrix manipulations [3]. We study the propagation of TE and TM electromagnetic waves in 2D photonic crystals made of a periodic array of cylindrical holes in a dispersionless dielectric host. Our macroscopic theory not only allows the calculation of the photonic band structure of the system, but also, the characterization of the polarization of its normal modes. We compute a macroscopic magnetic permeability from the spatial dispersion of the macroscopic dielectric response.

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**Cell-interaction and Cytotoxicity of Titanium Dioxide Nanoparticles**

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Nanomaterials are used in a wide variety of applications ranging from industrial uses (pigments, catalysts) to biomedical applications (controlled release systems, diagnostics). Because its use is in sharp increase, concern for knowing the type of interactions they have with biological systems has also increased. Many studies have shown that their toxicological effects are directly related to the nature and chemical properties of each material. Because of Titanium oxide is considered non-toxic, biocompatible and unreactive, it has been the focus of attention in several investigations for their effects at the molecular level when interacting with cells. However, due to the lack of suitable equipment and techniques to track in vitro and in vivo behavior its applications are still bounded. One alternative to monitoring this type of materials is fluorescent labeling. This procedure involves surface modification of the material (mainly amino groups) and further coupling with fluorophores. In the present work, we used two modifying agents to functionalize the surface of TiO<sub>2</sub> materials and were coupled to Fluorescein isothiocyanate -FITC-. The materials were characterized by UV-visible and Infrared spectroscopies, scanning electron microscopy and fluorescence microscopy. In order to study the effect of materials into cells, SH-SY5Y human neuroblastoma cells were incubated with different particle concentrations. Images of labeled materials and cells were taken by epifluorescence and confocal microscopies. MTT assay showed that Pt(acac)<sub>2</sub>-TiO<sub>2</sub> and TiO<sub>2</sub>-ac exhibited cytotoxic effect and that some relevant interactions take place at cell membrane level.

## Effect of Surface Functionalization of Carbon Nanotubes on the Dispersion of Platinum Nanoparticles

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Surface functionalization of carbon nanotubes (CNTs) has been used to improve the incorporation of metal nanoparticles on their surface [1]. In this work we report the effect of the surface chemical functionalization of CNTs on the dispersion of platinum nanoparticles. Platinum nanoparticles were incorporated following a vapor-phase impregnation method using metal-acetylacetonate as precursor [2]. The main functional groups observed at the surface of CNTs were carbonyl and carboxyl groups as a result of their treatment in a HNO<sub>3</sub>/H<sub>2</sub>SO<sub>4</sub> acid solution. HR-SEM observations revealed that highly dispersed platinum nanoparticles can be obtained on the surface of functionalized CNTs compared to pristine CNTs. The high dispersion of platinum nanoparticles remains unaffected even after an ultrasonic bath treatment for 15 min. Highly dispersed platinum nanoparticles on CNTs showed very attractive properties as electrodes for the hydrogen evolution reaction in proton exchange membrane electrolyzers.

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## Preparation of Zn(OH)<sub>2</sub> as Precursor for Obtaining ZnO

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At present the scientific and technological progress requires optimization or generation of new materials. Therefore it is vitally important to also have alternative techniques in materials synthesis. In this paper, the synthesis of ZnO based first obtaining chemical precipitation of Zn(OH)<sub>2</sub> and then calcined to obtain the ZnO. To obtain the precipitate, a solution of ZnSO<sub>4(aq)</sub> to which was added an alkaline solution of NH<sub>4</sub>OH, NaOH and KOH. The reaction was conducted at room temperature conditions and stoichiometry. In Figure 1. Shows XRD patterns of the samples were obtained with the presence of other crystalline phases in addition to the wurtzite, but are different to those reported by Masuda [1]. These samples are analyzed by Scanning Electron Microscopy to identify the particle morphology of checking that each sample has particle morphology. It is found that the samples calcined at 300 °C present the smallest particle size of glass or calculated by

Scherrer's Law. The case of NH<sub>4</sub>OH which showed a size of 90 to 100 nm.

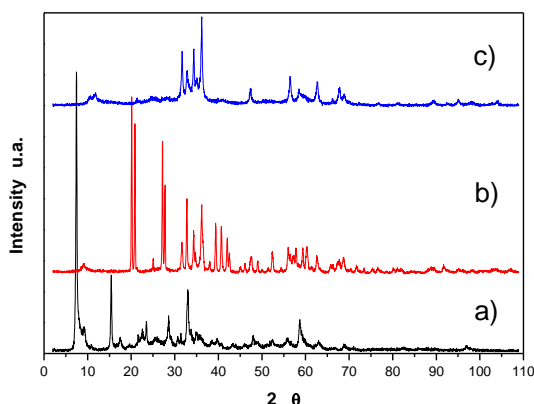


Figure 1. The XRD patterns of precipitate a) NH<sub>4</sub>OH, b) NaOH y c) KOH.

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## Evaluation of Rosiglitazone-loaded Chitosan Nanoparticles on Calcium Handling in Rat Cardiomyocytes

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Rosiglitazone administration to control hyperglycemia in Type 2 Diabetes Mellitus has been associated with adverse cardiovascular side-effects and hence its clinical usage is restricted<sup>[1]</sup>. One way to limit the undesirable Rosiglitazone side-effects is through the implementation of drug delivery with nanoparticles. Thus, our main aim is to administer rosiglitazone encapsulated in chitosan nanoparticles to animals that have developed Metabolic Syndrome and evaluate its effects on Calcium handling in isolated cardiomyocytes. In addition, we evaluate the effect of acute administration of 1) Rosiglitazone-loaded nanoparticles, 2) Rosiglitazone-free nanoparticles, and 3) Rosiglitazone alone (100µM) on Ca<sup>2+</sup> sparks and Ca<sup>2+</sup> transients of freshly isolated rat cardiomyocytes using confocal microscopy<sup>[2]</sup> for every five minutes until fifteen minutes in same cells. Rosiglitazone-loaded chitosan nanoparticles were synthesized by ionic gelation method for three different concentrations of chitosan and tripolyphosphate (TPP), i.e, 1:1, 2:1 and 3:1 respectively. The size of the particles were below 100nm for the 2:1 and 3:1 chitosan:TPP ratio (Figure 1) and 300 nm for 1:1 ratio. Ca<sup>2+</sup> spark properties (i.e. amplitude, duration, size, etc.) were not modified by 100 µM Rosiglitazone at the mentioned times. Evaluation of chitosan nanoparticles in reducing cardiac side effects of rosiglitazone *in vivo* is yet to be confirmed.

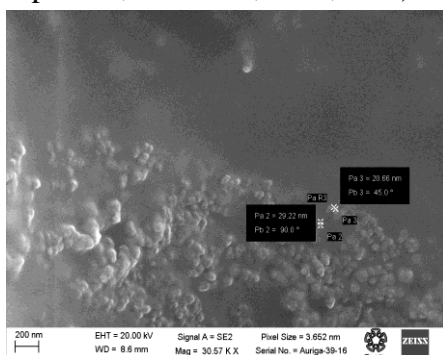


Figure 1. SEM micrograph of chitosan nanoparticle (2:1 chitosan:TPP ratio) prepared by ionic gelation method.

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