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para aplicaciones en energía solar, medio ambiente y salud

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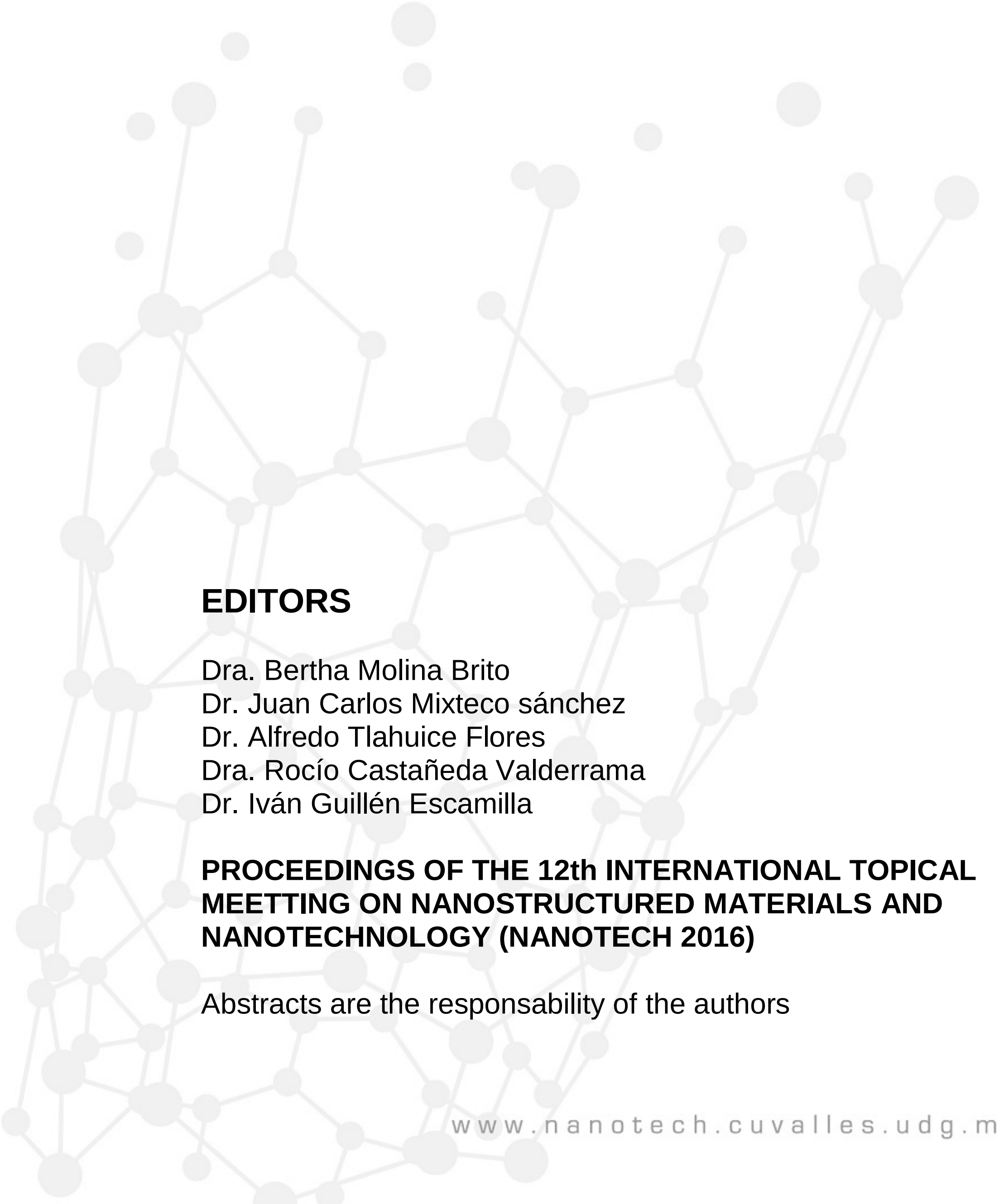

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PROCEEDINGS OF THE 12th INTERNATIONAL TOPICAL MEETTING ON NANOSTRUCTURED MATERIALS AND NANOTECHNOLOGY (NANOTECH 2016)

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12TH INTERNATIONAL TOPICAL MEETING ON NANOSTRUCTURED MATERIALS AND NANOTECHNOLOGY (NANOTECH 2016)

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INTRODUCTION

Dear participants of the 12th Nanotech congress:

It was a pleasure for the organizing committee to have you as our guest, and we look forward to the opportunity to do so again. This annual congress is the convergence place of the scientific community dedicated to the nanoscience and nanotechnology areas, likewise it is the ideal space for the presentation and discussion of ideas and projects in this field.

In this edition, ninety six posters were accepted and presented in three mural sessions and sixteen plenary lectures were held on topics of particular interest in the nanoscience and nanotechnolgy. Additionally, the activities of the third conference of nanomaterials for applications in energy, environment and health, the annual meetings of the Nanosciences Division of the Mexican Physics Society and the CONACyT Mexican Nanoscience and Nanotechnology theme network were hosted. Finally, four mini courses were taught to undergraduate and graduate students.

This congress certainly favored thematic and interdisciplinary discussions and narrowed collaborations between several national and international academic groups. This meeting also provided the support to incorporate young graduates in the nanoscience and nanotechnology industry, increasing in this way the impact of this discipline in our country at an international level.

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

Organizing Committee of the 12th Nanotech Congress

PLENARY SESSION

Organic functionalization of two dimensional systems

Pamela Rubio-Pereda[a], Diego Morachis Galindo[a], and Noboru Takeuchi[b]

[a]Centro de Investigación Científica y de Educación Superior de Ensenada 3918, Código Postal 22860, Ensenada, Baja California, Mexico

[b]Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Apartado Postal 14, Código Postal 22800, Ensenada, Baja California, Mexico

E-mail: takeuchi@cnyn.unam.mx

The adsorption of organic molecules onto surfaces is a topic of increased interest in some scientific and technological fields, since the molecular interactions at the molecule/surface interface play an important role in several applications. For example, with the adsorption of organic molecules, material surfaces can be provided with unique characteristics of the organic molecules, such as their absorption spectrum, chemical affinity and hydrophobicity/hydrophilicity. This process is known as organic functionalization, whose ultimate goal is the production of novel nano-electronic devices with properties such as light emission, light detection and chemical sensitivity. In this work, we study the adsorption of unsaturated hydrocarbons, onto material surfaces of two dimensional systems, such as graphene, silicene and germanene. Recent achievements associated with graphene have led to the research of analogue two-dimensional structures, such as silicene and germanene. In general, these systems are promising substrates for organic functionalization.

We thank financial support from Conacyt Project 164485 and DGAPA project IN100516. Calculations were performed in the DGCTIC-UNAM supercomputing center, project SC16-1-IG-31.

Nanophotonics for biomedical and optoelectronics applications

Elder De la Rosa

Centro de Investigaciones en Optica, A.P. 1-948, León, Gto. 37150 México

E-mail: elder@cio.mx

Optical and electronics properties of semiconductor nanocrystals or quantum dots (QDs) and ceramic nanocrystals can be tuned by controlling the size and composition, such characteristics make them excellent candidate for applications on biomedicine and optoelectronic devices such as displays, solid-state lighting, photodetectors and solar cells devices. Here in this work, it is discussed the luminescence and electronic properties of such functional nanomaterials and proposed some application for imaging and detection of analytes. It is also discussed different architecture to optimize the charge transport and then enhancing the efficiency of LEDs and solar cells based on QDs and ceramic nanocrystals. Hybrid QD-LED and pLED combined with nanocrystals were proposed and analyzed the electro- and photo-luminescence properties in terms of size and composition of nanocrystals, and the appropriate architecture that include organic and inorganic hole and electron transport film to maximize the emission efficiency.

One dimensional nanomaterials for energy storage application

Marina Elizabeth Rincón González

Instituto de Energías Renovables, Universidad Nacional Autónoma de México

E-mail: merg@ier.unam.mx

Material innovation and low capex manufacturing processes are required to accelerate the development and appropriation of electrochemical power sources such as batteries and super-capacitors. These devices are important not only to power the gadgets of modern life, but also to make the transition from fossil-fuels to Renewable Energy technologies and electric vehicles. Here we present the use of one dimensional core-shell structures based on nano carbon as anodes for Li-ion batteries. Modification of the highly reversible TiO_2 shell with oxides with larger theoretical capacitance was implemented to improve the performance of electrodes based on 1D-MWCNT@TiO_2. Theoretical calculations provided a better understanding of the basic phenomena at the carbon/oxide interfaces, particularly those related to the stability of the conductive carbon core, which was found very sensitive to the symmetry and thickness of the oxide deposition.

Physical properties of semiconductor nanostructures: First principles studies

F. Sánchez-Ochoa[1] , J. M. Galicia-Hernández[1] , J. Guerrero-Sánchez[2] , Gregorio H. Cocoletzi[1] , Noboru Takeuchi[2] , A. Sánchez-Castillo[3]

[1]BUAP, Instituto de Física “Ing. Luis Rivera Terrazas”

[2]UNAM, Centro de Nanociencias y Nanotecnología

[3]UAEH, Escuela Superior de Apan

E-mail: cocoletz@ifuap.buap.mx

Physical properties of semiconductor surfaces and nanostructures are of current interest in the material sciences because of the multiple technological applications. The nanostructures include 2D layers, 1D nanowires and nanotubes, and nanoparticles which have been extensively investigated both experimental and theoretically. Graphene and 2D boron nitride layers (a graphene-like system) may be considered as good examples of low dimensional systems with applications in the nano-optoelectronic industry. A great variety of devices include as part of them the graphene layer, namely; vertical field effect transistors, gas sensors, and organic light-emitting diodes (OLEDs). In this presentation we will describe some first principles total energy studies of semiconductor surfaces and nanostructures. Examples of semiconductor low dimensional systems will be considered to describe calculations of structural, electronic, optical and transport properties.

Vibrational spectroscopy of metal cluster complexes with a Free Electron Laser: investigating the chemistry on a small surface

A. Fielicke

Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany

E-mail: fielicke@physik.tu-berlin.de

Transition metal clusters are frequently used as model systems for low coordinated sites of extended surfaces and their study can provide valuable insights into the mechanisms of surface reactions. In many cases, however, there is still a lack of information on their structures and the relationship between structure and chemical behaviour. Using vibrational spectroscopy of gas-phase clusters one can obtain information about the clusters' structure or the behaviour of adsorbed species. The latter provides valuable insights into the binding geometry, the activation of bonds within the ligands or reactions occurring on the clusters' surface. Cluster size specific data can be obtained using infrared multiple photon dissociation spectroscopy. To cover the required spectral range from the far to the mid-IR our experiments make use of IR free electron lasers. The talk will discuss exemplary studies about structures of clusters of the platinum group metals [1] and the activation of carbon dioxide by anionic cobalt [3] and rhodium clusters.

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Formation and Atomic Structure of Hierarchical Boron Nitride Nanostructures

R. A. Guirado-López

Instituto de Física “Manuel Sandoval Vallarta”, Universidad Autónoma de San Luis Potosí,
Álvaro Obregón 64, 78000, San Luis Potosí, SLP, México

E-mail: guirado@ifisica.uaslp.mx

In this work we report a combined experimental and theoretical study of boron nitride (BN) nanostructures synthesized by ball milling methodology. The BN nanostructures were obtained using *h*-BN powder under low vacuum conditions and steel balls of different sizes. The HRTEM images of our samples show the formation of spheroidal BN nanoparticles with diameters as small as ~7 nm which self-assemble into different hierarchical nanostructures such as two-dimensional layered materials, spheroidal configurations, and one-dimensional solid BN chains. The Raman spectra reveals an intense absorption band in the 300—600 cm^{-1} region, which is absent in the spectra of BN nanotubes, previously synthesized BN nanoparticles, as well as in all bulk boron-nitride polymorphs. Density functional theory calculations show that the Raman spectra is consistent with the formation of fullerene-like BN particles which also exhibit an intense absorption band in the 200—800 cm^{-1} range dominated by a complex mixture of tangential, stretching, and radial breathing modes. Finally, by means of electron-beam irradiation experiments additional structural transformations can be induce on our hierarchical BN particles consisting in the formation of nano-holes of the order of 5 nm. Our here-reported BN nanostructures might lead to a wide range of potential applications.

Keywords: boron nitride, ball milling, density functional theory

Quantum-mechanical modeling of metal nano-architectures in catalysis and optics

A. Fortunelli

CNR-ICCOM, via G. Moruzzi 1, Pisa, 56124, Italy;

E-mail: alessandro.fortunelli@cnr.it, afloer@caltech.edu

I will present some results of our efforts exploring a predictive computational nanomaterials science–modeling materials with nanoscale structural features and searching for associated novel phenomena and properties, with particular attention to nano-architectured metal systems and their kinetics and dynamic phenomena, such as structural and electron dynamics. Ours strategy starts from fundamentals methods and concepts drawn from quantum mechanical approaches and aims at achieving accurate predictions under realistic conditions and environment.

First, the compositional and structural freedom of nanostructured systems calls for developing and implementing exhaustive search algorithms able to investigate the novel structural motifs, paths and mechanisms that such systems exhibit (“nanostructure problem”). In this context, I will briefly discuss a Reactive Glocal Optimization (RGO) approach as a computational protocol able to explore the reactive phase space of these systems in the presence of reactant molecules1, with examples of application to the thermodynamics and kinetics of elemental diffusion in alloyed systems2.

The natural deployment of such techniques is in the field of catalysis. Starting from the smallest systems, sub-nanometer (or “ultranano”) supported metal clusters (containing up to 10-20 metal atoms) represent a new class of materials which have been shown in several cases to exhibit superior catalytic properties in efficiency and selectivity with respect to traditional catalytic systems in addition to optimizing atom-economy efficiency. I will show how the application of systematic sampling under realistic conditions naturally leads to the concept of ligand/surface catalytic complex. The simultaneous presence on the metal catalyst of ligands and chemical species at various stages of the reaction and the non-linear interactions among them and with the support as a norm translates into the formation in-situ and under reaction conditions of a complex aggregate which acts as the real catalytically active species. This idea will be discussed and illustrated with a few selected examples3, highlighting its relationship to methods and results developed in the field of homogeneous catalysis4.

Moving to larger systems, results will be first reported on particle restructuring under realistic conditions and its relevance to carbon nanotube growth, (selective) oxidation reaction, and ammonia synthesis. Going to the extreme, it will be then shown how harsh reactive ligands can lead to phase transformations from nanocrystals to nanoporous particles via dealloying, as for Ni-Pt nanostructures under electrochemical oxygen reduction reaction (ORR) conditions5. Such “exotic” nanostructures obtained by electrochemical leaching of more electropositive metals (e.g., Ni) from nano- architectured alloys with another metal (e.g., Pt) typically exhibit continuously connected cavities (pores) of nanoscale size, and have attracted explosive interest in the last 15 years due to their unique properties in catalysis, sensors, and opto-electronic devices. However, lack of fundamental knowledge still remains on these systems concerning their geometric features and the relationships with the corresponding properties. A relationship will here be proposed between surface coordination environment and catalytic function and the origin of enhanced catalytic performance of these systems in the ORR, which is the rate determining step in low-temperature hydrogen fuel cells for sustainable and energy-efficient electrical power, with the final goal of designing Pt metallic systems with optimal catalytic activity.

Moving to electron dynamics, the absorption spectra of metal nanostructures will be explored using time-dependent density-functional-theory (TDDFT) methods. The sensitivity of Surface Plasmon Resonances (SPR)6 to the nanostructure environment and the possible damping of the absorption intensity in the visible region due to adsorbed species is a first issue which limits applications in molecule detection via Raman spectroscopy, enhanced plasmonic phenomena in metal nanogaps, biosensing, etc. Two different strategies will be investigated to overcome this issue and achieve intense SPR peaks in the whole near-IR/vis region. The first strategy is based on molecule/nanostructure resonance coupled with plamon/plamon interactions due to proximity effects. The coupling between the plasmonic modes of Au nanowires at close distances and those involving the interaction of the wires with adsorbed ligand species will be explored, and the search for synergic interactions in the optical response (‘hot- spot’ enhancement of response fields) will be discussed7. The second strategy is based on fine tuning the chemical features of the ligands8,9. Focusing on thiolated AuN(SR)M nanoclusters of well-defined atomistic structure, I will show how large enhancements in absorption in the optical region can be achieved by tuning the steric and electronic properties of the SR ligands. Charge decompression via steric hindrance and delocalization via conjugation to achieve optimal band alignment will be used as guiding principles leading to a resonance phenomenon in which many excitations, of composite Au/S/R character and involving the nanocluster as a whole, crowd in a narrow energy interval. This strategy allows one to circumvent the issue of SPR damping by the environment (SPR “re-birth”), and represents a step forward toward the goal of an in-silico design of nanocrystals with desired optical properties.

If time will allow, dielectric (oxide) ultrathin films grown on metal or semiconducting surfaces are examples of so-called 2D materials that have attracted an explosive interest in view of many applications, including transport and electronic devices. I will show how an interplay of theory and experiment working in close synergy is mandatory to arrive at a correct elucidation of the structural properties of such complex materials, and how such a detailed information opens the way to a full understanding and possibly control of the response properties of such systems10. In particular, an in-depth analysis of the charge and electrostatic potential at the metal/semiconductor junction to single out physical quantities such the work function, band bending and charge transfer at the interface allows one to shed light on electronic transport interfacial phenomena via quantum approaches11 and provides a link between the knowledge accumulated on model surface science systems and technological electronic devices based on 2D oxide phases.

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Rewritable Organic Memory Devices using Carbon Nanostructures/PEDOT: PSS nanocomposites

R. López-Sandoval

Instituto Potosino de Investigación Científica y Tecnológica, San Luis Potosí, SLP, México

E-mail: sandov@ipicyt.edu.mx

In this work, we talk about non-volatile memory devices based on resistive switching mechanism. A resistive switching memory is generally built by a capacitor like metal-insulator or semiconductor-metal (MIM) structure. In particular, we focus in organic resistive memory where the insulator layer is a multiwalled-carbon-nanotubes/PEDOT: PSS nanocomposite. We show that an essential parameter on the properties of memory devices is the metals used as electrodes. In general, in our memory device for having the resistive switching is necessary that one of the electrodes is an electrode of Al. This is because the aluminum always presents a native oxide layer, which can be electroformed to have resistive switching. In addition, physical and chemical properties of this native Al oxide layer can be modified using UV ozone treatment, which has important consequences on the resistive switching properties. Finally, it is essential that the carbon nanotubes are embedded in the PEDOT: PSS polymer matrix in order that our devices show a significant number of write-read-erase-read cycles. Moreover, depending on the type of carbon nanotube used in the memory device, i.e. doped with nitrogen, or functionalized with O groups, or pristine, the electrical properties of the memories are different.

Laboratorio Nacional de Nanotecnología (NaNoTeCh) - National Nanotechnology Laboratory

Francisco Espinoza Magaña

CIMAV - Unidad Saltillo, Miguel de Cervantes 120, Complejo Industrial Chihuahua Chihuahua, Chih. México. C.P. 31136.

E-mail: francisco.espinosa@cimav.edu.mx

The National Nanotechnology Laboratory (NanoTeCh) is located on site at CIMAV, and is dedicated to impulse and to promote nanoscience and nanotechnology research and development in Mexico.

The National Nanotechnology Laboratory is to serve as a node of the National Network of the Nanotechnology Laboratories created in 2006, as a result of a call for proposals issued by CONACYT to create a network of national laboratories and scientific infrastructure for technological development in Mexico, to promote training of human resources, scientific research and the development of specific applications in synthesis, characterization and applications of nanotechnology systems, providing a space for collaboration and support for institutions and businesses supporting the academic, productive and social sectors in general. Since its inception, the Nanotechnology National Laboratory has supported a large number of universities and research centers throughout the country of Mexico and abroad.

Nanotech technical capacities include three transmission electron microscopes, three scanning electron microscopes, one focused ion beam, two atomic force microscopes, three X-ray diffractometers and one micro Raman spectrometer.

Hydrogen Storage in Graphene

S. Heun

NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, 56127 Pisa, Italy.

E-mail: stefan.heun@nano.cnr.it

The realization of innovative hydrogen storage materials has worldwide strategic importance. Graphene has recently attracted attention as a promising hydrogen storage medium. Indeed, graphene is lightweight, chemically stable, and exhibits attractive physico-chemical properties for hydrogen adsorption. Furthermore, the interaction between hydrogen and graphene can be controlled by chemical functionalization.

The energetics of the chemisorption of hydrogen on graphene can be modified by the local curvature of the graphene sheet. Based on scanning tunneling microscopy (STM) we report on site-selective adsorption of atomic hydrogen on convexly warped regions of monolayer graphene grown on SiC(0001). This system exhibits an intrinsic curvature owing to the interaction with the substrate [1]. We show that at low coverage hydrogen is found on convex areas of the graphene lattice [2]. No hydrogen is detected on concave regions. These findings are in agreement with theoretical models which suggest that both binding energy and adsorption barrier can be tuned by controlling the local curvature of the graphene lattice. This curvature-dependence combined with the known graphene flexibility may be exploited for storage and controlled release of hydrogen at room temperature.

Theoretical studies regarding metal atoms (e.g. Ti, Li) deposited on graphene suggest that such materials can adsorb up to 8 wt% gravimetric density of hydrogen. We investigate the deposition of Ti on graphene and its potential for hydrogen storage [3]. The Ti atoms form small islands (diameter ~ 10 nm). The Ti-covered graphene was exposed to molecular hydrogen, and the hydrogen desorption dynamics was measured by thermal desorption spectroscopy. Our data demonstrate the stability of hydrogen binding at room temperature and show that

the hydrogen desorbs at moderate temperatures – both ideally matching technical requirements for hydrogen storage. First principle calculations clarify the multi-bonding state between hydrogen and the graphene-supported Ti clusters [4]. To further increase the hydrogen uptake of these samples, we employ controlled surface modifications to increase the active surface for hydrogen adsorption by decreasing the size of the Ti-islands and increasing their density [5].

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Chitosan based nanocomposites for biomedical and sensor applications

Evgen Prokhorov

CINVESTAV-Unidad Querétaro. Querétaro, Libramiento Norponiente 2000, Queretaro, México.

E-mail: prokhorov@cinvestav.mx

Citosan (CS) is a suitable matrix material for stabilization and homogeneous nanoparticles (NPs) dispersion in the polymer environment. Properties of nanocomposites essentially dependent on the high surface area of the NPs which in turn depend on the dimension and concentration of NPs. Different routes of synthesis of polymer-NPs composites have been proposed. The dimension of NPs can be obtained from TEM or SEM measurements but problem appears how to control NPs concentration.

Additionally, one of the most important question of nanotechnology is how to compare properties of nanocomposites obtained using different methods of preparation (precursors, reducing agents, temperature, etc.) and how to find optimum concentration of NPs with the highest surface area in the composites? In this work chitosan (CS) based nanocomposites with high conductivity silver (AgNPs), gold (AuNPs), clay nanoparticles and multiwall carbon nanotubes have been investigated and relation between electrical properties and optimum concentration of NPs for application in biomedicine and sensors have been found.

It was shown that the percolation threshold (obtained from impedance measurements) represents a critical concentration above which NPs agglomeration takes place such that the effective surface area of the nanocomposite decrease. Herein we report the successful production of chitosan based nanocomposites: a) CS-Ag films with antibacterial properties, b) CS-Au sensor for detection of Cu++, c) CS-nanoclay sensor for detection of NO3- and CS-carbon nanotubes for vapour sensing. For all these applications the best functional performance of nanocomposites has been observed when NPs concentration increases and approaches the percolation threshold. The obtained relationship between electrical percolation threshold and functional properties of polymer nanocomposites is of primary importance in the design of high-performance applications.

Keywords: chitosan, conductivity nanoparticles, percolation threshold.

Nanomaterials for solar energy conversion systems

Gerko Oskam

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

E-mail: gerko.oskam@cinvestav.mx

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

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

In the solar fuels research project, we use a combinatorial technique to find new metal oxide nanomaterials for solar water splitting. In addition, we use advanced (photo)electrochemical methods in order to study the fundamental processes taking place in promising nanomaterial, analyzing the hole transport and recombination properties using intensity-modulated methods, including photovoltage (IMPV) and photocurrent spectroscopy (IMPS). We have recently obtained interesting results for the p-type semiconductor $CuBi_2O_4$.

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

Development of hydrodesulfurization catalysts based on transition metal sulfides

Sergio Fuentes Moyado
Departamento de Nanocatálisis, Centro de Nanociencias y Nanotecnología Universidad Nacional Autónoma de México, campus Ensenada.
E-mail: fuentes@cnyn.unam.mx

The environment protection in the case of air requires the production of ultra low sulfur fuels for use in transportation. In Mexico the required level of sulfur in fuels is regulated by NOM 086 that indicates that gasoline has to be less than 30 ppm and 10 for diesel. Therefore the Pemex refineries need to improve catalysts used in hydrodesulfurization units to reach those levels. Indeed, the challenge is even more demanding for Mexican refineries that process stocks derived from heavy oil as the Maya which contain more than 3 wt %. This work presents results about the development of scalable prototypes of CoMo and NiMo catalysts both in bulk form or suported on gamma-alumina designed to process heavy oil fractions derived from maya crude oil.

The bulk catalysts were prepared by decomposition of alkylammonium thiosalts of Mo and W, including Ni or Co as promoters. The obtained catalysts presented high surface area, high catalytic activity, high carbon content and they were very selectives for hydrogenation path.

In the case of supported catalysts three cases were investigated:

a) Silica based mesoporous materials SBA-15 and KIT-6 covered by alumina or titania which improve the dispersión of MoS2 nanostructures and ameliorate the catalytic activity favoring the direct hydrodesulfurization path.

b) Alumina nanorods which induce the formation of low dimensionality WS2 and improve the catalytic activity for reactions HDS of DBT y 4,6 DM-DBT.

c) Alumina promoted with Y zeolite for preparation of CoMo and NiMo catalysts used in the hydrotreating of heavy oil fractions as light gasoil (LGO) to produce ultra low sulfur fuels. Pilot plant results show that prototypes developed are able to produce ultra low sulfur diesel under similar conditions as those in refinery plants even in the case where high contents of refractory charges as light cycle oil (LCO) are introduced.

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From synthesis to application of photovoltaic perovskite nanowires

László Forró

Laboratory of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne, CH-1015, Lausanne.

E-mail: laszlo.forro@epfl.ch

In the last few years, the organolead halide perovskite CH3NH3PbI3 and its derivatives have been found to be very efficient light harvesters and ambipolar semiconductors revolutionizing the field of solid-state solar cells. Its low temperature fabrication process allowed to design simpler solar cell structures (i.e.from mesoscopic to planar junctions) which yielded efficiencies exceeding 20%. The major research area in this field is photovoltaic device engineering although other applications as solar water splitting, field effect transistors (FETs), ultra-broadband photodetectors, thermoelectric devices, light emitting diodes and lasers are being explored as well.

Recently, we have shown that nanowires of this photovoltaic perovskite can be synthesized, which in association with carbon nanostructures (carbon nanotubes and graphene) make outstanding composites with rapid and strong photoresponse. They can serve as conducting electrodes, or as central components of detectors. The performance of several miniature devices based on these composite structures will be demonstrated. Our latest findings on the guided growth of perovskite nanowires by solvatomorphgraphoepitaxy will be presented. This method turned out to be a fairly simple approach to overcome the spatially random surface nucleation. The process allows the synthesis of extremely long (centimeters) and thin (a few nanometers) nanowires with a morphology defined by the shape of nanostructured open fluidic channels. This low-temperature solution-growth method could open up an entirely new spectrum of architectural designs of organometallic-halide-perovskite-based heterojunctions and tandem solar cells, LEDs and other optoelectronic devices.

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Understanding Optical Absorption Spectrum of Copper Sulfide Nanoparticles

Jonathan C. Luque-Ceballos,[a] Alvaro Posada-Borbón,[b] María E. Trujillo-Camacho,[c] Ronaldo Herrera-Urbina,[c] R. Aceves,[a] Alvaro Posada-Amarillas[a]

[a]Departamento de Investigación en Física, Universidad de Sonora

[b]MSc in Applied Physics Program, Chalmers University of Technology

[c]Departamento de Ingeniería Química y Metalurgia, Universidad de Sonora

E-mail: posada@cifus.uson.mx

Copper sulfide semiconducting nanoparticles have attracted considerable attention because of their outstanding photochemical properties. Absorbance and transmittance of these nanoparticles have been measured and utilized to estimate the energy band gap which is about 2.29 eV. Their structural characterization by means of TEM and XRD measurements has shown an hexagonal structure characteristic of covellite phase, and a main Raman peak has been observed at about 474 cm^{-1}. Utilizing the static and dynamical approaches of Density Functional Theory and a simple ground-state structural model which resembles the covellite arrangement of atoms, the theoretical Raman activity was obtained at 489 cm^{-1}, corresponding to a symmetrical stretching mode of a three-membered fragment of sulfur atoms, of a C_{2v} symmetry pentamer cluster structure. The experimental UV-vis absorbance spectrum is explained in terms of calculated excited state transitions in the observed energy range. The absorption peaks are assigned mainly to σ→σ*, π→π*, and σ→π* type transitions. The photocatalytic activity of CuS nanocrystals is examined in the UV and visible regions.

Ligand effects on the optical and chiroptical properties of thiolated gold clusters

A. Tlahuice-Flores

CICFIM-Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL 66450.

E-mail: tlahuicef@gmail.com

The effect of ligands (chiral and achiral) protecting thiolated clusters has been studied based on density functional theory (DFT) and its corrected long-range interaction (DFT-D) approach. It was found that the electronic properties (energy levels) depend on the specific ligands, which induce distinct distortions on the Au–S framework. The ultimate goal is to determine if simplification of ligand as -SCH_3 is able to reproduce the displayed vibrational, bonding, optical and chiroptical properties. Moreover, it is important to find if calculated profiles display more intense signals which is expected to future applications as chemical sensors.

Applications of nanoscale inorganic materials for solar energy uses, environmental protection and health preservation

David Díaz[♦], I. Zumeta-Dubé[♦], J. Rizo-Estrada[♦], D. Velasco-Arias[♦] and Hernández-Delgadillo R[♣].

[♦]Facultad de Química, Universidad Nacional Autónoma de México .

[♣]Facultad de Ciencias Biológicas, Instituto de Biotecnologia, Universidad Autónoma de Nuevo León, Monterrey, México.

E-mail: david@unam.mx

In this oral contribution three lucky cases, where some common and inexpensive inorganic nanomaterials are involved with applications of main topics of this colloquium, will be discussed.

1. In the first case we sensitized TiO2 electrodes with QDs obtained by the SILAR technique, starting from aqueous solutions of Bi(NO3)3 as the cation precursor and Na2S as the sulfide source. In a second variant, we used a similar procedure, but the Na2S solution was replaced by elemental sulfur vapor as precursor. We found that an immersion time of 30 min leads to an efficient QDs deposition into the TiO2 porosities closer to the substrate. It was found that the presence of sodium ions in the reaction system does not directly lead to the formation of Bi2S3 on the porous TiO2 layer. Additionally, the I g I w ph I Th − I g (J−V) characteristic and the photocurrent time stability revealed: (i) the much better performance of Bi2S3 QDs sensitized photoelectrodes obtained using elemental sulfur vapor as precursor and (ii) the inconvenience of sodium ions inclusion in the attempted synthesis procedure [1].

2. A straightforward, environmental friendly and economical one-step degradation method of methyl-parathion (MP) -- a common, persistent, neurotoxic, organophosphorus pesticide -- was achieved through an aqueous suspension of copper (I) oxide nanoparticles (NPs). This type of contaminated rinse waters come from fruits previously sprayed with this bug killer. 1H nuclear magnetic resonance (NMR) results show that the hydrolysis of MP leads to the formation of 4-nitrophenol as the most common reaction product and the P=S of the MP becomes P=O, confirmed by 31P NMR. UV-visible spectra suggest the reaction follows a pseudo first-order kinetic procedure. MP degradation was established to be occurring

because of the basicity properties of Cu2O NPs which increase with decreasing particle size. Our results support the potential application for the treatment of water contaminated with organophosphate pesticides [2].

3. The objective of this investigation was to evaluate the fungicidal activity of Bi2O3 nanoparticles against Candida albicans, and their antibiofilm capabilities. Our results show that aqueous colloidal bismuth oxide nanoparticles display antimicrobial activity against C. albicans growth and a complete inhibition of biofilm formation. These results are better than those obtained with the most effective oral antiseptic and commercial antifungal agents. These outcomes suggest that bismuth oxide colloidal nanoparticles could be a very interesting candidate as a fungicidal agent to be incorporated into an oral antiseptic [3].

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Chirality at the Nanoscale: Geometric quantification of chirality in Bare and Ligand-Protected metal clusters

J. Jesús Pelayo[1], Robert L. Whetten[2], Ignacio L. Garzón[1]

[1] Instituto de Física, Universidad Nacional Autónoma de México, México D.F., México.

[2] Department of Physics and Astronomy, University of Texas, San Antonio, 78249 San Antonio, Texas, USA.

E-mail: garzon@fisica.unam.mx

Chirality has been found as a relevant property of nanomaterials, including ligand-protected metal clusters and nanorods [1-4]. This property is not only crucial in nanotechnology developments related with asymmetric catalysis and chiroptical phenomena, but also generates fundamental questions on the existence of chirality at the nanoscale. In fact, x-ray total structure determination, electron diffraction studies, NMR and circular dichroism spectroscopies, as well as theoretical calculations performed on gold clusters protected with thiolate or phosphine ligands have confirmed the existence of chiral structures in the size range of 18-144 Au atoms. In this work [5], we realize a comparative analysis of the degree or amount of chirality existing in chiral ligand- protected gold clusters (LPGC), through a geometric quantification, using the Hausdorff chirality measure (HCM) [6]. The calculated HCM values provide a quantitative framework to compare, classify, and gain insight into the origin of chirality. Interestingly, these values are consistent with the current knowledge on the different sources of chirality: achiral cores and chiral arrangement of ligands in, for example, Au102(SR)44 and Au38 (SR)24, or intrinsically chiral cores, like in Au52(SR)32 and Au20 protected with phosphine ligands. Our calculations are also helpful to assign an index of chirality, and classify as chiral several recently synthesized and structurally solved LPGC that, in first instance, were not identified as such. The calculated HCM values are used to extract trends on how chirality is spatially distributed in LPGC, and correlate them with optical activity measurements. The main trend indicates that the Au-S interface has the dominant role in the chirality of LPGC [5].

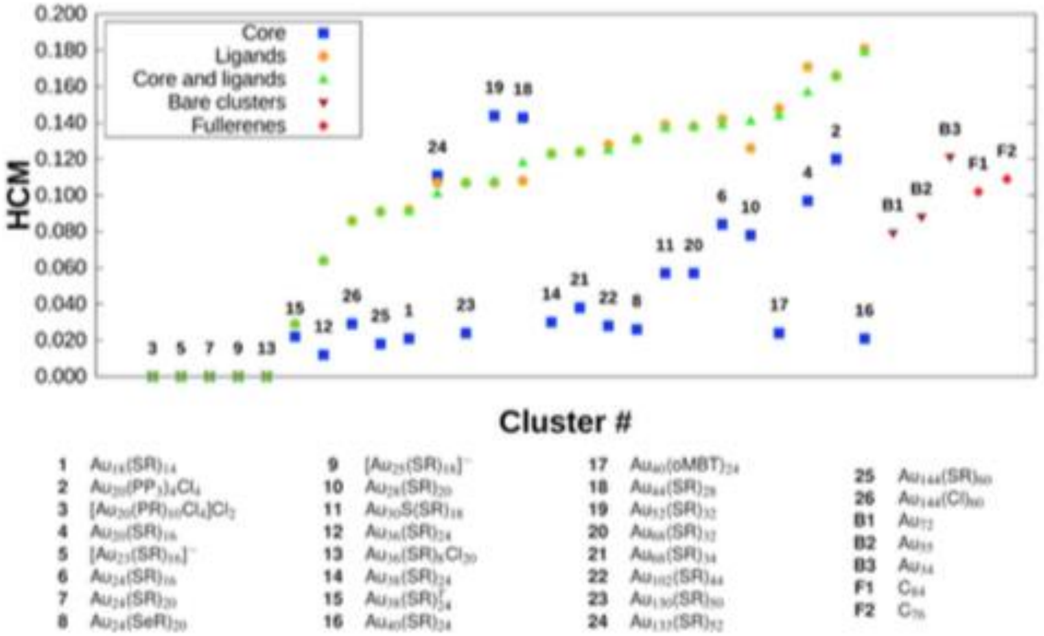

Fig. 1 Geometric chirality (HCM) values for 26 ligand-protected gold clusters. The numbers in black above the blue squares denote the cluster number (index).

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POSTER SESSION

Collection and reuse of nanowaste: towards a sustainable nanotechnology

M.S. Cruz Leal, O. Goiz, C. Felipe, F. Chávez, G. F. Pérez Sánchez, P. Zaca

Unidad Profesional Interdisciplinaria de Biotecnología, Instituto Politécnico Nacional

E-mail: xaraicruz@gmail.com

In this work, the nanowastes generated during the synthesis of nanomaterials by using the HFCVD technique were recovered and studied. This material was used for photo-degradation of organic matter. The results showed that the nanowaste can be recycled if it exhibit similar characteristics to the synbtehsized nanomaterial.

Use of nanowaste for photo-degradation of organic matter and catalytic soot oxidation

M.S. Cruz Leal, O. Goiz, C. Felipe, F. Chávez, G. F. Pérez Sánchez, P. Zaca Morán, J. Flores Moreno

Unidad Profesional Interdisciplinaria de Biotecnología, Instituto Politécnico Nacional

E-mail: ogoiza@gmail.com

In this work, the nanowastes generated during the synthesis of nanomaterials by using the HFCVD technique were recovered and studied. This material was used for catalytic soot oxidation. The results showed that the nanowaste can be recycled if it exhibit similar characteristics to the synbtehsized nanomaterial.

Treatment of Vinasse from Tequila by Coagulation-Flocculation and Heterogeneous Photocatalysis using TiO2 Nanoparticles

[*1]Alicia Rodríguez Arreola, [1]Alejandra Carreon-Alvarez, [1]Marciano SanchezTizapa, [1]Rocío Castañeda Valderrama, [2]José Luis Rodríguez López, [1]Lorenza Augusta Cortés Villegas.

[1]Departamento de Ciencias Exactas y Naturales. Centro Universitario de los Valles (CUVALLES). Universidad de Guadalajara. Carretera Guadalajara-Ameca Km. 45.5, C.P. 46600.

[2]Instituto Potosino de Investigación Científica y Tecnológica (IPICYT), Camino a la Presa San José 2055, Col. Lomas 4a sección, San Luis Potosí, S.L.P. 78216, México.

*E-mail: ra.alici@gmail.com

In this study is reported the treatment of tequila vinasse by heterogeneous photocatalysis using titanium dioxide nanoparticles (NPs-TiO2). Tequila vinasse was pretreated by physical-chemical coagulation-flocculation. It was used aluminum sulfate (Al2(SO4)3(14-18) H2O) and calcium hydroxide (Ca(OH)2) as a precipitating agent. Tequila vinasse was characterized before and after treatment by measuring the pH, the determination of the chemical oxygen demand (COD), colour and total suspended solids (TSS). Moreover, the NPs-TiO2were synthesized by the sol-gel and annealing at 400 °C for 1 h in air atmosphere. The NPs-TiO2 were characterized by X-ray diffraction (XRD), spectroscopy ultraviolet light absorption, transmission electron microscopy (TEM) and Raman spectroscopy. By XRD was found in the annealed samples, the anatase phase of TiO2 which presents the most active phase in photocatalysis. In the treatment of vinasse was used a type of batch reactor with continuous stirring, in which 200 mg of NPs-TiO2 were added to 200 mL of clarified tequila and hydrogen peroxide (H2O2) as highly oxidizing agent andfinally was irradiated for 3 hours with ultraviolet light as an energy source. The photocatalysis heterogeneous process coupled with the coagulation-flocculation process were considered as efficient as it was possible to obtain percentages of reduction of 70, 86 and 99%, for COD, color and SST, respectively.

KEYWORDS: vinasse, heterogeneous photocatalysis; TiO2 nanoparticles; sol-gel; coagulation-flocculation.

Synthesis optimization of magnetite nanoparticles by coprecipitation method

D. Ravelo[1], H. T. Yee[1], J. A. Ortega[1], H. Balmori[2], C. R. Diaz[3]

[1]Escuela Superior de Física y Matemáticas, Instituto Politécnico Nacional, Edificio 9, U.P. A.L.M., Col. San Pedro Zacatenco, C.P. 07738, México D.F., México.

[2]Centro de Nanociencias y Micro y Nanotecnologías (CNMN), Instituto Politécnico Nacional (IPN), Unidad Profesional Adolfo López Mateos, Zacatenco, Delegación Gustavo A. Madero, C.P. 07738, Ciudad de México, México.

[3]Centro de Biomateriales, Universidad de La Habana (BIOMAT), Avenida Universidad s/n entre G y Ronda, Vedado, apartado postal 6323, La Habana, Cuba.

E-mail: david.raveloacua258@gmail.com.

An optimized synthesis of iron oxide (〖Fe〗_3 O_4) nanoparticles was conducted by coprecipitation using a solution composed of ferrous chloride, ferric chloride, and hydrochloric acid as a cationic solution and ammonium hydroxide as an alkaline solution. Two methods were used, classical coprecipitation synthesis and the optimized coprecipitation synthesis (where experimental conditions are kept constant) to compare the respective agglomeration and crystallite size of the nanoparticles produced; the usual agglomeration caused by these procedures is avoided by applying a coating of tetraethyl orthosilicate (TEOS). The magnetite nanoparticles were characterized by X Ray Diffraction (XRD), Infrared Spectroscopy (FT.IR), Scattering Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and magnetic measurements with a magnetometer (SQUID). These techniques revealed that the synthesis produced spherical nanoparticles with diameters varying between 9-12 nm. The lack of oxidation in the synthesis process indicated stable nanoparticles.

Chiral phosphorus nanotubes: structure, bonding,and electronic properties

H. N. Fernández-Escamilla, J. J. Quijano-Briones, and A. Tlahuice-Flores

CICFIM-Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL 66450.

The study of black phosphorus nanotubes (PNTs) had been devoted to zigzag and armchair structures, with no consideration of chiral structures to date. In this work, we studied the structural and electronic (band structure) properties of chiral nanotubes using a periodic plane wave-pseudopotential approach. We found that some chiral nanotubes display similar bandgaps and binding energies per atom (BEA) as armchair PNTs and Born–Oppenheimer molecular dynamics (BOMD) calculations attest their thermal stability. Interestingly, we determined that the bandgap is tuned by varying the PNTs chirality and it is not related to their diameters. This feature can be exploited in optical and electronic applications wherein a direct and sizable bandgap is required.

Keywords: Phosphorene,chiral nanotube, band structure.

Doped penta-graphene and hydrogenation of its related structures: a structural and electronic DFT-D study

J. J. Quijano-Briones, H. N. Fernández-Escamilla and A. Tlahuice-Flores

CICFIM-Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL 66450.

The structure of penta-graphene (penta-C), an irregular pentagonal two-dimensional (2D) structure, has been predicted recently. In this work we carried out a dispersion-corrected density functional theory (DFT-D) study of the penta-C doped with Si, Ge and Sn atoms and its related hydrogenated penta-C structures (H–penta-C–X). We predict various new structures as thermally stable based on Born–Oppenheimer molecular dynamics (BOMD) calculations. Moreover, their dynamical stability is attested by phonon dispersions spectra. In general, we found that the bandgap value of doped structures reduces, while H–penta-C–X show large bandgap values. This feature can be exploited for potential uses of hydrogenated doped-penta-C structures as dielectric layers in electronic devices.

Keywords: Pentagraphene, DFT-D, Electronic structure.

Immobilization of Candida antarctica, Rhizomucor miehie and Thermomyces lanuginosus lipases on a functionalized layered double hydroxide with sodium dodecyl sulfate

A. J. Mendoza, G. G. Carbajal-Arizaga, J. A. Córdova-López, J. C. Meteo-Diaz, J. J. Flores-Rivera, J. Barajas-Vargas

Centro Universitario de Ciencias Exactas e Ingeniería, Univerdad de Guadalajara.

E-mail: jama8507_@hotmail.com

In this study, MgAl (4:1)–LDHs (layered double hydroxides) intercalated with sodium dodecyl sulfate (0.96, 0.90, 0.54 y 0.18%) were prepared by coprecipitation method. The existence of hidrofobic part in LDHs improved the charge of protein on the support for Candida antarctica lipase, Rhizomucor miehie lipase and Thermomyces lanuginosus lipase by hydrophobic adsorption on the surface support. The best support for C. antarctica lipase was MgAl (4:1) _SDS (0.18%) with 89.7 (mg) protein adsorbed/ (g) of support and 209.95 (U) protein/ (g) of support. For the case R. miehie lipase was MgAl (4:1)_SDS(0.96%) with 82.86 (mg) of protein/ (g) of support and 237.97 (U) protein/ (g) of support and finally for T. lanuginosus lipase the results were MgAl (4:1)_SDS(0.96%) support, 62 (mg) protein adsorbed/(g) of support and 93.27 (U) protein/ (g) of support. The support with and without enzymes were characterized by Powder X–Ray Diffraction (XRD), Infrared spectroscopy by Fourier Transform (FT-IR), etc.

Moreover, the immobilized enzymes were probed in hydrolysis with p-NPB sustrate. They were higher temperatura resistence, similar pH value and better thermoestability in hydrolysis with p-NPB sustrate.

Besides, they were probed for the synthesis of Caffeic acid phenethyl ester (CAPE) in organic solvents with good results.

Photochemical Synthesis of Flat Silver Nanoparticles

P.E. Cardoso-Avila[1], M.M. Martinez García[1], A. Martinez Hernandez[2], J.L. Pichardo-Molina[1]

[1]Laboratorio de Espectroscopia Biomédica y Nanomateriales, Centro de investigaciones en Óptica, A.C., León, México.

[2]Universidad Tecnológica de Tulancingo.

Flat Silver Nanoparticles (FS-NPs) were obtained by means of a photochemical transformation process. Small spherical NPs synthetized by chemical reduction show an excellent colloidal stability, as they can be stored for months without aggregation or any change in morphology. But as soon as the spherical silver NPs (plasmon band around 400nm) are irradiated with green and red LEDs to promote the photochemical process. The use of these out-of-resonance light sources allowed us to tune the plasmon band in the red region of the visible spectra. UV-Vis spectroscopy was used to study the growth kinetics and the optical characterization of these colloids. On the other hand SEM and DLS allowed us to determine the morphology and size distribution. We have developed a fast and low cost photochemical method to synthetize flat silver NPs with a plasmon band in the red region of the visible spectra while maintaining a small size.

Influence of the reaction conditions on the particle size and morphology modulation of TiO_2 obtained by a microwave assisted method

Ana Laura Sánchez-Romero[1], José Luis Sosa-Sánchez[1], José Alberto Luna-López[1], Adan Luna-Flores[1,2]

[1]Centro de Investigación en dispositivos Semiconductores, Instituto de Ciencias BUAP, 14 sur y Av. San Claudio,edificio 103D Ciudad Universitaria, Puebla, Pue, C.P. 72570, México.

[2]Facultad de Ingeniería Química, BUAP. Av. San Claudio, Ciudad Universitaria, Puebla, Pue., C.P. 72570, México.

The development of new synthetic strategies to obtain advanced functional materials and in particular nanostructured semiconductor oxides is of high relevance for the advance of science and technology. This is so, because these materials constitute one of the building blocks to assemble, in a bottom-up approach, more complex structures that can find an application in the fields of energy conversion and photocatalysis.Titanium dioxide (TiO_2) is one of the most widely studied materials due to its advantageous properties such as photophysical activity, great stability, big surface area per volume unit, catalytic, and non-toxic behavior. However, its wide bandgap (3.2 eV) and the well documented recombination process for their photo generated electron-hole pair affect their efficiency in catalytic and photovoltaic applications. In this work, we report an improved microwave assisted synthesis of TiO_2 in which the effect of the thermal treatment for both the microwave reaction and the calcination process on the particle size and morphology of the products was determined. In addition, the effect of the use of surfactants such as Triton X-100 and doping agents (HF and other fluorine compounds) to improve its photocatalytic performance for the degradation of organic dyes is also determined. The characterization of the TiO_2 products was carried out by x-ray diffraction, SEM, BET method and FT-IR. We also carried out photocatalytic activity tests of the synthesized material to evaluate the degradation of the Rhodamine B compound.

Keywords: synthesis of TiO_2, nanometric size and morphology and photocatalytic activity.

Synthesis and characterization of nanomaterials based layered double hydroxides functionalized with biologically active molecules

Osvaldo Gutiérrez Guzmán[1], Gregorio Guadalupe Carbajal Arízaga[2], Jenny Arratia-Quijada[1]

[1]CUTonalá, Av. Nuevo Periférico No. 555 Ejido San José Tatepozco, C.P. 45425, Tonalá, Jalisco, México.

[2]CUCEI, Departamento de Química, Blvd. Marcelino García Barragán No. 1421, C.P. 44430, Guadalajara, Jalisco, México.

The double hydroxides laminate (HDLs) they are synthetic compounds also acquaintances like anionic clays or synthetic clays, there are formed by sheets of metallic hydroxides loaded positively that are stabilized by anions you will interlaminate. The HDLs possess the such only properties as the capacity of exchange controlled of anions, the great chemical stability, the solubility dependent on the pH, the property of controlled liberation, excellent biocompatibility, and low toxicity, for what they have showed diverse applications in the biomedical area as selective sensors of molecules, carriers of biologically active molecules and agents theranostics. The present work there proposes the functionalization of such biological active molecules as collagen, hidroxi-methyl butirato (HMB) and gallic acid in HDLs them carriers apply as agents of these molecules supporting his biological activity. The synthesis of the functioned HDLs was realized by means of co-precipitation of you go out in alkaline way, reconstruction or ionic exchange. The physicochemical characterization of the materials was realized by means of bosses of diffraction of X-rays and analysis of infrared. The size of particle I determine with Debye Scherrer's equation. Since results of this work obtained HDLs Zn -Al (2/1)) functioned with collagen and HMB, and Mg/Al (2.5/1) functioned with gallic acid. The nanomaterial's present a size of particle estimated of 3.84 nm. The biological activity of the HDLs functioned with the different biological active molecules obtained in this work will be realized in future biological tests using models of sarcopenia.

Synthesis and caracterization of nanocomposites comprised of layered double hydroxides and biomolecules (chitosan or lignin) for their use as adsorbents

Rodolfo Ortiz[1], Cesar M. Gómez[1,2], Orfil González[1], Gregorio G. Carbajal[2]

[1]Departamento de Ingeniería Química, Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421, Guadalajara, 44430, México.

[2]Departamento de Química, Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421, Guadalajara, 44430, México.

E-mail: ortizrodolfo2000@yahoo.com.mx

Adsorption is one of the most promising techniques applied for the water decontamination from organic pollutants and heavy metals. To achieve this goal, materials like nanocomposites possess a series of unique physical and chemical properties. A very important one is that most of the atoms that have high chemical activity and adsorption capacity are on the surface of the nanocomposites. Layered double hydroxides (LDH) are a class of synthetic anionic clays at nanoscale consisting of positively charged hydroxyl layers of bivalent and trivalent metal ions with exchangeable interlayer anions. In recent years, many studies have focused on the application of LDH in environmental remediation of different pollutants. In this study, nanocomposites of chitosan-LDH (CLDH) and lignin-LDH (LLDH) were synthesized for adsorption of the heavy metal Cr6+. The raw chitosan, raw lignin, unsupported LDH, CLDH and LLDH were characterized by X-Ray diffraction (XRD), transmission electron microscopy (TEM) and Fourier transform infrared spectroscopy (FTIR). Batch adsorption experiments were performed for determining the pollutant adsorption characteristics of CLDH and LLDH. The amounts of heavy metal adsorbed at variable concentrations were determined by an indirect colorimetric method based in the reaction between diphenylcarbazide and the Cr6+ that produced red-violet color complexes. Equilibrium isotherm data were analyzed by the Langmuir, Freundlich and Dubinin-Radushkevich equations using non-linear regression analysis.

Keywords: Nanocomposites; layered double hydroxides; adsorption; chitosan; lignin; chromium.

Study of the effect of the amount of adsorbent in the lignocellulosic waste and magnetite nanoparticulate composite for removing zinc and chromium (VI) in synthetic solutions

Tanya Medina, Víctor H. Guerrero, Christopher Asimbaya, David Alvear

Department of Materials, New Materials Laboratory, National Polytechnic School
Ladron de Guevera E11-253, Quito 170517

In this study, removals of zinc and chromium (VI) of different aqueous solutions were performed by using magnetite nanocomposites with three types of lignocellulosic waste (laurel, canelo and eucalyptus). Magnetite nanoparticles were obtained by co-precipitation method of ferric and ferrous salts in sodium hydroxide aqueous solution. For the nanocomposite synthesis, each lignocellulosic waste was added to magnetite to the same conditions that were, stirring of 1 000 min-1 with a reaction time of 45 min at 50 °C. Both magnetite as the nanocomposite were characterized by Raman Spectroscopy. Removal tests were performed with different contact times and stoichiometric ratios of 1:1 and 3:1 (lignocellulosic waste/magnetite). The maximum rate of zinc removal was reached with 60 min of contact time, with a synthetic solution initial concentration of 50 mg/L of zinc, at pH 6 and stirring of 150 min-1; while for the removal of chromium (VI), the maximum rate were obtained at 30 min of contact time at 25 °C, pH 2,5, and stirring of 200 min-1 of the synthetic solution with an initial concentration of 20 mg/L of chromium (VI). The lignocellulosic waste of the nanocomposite in 3:1 ratio, which allowed a greater adsorption of metal ions, was the laurel with zinc removal percentages of about 97%, and 99% for chromium (VI).

Keywords: magnetite, lignocellulosic waste, metal ions.

SERS- effect of Au/SiO_2 Core- Shell nanoparticles, in the detection of glucose

K. de Lázaro- Gasca[1], Ma. D L. Ruiz- Peralta[1], E. Rubio- Rosas[2]

[1]Facultad de Ingeniería Química- BUAP, Av. San Claudio, S/N, C. P. 72570, Ciudad Universitaria, Cd. de Puebla, Puebla, México

[2]Centro Universitario de Vinculación y Transferencia de Tecnología, Benemérita Universidad Autónoma de Puebla. Av. San Claudio, S/N, C. P. 72570, Ciudad Universitaria, Cd. de Puebla, Puebla, México

Core-shell nanoparticles have been applied due to improved properties such as less cytotoxicity, compatibility, better conjugation to other bioactive molecules, improved thermal stability and chemical, detection of biological molecules [1]. The sensitivity in detection of biological molecules by Raman spectroscopy can be strongly driven and, in some cases, extending to the level of single molecule detection. An example of this is the SERS effect [2]. In this work Au/SiO_2 nanoparticles with spherical like morphology were fabricated in two steps, Au nanoparticles were synthesized by chemical reduction, while SiO_2 shell was prepared by Stöber method ; changing the synthesis (hydrolysis and condensation reactions) conditions it could be control the shell thickness. The DRX results show two phases present assigned to Au fcc and SiO_2 amorphous phase, the ICP was carried out to determine elemental composition of the nanoparticles; TEM results show different shell thickness, and, apparently particle- particle aggregation is the main mechanism involved in the shell formation; functionalization of Au / SiO_2 surface was performed in order to detect Glucose from 2 mM to 6 mM similar concentration present in blood.

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Pectin matrix as a freeze-drying storage method for gold nanoparticles

Daniel Jáuregui Gómez, Oscar Miguel Bermejo Gallardo, Francisco Carvajal Ramos, Alberto Gutiérrez Becerra.

Engineering Department, University of Guadalajara. Av. Nuevo Periférico Oriente 555, Tonalá 45425, México.

E-mail: ing.danieljauregui25@gmail.com

Nowadays there are an increasing number of studies focused on the application of metallic nanoparticles in different scientific fields e.g. biotechnology, catalysis, energy storage, advanced materials, etc. Depending on the application, it is necessary to have nanoparticles with specific size, size distribution and shape. To satisfy this condition, several synthesis methods have been proposed.

One of the most common method consists in the reduction of a metallic ion with a reducing agent followed by the addition of a capping agent. According to different results published regarding this matter, this type of systems are able to control the size and shape of the metallic nanoparticles, but only for a short period of time. For instance, to synthesize gold nanoparticles, sodium citrate is typically used because it acts as both, reducing and capping agent, nevertheless, the stabilization of the nanoparticles rarely lasts more than two months. Increasing the stability of nanoparticles avoiding their aggomeration or chemical decomposition is of extremely interest in nanotechnology. In this work, we propose a method that allows to store gold nanoparticles for a prolonged time.

Gold nanoparticles synthesized by the reduction of gold ions with ascorbic acid, are stabilized with pectin. When the gold nanoparticles-pectin mixture is lyophilized, a sponge-like solid is obtained. Due to the low amount of remaining water in the dry pectin matrix, nanoparticles agglomeration is negligible, making the freeze-drying pectin matrix a cheap, fast, environmentally friendly and biocompatible method to store nanoparticles. By just adding water, the matrix containing gold nanoparticles can be redispersed for the required application. The system was characterized before and after lyophilization by means of UV-vis spectroscopy, X-ray diffraction and Electron microscopy. The results show that lyophilization does not modify the size, size distribution and shape of the gold nanoparticles.

Keywords: Gold nanoparticles; pectin; storage; freeze-drying.

Improvement of hydrolysis method by SOL-GEL process assisted by microwave technique TiO_2 of nanoparticles

Felipe de Jesus MORALES[1], Marco Antonio Alaniz Hernandez[2], Maria de la Luz Mota Gonzales[2,3], Carlos Ivan Rodriguez Rodriguez[1], Amanda Carrillo Castillo[2]

[1]Universidad Tecnologica de Ciudad Juarez, No.3051, Lote Bravo II, Ciudad Juarez Chihuahua. CP 32695, Mexico.

[2]Instituto de Ingenieria y Tecnologia, Universidad Autonoma de Ciudad Juarez. Cd. Juarez Chihuahua. CP 32310, Mexico.

[3]CONACYT, Direccion Adjunta al Desarrollo Cientifico, Direccion de Catedras, Insurgentes Sur 1582, Credito Constructor, D.F, Benito Juarez, Ciudad de Mexico, 03940, Mexico.

Titanium Dioxide (TiO_2), otherwise known as Titania, has being an interesting subject for study due to its various properties, such as; bio compatibility, Semi conductivity, Anti-Septic, UV-Ray absorption and photocatalitic properties among others. One of the biggest problems with the study of Titania it’s the high cost on the general market, due to the most useful crystalline phase for study being Anatase difficult to reach, and the expenses of time it takes when synthesizing. In this work it’s reported the synthesis of Titania nanoparticles obtained by sol-gel process at low temperatures assisted by the microwave technique. It was utilized a source of Titanium (Ti) ions, titanium Isopropoxide, water as a solvent and Isopropilic alcohol. It was found that the size of the nanoparticles is dependant of de Ti ions concentration, the sizes located in a range from 20 to 80 nanometers. The nanoparticles where characterized via XPS and UV-Ray spectroscopy, X-Ray Diffraction (XRD) and where also scanned via Scanning Electron Microscopy (SEM).

Keywords: TiO_2, Sol-Gel, Nanotechnology.

Optical properties of different sequences of nucleotides RNA type of the DIS of the HIV-1 genome from TD-DFT calculations

Pedro Francisco-Santiago[1], Jorge Ramón Soto-Mercado[1], Luis Enrique Sansores-Cuevas[2], Bertha Molina Brito[1]

[1]Facultad de Ciencias, Av. Universidad 3000, Circuito Exterior S/N, Ciudad Universitaria, Coyoacán, 04510, México, D.F.

[2]Instituto de Investigaciones en Materiales, Av. Universidad 3000, Circuito Exterior S/N, Ciudad Universitaria, Coyoacán, 04510, México, D.F.

In this work we carried out a TD-DFT study to predict optical properties of different pyrimidine and purine sequences, which conforming the Dimerization Initiation Site (DIS) of the HIV-I genome [1]. The sequences RNA type here study are; 5'-CA-3' , 5'-UG-3', 5'-UGC-3',5'-CACA-3', 5'-AAUG-3', 5'-CACACA-3', 5'-GUGCAC-3' and 5'-UGAAGU-3'. To approach the exchange and correlation interactions we used the GGA-PBE functional with the Grimme Dispersion-3 term, within the ZORA scalar approximation. The TZP bases were used to model each atom in all cases. Additionally, we used the water as solvent to study its influence in the optical properties of the nuclei bases sequences above described, for which, we employed the Conductor-like Screening Model (COSMO) [2] to model the interaction among the solvent and RNA sequences. Comparing the UV-vis spectra calculated with and without dispersion term and solvent, it can be observed an ultraviolet-shift, which is more pronounced when solvent is taken into account. Besides, for all chains we also calculated the CD (Circular Dichroism) spectra using the same methods above mentioned. A polarity change in the CD spectra is obtained when the dispersion term is included.

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Synthesis and characterization of copper and cobalt ferrites for removing arsenic (III, V) in water

Morales A. Corazón[a] Astudillo S. Pablo[a], Martínez V. Sergio[b]

[a]Universidad de Guadalajara-Campus Tonalá Av. Nuevo Periférico No. 555, Ejido San José Tatepozco, 48525 Tonalá, JAL 01 33 3540 3020

[b]Universidad Autónoma del Carmen-Facultad de Ingeniería Av. Central S/N esq. con Fraccionamiento mundo maya 24115, Ciudad del Carmen, CAMP 381 10 18 ext. 1702

E-mail: crzn04@gmail.com

Nowadays an important challenge corresponds to the removal of heavy metals and inorganic harmful substances to the health, specifically arsenic (As), which in many cases also causes a severe damage to the environment [1]. In this framwork, the development of technologically viable and accessible alternatives to remove As from water constitutes a priority need for many places with high concentrations of As in the water. The aim of this work is to implement a low-cost methodology in the water treatment, and specifically in the removal of the As. For this reason, magnetic nanoparticles have been obtained based on M X Fe 3-xO 4 (where M = Fe, Cu and / or Co and X = 0 or 1) using the method proposed by Massart [2]. This nanoparticles have been characterized by means of diffraction of X-rays, magnetometry, scanning electron microscope and raman spectroscopy. Likewise, nanoparticles kinetic adsorption was determined using As in trivalent and pentavalent conditions where it can be seen the viability of using magnetic nanoparticles as arsenic removal agents.

Key words: Adsorption, arsenic, nanoparticles, water.

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NaYF$_4$:Yb-Er Up-Converter material, as scattering layer in sesitized solar cell

V.H. Romero[1], J. Pablo Guerrero[1], T. Lopez-Luke[2], D. Ramachari[2], Elder de la Rosa[2], C. A. Guzmán[1], B. Rangel Sulbaran[1].

[1]Centro Universitario de Tonalá de la Universidad de Guadalajara, División de Ciencias, Tonalá Jal. Nuevo Periférico #555, 48525, México.

[2]Centro de Investigaciones en Óptica, A. P. 1-948, León Gto. 37160, México

In the last decade, significant advances have been achieved in the development of Quantum Dot sensitized solar cell. A typical configuration of these systems consists of two layers of semiconductor material, where the second one, furthermore of interaction with the sensitizers, it works as scattering layer. In this work, was incorporated an additional layer of submicron NaYF$_4$:Yb-Er powder. we found that this extra layer, works as scattering layer and as luminescent layer.? Each layer of the solar cell, absorbs different regions of the visible spectrum of solar radiation. Firstly the UV region is absorbed by the TiO$_2$ layers, while the region centered at 550 nm is absorbed by QD (CdS), and finally the last layer of NaYF$_4$:Yb-Er absorbs the IR region, and they have visible emission under up-conversion process, that are absorbed by the quantum dots. This last layer in addition to the luminescence process, also functions as a scattering layer. The results show an improvement of 25.5% compared with samples without NaYF$_4$-RE layer. The different molar ratios of rare earth, indicate an effect by up-conversion processes, while samples undoped reveal an increase efficiency of 17.5% associated to the scattering effect.

Keywords: QDSSC, Up-Conversion, Scattering Layer.

Development and Characterization of Absorbing Films of Terahertz Radiaction

Carlos Jesús Correa-González, Donato Valdez-Pérez, Eloy Ramirez-Garcia, Mauro Alberto Enciso-Aguilar.

Instituto Politécnico Nacional, UPALM, ESIME-Zac, Av. Instituto Politécnico Nacional s/n, San Pedro Zacatenco, 07738, Ciudad de México, México.

Email: carlos_correa_6@hotmail.com

Recently some research groups have demonstrated that nanostructured films present absorbance peaks within the Terahertz (THz) band. In [1, 2] researchers have found absorbance between 20 to 50 THz for hydroxylated carbon nanotubes (CNTs-OH) and boron nitride (BN) films. Moreover, some theoretical studies suggested that graphene (G) absorbs electromagnetic energy at around 3 THz [3]. These results demonstrate that nanostructures may be useful to develop detectors in the THz regime.

This work is devoted in describing the fabrication and characterization of self-assembled thin films with nanostructures that absorb electromagnetic energy within the THz range. We used the Langmuir-Blodgett balance (LBB) technique to deposit the nanostructured films. Further, we used silicon, silicon oxide, or cyclic olefin copolymer (TOPAS) as substrates. Another remarkable feature of this work is that we were able to control the number of layers of the different nanomaterials. We characterized samples having 2, 6, 10 and 20 monolayers.

We discuss the nanostructured film development and characterization results using THz time domain, Raman and infrared spectroscopies techniques, and show that the absorption is within the THz range. This latter property of these films demonstrates that they may be useful for developing THz sensors. Our main goal in the near future is to develop sensors for their possible application in THz telecommunication systems.

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Keywords: THz Absorbing Films, Langmuir-Blodgett Balance, Spectroscopy Techniques.

Theoretical Study on Silver Complexes with Methanetiols

M. A. Colín-Valero, J. R. Soto-Mercado, B. Molina-Brito

Facultad de Ciencias, Universidad Nacional Autónoma de México, Av. Universidad 3000, Circuito Exterior S/N, Ciudad Universitaria, Coyoacán, C. P. 04510, Cd. de México.

The antimicrobial properties of the silver are well known since time ago; but, only recently, silver molecular complexes were discovered as antiviral agents, capable to block proteins, the reverse transcriptase or interact with RNA molecules. In this work, geometry optimizations and frequency calculations were carried out within the framework of the density functional theory (DFT) in order to characterize the most relevant structural and electronic properties of the subnanometer bare Ag_n (n = 1-3) clusters and $Ag_n(SCH_3)_m$ (n = 1-3, m = 1, ..., n + 1) silver complexes. The exchange-correlation term was approached by the GGA-PBE functional within the zeroth order regular approximation (ZORA), in conjunction with the triple-ζ basis doubly polarized (TZ2P). The results obtained for bare silver clusters are in good agreement with previous results found in the literature. On the other hand, according with our calculations we observed that the methanethiol prefers a bridge arrangement or configuration trans; while, from a Mülliken population analysis, we found a concentration of the electronic charge on the sulfur and hydrogen atoms. In this work we also report the silver complexes bond lengths and their HOMO-LUMO energy gap.

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Keywords: silver, methanetiols, DFT.

Synthesis and characterization of Nano sized ZIF-8

A. Sainz-Vidal, J. M. Saniger

Centro de Ciencia Aplicada y Desarrollo Tecnológico (CCADET), Universidad Nacional Autónoma de México (UNAM), Circuito Exterior S/N, Ciudad Universitaria, Ciudad de México 04510, México.

E. mail address: arianee.sainz@ccadet.unam.mx

Zeolite imidazolate frameworks (ZIFs) are a particular class of metal-organic frameworks (MOFs) constructed by the union of the imidazole or its derivatives with tetrahedral metal cations binding nitrogen atoms. One of the most studied member in this group is the Zn (2-methylimidazole)2 (ZIF-8) due to its structure stability and flexibility, which make it a promising candidate for gas storage, catalysis, etc. A useful tool to increase the superficial area and enhance the properties, especially those related to surface phenomena i.e. gas adsorption, is the reduction of the material dimensions. In this work, it is investigated the effect of different anions on the ZIF-8 crystals shape and size. Here, the method in aqueous solution reported by Yichang Pan and coworkers was employed, with some variations, for the material synthesis. For this method, the $ZnCl_2$ was used to replace $Zn(NO_3)_2{\cdot}6H_2O$ as metal source. Additionally, DRX, TGA, IR, SEM and N2 adsorption/desorption techniques were performed for the characterization of the obtained material. Hence, corroborating the obtention of nanocrystals of ZIF-8 hexagonal shaped. In conclusion, the particles exhibited smaller size (~ 50 nm) and a highly homogeneous size distribution. As contrasted against the rounded shaped ZIF-8 (~ 85 nm), prepared by $Zn(NO_3)_2$. $6H_2O$.

Keywords: ZIF-8, nanocrystals, synthesis, aqueous solution.

Synthesis of TiO_2 doped gold nanoparticles and their application in the adsorption of metals

Faridy Didier Salazar Martínez[1], Daniel Cruz González[1], M. Juárez Meneses[2], Valeria Jordana González Coronel[1], Nancy Tepale Ochoa[1]

[1]Facultad de Ingeniería Química, Benemérita Universidad Autónoma de Puebla, C.P. 72570, Puebla, Pue., México

[2]Centro Universitario de Vinculación y Transferencia de Tecnología, Benemérita Universidad Autónoma de Puebla, Prol. 24 sur y Av. San Claudio S/N, Puebla, Pue. 72570, México

The textile industry is one of those with a higher consumption of water and wastewater generated due to the process contain a large number of pollutants of various nature such as chlorinated paraffins, chlorophenols, chlorobenzenes, heavy metals, among others. Sorption of a sample of textile wastewater using TiO_2-Au system has been investigated during four hours. The system TiO_2-Au was synthesized by the modified method of combustion and was characterized by x-ray diffraction and SEM. Sorption analysis of heavy metals established in the official Mexican norms NOM-001-SEMARNAT-1996, NOM-002-SEMARNAT-1996 and NOM-003-SEMARNAT-1997, showed a decrease of Cadmium and chrome (73% and 51% respectively). On the other hand, Arsenic, Copper, Nickel, Lead and Zinc; not shown changes. Additionally, were identified Iron, Manganese, Molybdenum, Strontium and Vanadium. TiO2-Au system showed good capacity to adsorb Iron (99%), Manganese (61%) and Vanadium (76%). However, was not observed adsorption capacity for Strontium and Molybdenum.

Size evolution relativistic DFT-QTAIM study on the gold cluster complexes Au_m-S-C_nH_{2n}-S'-Au_m' (n=2-5; m=4,13,20,28)

Juan I. Rodríguez[1]*, Emilbus A. Uribe[2], María I. Baltazar-Méndez[1], Jochen Autschbach[3], F.L. Castillo-Alvarado[1]

[1] Escuela Superior de Física y Matemáticas, Instituto Politécnico Nacional, Edificio 9, U.P. A.L.M., Col. San Pedro Zacatenco, C.P. 07738, México D.F., México.

[2] Departamento de Ciencias Básicas, Universidad Santo Tomás, Carrera 9 No. 51-11, Bogotá, Colombia.

[3] Department of Chemistry, University at Buffalo, State University of New York, Buffalo, 14260-3000 New York, USA.

We introduce relativistic density functional theory (DFT) calculations on the gold cluster complexes (cluster-molecule-cluster) Au_4-S-C_nH_{2n}-S'-Au_4' (n=2-5; M=4,13,20,28). The structural, electronic and relativistic (ZORA) Bader's quantum theory of atoms in molecules (QTAIM) properties of the two lowest-energy complex isomers were computed as a function of the alkanedithiol size (n) and cluster size (m). The lowest-energy isomer is a triplet spin state independently of the complex size. According to QTAIM, the Au-Au and S-Au bonds are classified as closed shell (non-covalent) type, the S-Au bond have some of electrostatic character though. The HOMO-LUMO gap of the cluster complexes shows a zigzag behavior typical of gold nanoclusters with respect to the size of the alkanedithiol chain (n).

Charge mobility study on the gold cluster complexes Au_4-S-C_nH_{2n}-S'-Au_4' (n=2-5)

Juan I. Rodríguez[1]*, Emilbus A. Uribe[2], Daniel Trujillo-González[1] Jochen Autschbach[3], F.L. Castillo-Alvarado[1]

[1]Escuela Superior de Física y Matemáticas, Instituto Politécnico Nacional, Edificio 9, U.P. A.L.M., Col. San Pedro Zacatenco, C.P. 07738, México D.F., México.

[2]Departamento de Ciencias Básicas, Universidad Santo Tomás, Carrera 9 No. 51-11, Bogotá, Colombia.

[3]Department of Chemistry, University at Buffalo, State University of New York, Buffalo, 14260-3000 New York, USA.

We present the two lowest energy isomers for the complexes (cluster-dithiol-clsuter) Au_4-S-C_nH_{2n}-S'-Au_4' (n=2-5). A non-equilibrium Green's functions calculation is perdormed for each complex isomer in order to determine charge mobility as a funtion of the alkadithiol size (n). Based on these results, a discussion about the potential used of these systems as nanowires is introduced.

Flexible resistive organic memory using a Nitrogen doped carbon nanotubes + PEDOT:PSS composite

J.A. Ávila-Niño[1], I.A.Rosales-Gallegos[2], D. Hernández-Arriaga[2], M. Reyes-Reyes[2], R. López Sandoval[1]

[1]Advanced Materials Department, IPICYT, Camino a la Presa San José 2055, Col. Lomas 4a sección, San Luis Potosí 78216, Mexico.

[2]Instituto de Investigación en Comunicación Óptica, Universidad Autónoma de San Luis Potosí, Álvaro Obregón 64, San Luis Potosí 78000, Mexico.

Nowadays, organic materials have been used in the fabrication of electronic devices due their flexibility in comparison with the conventional electronics based on silicon. Among the memory technologies used in electronic components, the non-volatile memories have had great interest lately because they can retain the information even if the power is turning off in comparison with other memory technologies as SRAM and DRAM. An organic non-volatile memory device is presented in this work with the next configuration: Al/ PEDOT:PSS + Nitrogen doped carbon nanotubes (NCNTs)/Al sandwich architecture deposited on a plastic substrate. This memory is rewritable and present more than 500 write and read cycles. The carbon nanotubes used in these devices were functionalized in order to improve their miscibility in the PEDOT:PSS matrix and doped with nitrogen to improve their conductivity. It was found that the presence of the NCNTs is crucial to obtain a rewritable memory as well as the presence of a native aluminium oxide film formed on the bottom electrode. Different electrode configurations were fabricated and we found that using gold as bottom electrode the device not shows memory behaviour. Optical photographs show that when a voltage stress is applied to the memory devices, bubbles appear on the aluminium electrodes, which is related with the formation of electron traps in the native aluminium oxide layer that could be filled and unfilled when opposite polarity voltage sweeps are applied to the device. While the traps in the AlOx layer are the responsible of switching, the NCNTs embedded in the polymeric matrix plays a key role in their forming and memory behaviour.

Keywords: Organic electronics, non-volatile resistive memories, carbon nanotubes.

Presenting author email: avilanino84@gmail.com

Decoration of Graphene Oxide with Metallic Nanoparticles induced by light

A. Solís-Gómez, R. Sato-Berrú, J. M. Saniger

Centro de Ciencia Aplicada y Desarrollo Tecnológico (CCADET), Universidad Nacional Autónoma de México (UNAM), Circuito Exterior S/N, Ciudad Universitaria, Ciudad de México 04510, México.

E-mail address: araceli.solis@ccadet.unam.mx

The present investigation proposed a facile method for the decoration of graphene oxide (GO) with Gold (Au) and Silver (Ag) nanoparticles (NPs). The hybrid materials (Au–GO, Ag-GO) were prepared by in-situ reduction of HAuCl4 and AgNO3 into graphene oxide (GO) dispersions using sodium borohydride and sodium citrate as reductant; the growth of gold and silver nanoparticles was induced by the joint effect of light and chemical reductor. The resulting hybrid materials were characterized with UV–Vis and Raman spectroscopies. The shape and size distribution of nanoparticles into graphene oxide was studied by scanning electron microscopy and transmission electron microscopy. The nanocomposites will be tested as substrate for SERS.

Keywords: graphene oxide, nanoparticles, silver, gold, photoreduction.

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InAs quantum dots grown on InGaAs strain-compensating layers

M. Colunga-Saucedo[1], L.E. Rios-Saldaña[1], E. Eugenio-López1, J.A. Espinoza-Figueroa[1], I.E. Cortes-Mestizo[1], C. Mercado[1], A. Yu. Gorbatchev[2], V. H. Méndez-García[1]*

[1]Center for the Innovation and Application of Science and Technology, Universidad Autónoma de San Luis Potosí, Av. Sierra Leona #550, Col. Lomas 2a Secc. C.P. 78210, San Luis Potosí, México.

[2]Optical Communications Research Institute, Universidad Autónoma de San Luis Potosí, Av. Karakorum #1470, Lomas 2ª Secc. C.P. 78210, San Luis Potosí, México.

In the last few years the requirements for high performance electronic-optoelectronic devices and the increasing miniaturization in the field of microelectronics has encouraging the interest in low dimensional systems. As an example, the semiconductor quantum dots (QDs), also known as zero-dimensional systems are very promising for development of next generation technologies and appliances. Some examples of applications are high-efficiency LEDs, solar cells and quantum computing.[1] However there still are challenges to be overcome in order to reach the successful implementation of the QDs structures in common devices. Quantum dots are three-dimensional nano-islands of a low-band-gap semiconductor, which are enclosed in a wideband-gap semiconductor matrix. The QDs are commonly grown on dissimilar materials (different lattice constant) to propitiate the accumulation of strain at the interface, which is the main mechanism of the formation self-assembled QDs, and the subject of this investigation. In this work, the InAs QDs self-assembling on strain compensated GaAs/InGaAs eterostructures is reported. In order to modify the strain prior to the nucleation of the InAs QDs, a 20 nm thick InGaAs layer was grown below the GaAs layer. The ternary alloy InGaAs thickness, S, was varied from 1 to 5 nm and it regulates the strain during the growth of the QDs. The RHEED intensity showed changes in the InAs lattice relaxation depending on S. In particular, the InAs critical thickness (Hc) increases with increasing S. On the other hand, ex-situ Atomic force microscopy (AFM) measurements corroborated that by increasing S both the QDs density and diameter decreases.

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Lattice thermal conductivity by the Kubo-Greenwood formula applying Green function and the Landauer formalism in Au13 cluster and silicon nanowire

S. Peláez-Martínez,[a] L. F. Mendoza-Villegas,[a] J.A. Herrera-Carvajal,[a] F. Salazar-Posadas,[a] M. Cruz-Irisson,[a] L. A. Pérez-López.[b]

[a]ESIME-Culhuacán, Instituto Politécnico Nacional, Av. Santa Ana 1000, 04430, México, D.F., México.

[b]Instituto de Física, Universidad Nacional Autónoma de México, A.P. 20-364, 01000, México, D.F., México.

In this work we present a theoretical study of the lattice thermal conductivity [κ(T)] of a 13 atoms gold cluster (Au_{13}) and a silicon nanowire (SiNW) grown along [111] crystallographic direction passivated with hydrogen atoms. The study is performance using the density functional theory (DFT) in the generalized gradient approximation (GGA) and the density functional perturbed theory (DFPT) in order to find the force constants associated with the dynamic matrix and the vibrational frequencies spectrum. The thermal conductivity for both study systems is obtained by the Kubo formula, following the Green function formalism [1] for the Au_{13} cluster, and the Landauer formalism for the Si nanowire [2]. The results show that κ(T) for the Au_{13} starts at T=5K due the known acoustic gap [3], in contrast with the SiNW where κ(T) grows linear with T in the low temperature regime. Both systems converge to the classical limit at high temperatures. These result, show that the Green function and the Landauer formalisms are successful applied in the Kubo formula to obtain the lattice thermal conductivity in the harmonic approximation.

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Keywords: Thermal conductivity, Kubo formula, nanomaterials.

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Innovation model to eliminate corrosion on automotive parts using nanomateriales

Pérez-Zamorano Jorge[1, 2], Torres Luis Adolfo[2], Escamilla Jorge[2], Mena María Eugenia[3], García Luis[4]

[1]General Motors de México, S. de R.L. de C.V. Complejo Silao, Carretera Silao - Guanajuato km 7.1, Silao Guanajuato MX. CP 55300, jorge.perezzamorano@gm.com

[2]Universidad Iberoamericana León, Jorge Vértiz Campero, 1640, Cañada de Alfaro, León Gto. MX. C.P. 37238, adolfo.torres@iberoleon.mx , 174671-5@iberoleon.edu.mx

[3]Desarrollos y acabados en poliuretano, S.A. de C.V., Sigma 106, Industrial Delta, León Gto. MX, CP 37545, quenamena@gmail.com

[4]IXES Development Solutions, S. de R.L. de C.V. Cristal 110, Col San Rafael, Leon Guanajuato, MX, CP 37380, luis.garcia@ixes.mx

The automotive industry is facing a critical situation related to corrosion, the use of metal parts in their basic structures imply, to fight with corrosion, from their metal components, despite the high level of development of current coatings implemented.

Enterprises have been allocated significant dollar amount in their annual budgets [1], to keep corrosion under control and reduce the operational impact. Looking for alternatives, the current study, explains the impact that automotive industry is facing. The technological innovation from this proposal describes that, using nanomaterials and going in deep in the molecular structures [1], could be possible to find the way of modifying the molecular configuration and to find the physicochemical arrangement in its molecular structure to eliminate the destructive action from the oxygen on the metal surface. It is described the importance of the involvement from the companies and the synergy that must be created among Industry, University and Public sector.

The Technology transfer [2] process explained in several steps in this essay (Industrial need, link Academy-Industry, logistics and supply chain); shows the Industrial need requesting an urgent solution, following with the very important linkage that must exist between the Academy and Industrial area, registering the importance of investigation centers and laboratories installed inside companies as key factors. Finally, the start up from the Supply Chain and its logistic implications during distribution of finish goods described as well. The simple model described above, covers 360o solution. In other words, innovation means, value added to the solution for a problem that has impacted for many years the industry results.

Keywords: Nanomaterials, Technological Innovation, Automotive Industry.

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Production and Characterization of Photoactive Composite Materials Elaborated from Polymeric Compounds and Carbon Nanoparticles

I. J. Lozano-Chávez[1], L. A. Cortés-Villegas[2], P. D. Astudillo-Sánchez[1] and R. Garibay-Alonso[1]

[1]Departamento de Ingenierías, CUTonalá, Universidad de Guadalajara, Av. Nuevo Periférico No. 555, Ejido San José Tatepozco, C.P. 45425, Tonalá Jalisco, Mexico

[2]Departamento de Ciencias Exactas y Naturales, CUValles, Universidad de Guadalajara, Carretera Guadalajara Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, Mexico.

Thick film composed materials are prepared by incorporating carbon nanoparticles into photoactive polymeric matrixes for their deposition on transparent insulating substrates. In order to obtain a homogeneous dispersion into the polymeric matrixes, the carbon nanoparticles are previously disaggregated and functionalized by using a reflux method. The material for deposition is produced by mixing the photoactive polymer P3HT and carbon nanoparticles in several polar organic solvents. The deposited films are characterized by UV/VIS spectrophotometry.

Metallic bismuth nanobundles synthesized via solvothermal under acidic conditions

R. Borja Urby[2], U. Aleman Vega[1], N. Cayetano Castro[2], H. Dorantes Rosales[1]

[1]Escuela Superior de Industrias Químicas e Industrias Extractivas, Instituto Politécnico Nacional (IPN), Unidad Profesional Adolfo López Mateos, Zacatenco, Delegación Gustavo A. Madero, C.P. 07738, Ciudad de México, México.

[2]Centro de Nanociencias y Micro y Nanotecnologías (CNMN), Instituto Politécnico Nacional (IPN), Unidad Profesional Adolfo López Mateos, Zacatenco, Delegación Gustavo A. Madero, C.P. 07738, Ciudad de México, México.

E-mail: rborjau@ipn.mx

Synthesis of bismuth nanostructures needed for theoretical study of thermoelectric and photonic properties at the nano-scale, is nowadays a hot topic in the field of nanoscience. Association of size, shape, phase and purity of the synthesized material and its properties, will deliver clearer insight in how materials characteristic can be tailored for practical applications. In the present work, bismuth nanobundles are synthesized from bismuth nitrite pentahydrate in acidic conditions and short reaction times, via solvothermal reaction. Characterization by transmission electron microscopy of the as synthesized bismuth nanobundles as a function of reaction parameters: pH and temperature, shows nanobundles are made of metallic nanoparticles with size under 10 nm, which is in the proper range for future study and characterization of quantum confinement effects and Plasmon properties of bismuth nanostructures.

Keywords: Bismuth, Nanostructures, Thermoelect.

Effects of biosynthesized silver nanoparticles on cardiovascular parameters and molecular markers of inflammation in type II diabetes

A. Virgen-Ortiz[1]*, S. Limón-Miranda[2], C.T Salas-Villaseñor[3], A. Apolinar-Iribe[4], E. Rodríguez-León[4], R. Iñiguez-Palomares[4], E.A. Sánchez-Pastor[1].

[1]Centro Universitario de Investigaciones Biomédicas, UCOL. 2Depto. de Ciencias Químico Biológicas y Agropecuarias, URS-USON. 3Centro Universitario de los Lagos, UDG. 4Departamento de Física, USON.

*Corresponding address: Centro Universitario de Investigaciones Biomédicas, Universidad de Colima. Av. 25 de Julio 965, Col. Villa San Sebastián, Colima, Colima, México. C.P.2045. Telephone: +52 312 31 6 1000 ext. 47552. E-mail: avirgen@ucol.mx

The presence of inflammation markers has been studied in metabolic disorders such as diabetes mellitus. The main cytokines involved in the pathogenesis of type II diabetes are interleukin-1β (IL-1β), Tumor Necrosis Factor-alpha (TNF-α) and interleukin-6 (IL-6). The biosynthesis of metal nanoparticles using plant extracts or fruit plays an important role in the field of nanomedicine, these nanoparticles represent a novel therapeutic alternative of low-cost and less adverse effects for a wide variety of diseases. The aim of present study was evaluate the effect of biosynthesized silver nanoparticles (AgNPs), using the extract of Rumex hymenosepalus, on cardiovascular parameters and molecular markers of inflammation in rats with type II diabetes. For carry out all experiments, male rats of the Wistar strain were divided into experimental groups: 1) control non-treated, 2) control + AgNPs (1 mg/kg), 3) diabetic non-treated and 4) diabetic + AgNPs (1 mg/kg). Diabetes was induced by intraperitoneal administration of nicotinamide (120 mg / kg) followed by streptozotocin (65 mg/kg). The rats were considered diabetic when their blood glucose was greater than 200 mg / dL. The treated groups received for 3 months AgNPs. Postreatment, the blood pressure was measured using a non-invasive device for rats. Moreover, blood samples were collected by cardiac puncture and then serum was obtained by centrifugation. Serum levels of IL-1β, TNF-α and IL-6 in all groups were measured by ELISA method following the manufacturer's recommended protocol. Also, IL-1β, TNF-α and IL-6 were measured in hepatic and renal tissue. The chronic administration of

AgNPs resulted in decrease of the high blood pressure induced by diabetes. The treatment with AgNPs elicited decrease of IL-1β, TNF-α and IL-6 in serum, liver and kidney of diabetic rats. In conclusion, biosynthesized silver nanoparticles protect of the cardiovascular alterations, systemic and tissue inflammation induced by chronic diabetes.

Stability of X@Al_{12} clusters and their interaction with hydrogen and carbon monoxide complexes: A DFT study

D. Mora Herrera[1], A. Bautista Hernandez[1], AA Peláez Cid[1], Fernando Pérez[2] and, M. Salazar-Villanueva[1]**.

[1]Facultad de Ingeniería, Universidad Autónoma de Puebla, Apartado Postal J-39, CP 72570, Puebla, México

[2]Escuela de Ciencias, Universidad Autónoma "Benito Juárez" de Oaxaca ,México

DFT calculations were carried out to determine the electronic and structural properties of bare, hydrogenated and carbon monoxide X@Al_{12} clusters (X= atoms belonging to family of Carbon and Nitrogen). The atomic replacement was made at the center of each one of the clusters. According vibrational analysis, all of them are stables whereas the binding energy and electronic gap were enhanced compared to Al_{13} pristine cluster. The adsorption energy reveals that there are phenomena of physisorption and chemisorption for X@$Al_{12}H_{12}$ and X@Al_{12}CO clusters, respectively. These systems can be experimentally synthetized due to their values of Gibbs energy and they could be applied as gas sensors or some catalytic process.

keywords: Electronic structure and bonding characteristics, Density-functional theory, Interatomic distances and angles.

Synthesis of polyurethane nanoparticles by ultrasound assisted method

J. M. Andreu-Díaz[1], A. Estrada-Monje[2], M.C. Luna-Ríos[3]

[1]Universidad Iberoamericana León, Blvd. Jorge Vértiz Campero No. 1640, Fracciones Canadá de Alfaro, CP. 37238 León, Guanajuato, México

[2]CIATEC, A.C. Omega No. 201, Industrial Delta, León, Guanajuato, México, CP.37545.

[3]UPIIG- IPN, Av. Mineral de Valenciana 200, Industrial Puerto Interior, Silao de la Victoria, Guanajuato, Mexico. CP. 36275

One of the most important applications of polyurethanes is their use for biomedical and biotechnological purposes where PU microspheres find a major interest. For this reason, a series of polyurethane (PU) nanoparticles, based on 4, 4(-diphenylmethane diisocyanate and 1,4- butanediol were synthesized by a one-step method assisted by ultrasound, varying time, amplitude and frequency. The obtained PU nanoparticles were characterized by infrared spectroscopy (FT-IR), Transmission electron microscopy (TEM) and differential scanning calorimetry (DSC). FT-IR results demonstrates the formation of polyurethane, DSC denote the influence of cavitation in the crystalline arrangements of PU. TEM study suggests that the parameters of ultrasound have a great effect on the size of polyurethane nanoparticles obtained.

Keywords: ultrasound, polyurethane, nanoparticles.

Pseudo Jahn-Teller puckering instability in graphene-like 2D crystals

J.J. Castro[1], J.R.Soto[2], B. Molina[2]

[1]Departamento de Física, CINVESTAV del IPN, Apdo. Post. 14-740, 07000, México, D.F., México

[2]Facultad de Ciencias, Universidad Nacional Autónoma de México, Apdo. Post. 70-646, 04510 México D.F.,México

E-mail: jjcastro@fis.cinvestav.mx

Single-layer, free-standing silicene and germanene, the 2D graphene-like nanosheet crystals, have been theoretically predicted to have a 2D structure stabilized by an out-of-plane small buckled distortion, whose origin has been attributed to the pseudo Jahn-Teller (PJT) effect.

In this work we present a study of the PJT effect based on Density Functional Theory (DFT) and Time Dependent DFT (TD-DFT) calculations, of the ground and excited states responsible for the buckled structure. We analyse the planar D6h symmetry instability to a puckered D3d structure of the hexagonal honeycomb unit. It is shown that the usually assumed vibronic coupling of the ground state with only one excited state to explain planar instability, is inconsistent with the linear multilevel PJT effect theory.

We show that despite each system presents a buckled conformation with a PJT origin, their vibronic coupling might have different origins. Our model [1,2] allows a determination of the coupling constants and predicts simultaneously the Adiabatic Potential Energy Surface (APES) behaviour for the ground and excited states around the maximum symmetry point. The analysis is based on a scalar relativistic DFT and TD-DFT calculations in the Zero Order Regular Approximation (ZORA), as implemented in the ADF program.

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Keywords: 2D crystals, Pseudo Jahn-Teller Effect, Density Functional Theory

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Stable dispersion of nanosized synthetic clays

G. G. Carbajal Arízaga[1], M. G. Ventura Muñoz[1], S. J. S. Bravo Delgadillo[1], A. Villarruel-López[2], M. R. Torres-Vitela[2], L. E. Guerra Rodríguez[3], A. Viruete[1], C. Sánchez Jiménez[1].

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

[2]Departamento de Farmacobiología, Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421. C.P. 44430. Guadalajara, Jalisco, México.

[3]Facultad de Ciencias Aplicadas a la Industria. Universidad de Camagüey "Ignacio Agramonte Loinaz". Circunvalación Norte, km 5.5. C.P. 74650. Camagüey, Cuba.

Nanoscience studies matter composed by either metals, ceramics, organic polymers, ionic compounds or mixtures of them. Among these, anionic clays emerged three decades ago as matrices to prepare intercalation compounds through synthetic routes where low activation energy was required, and therefore, hundreds of new materials have been designed with these compounds during the last years. The pharmaceutical industry is one of the areas where more applications for synthetic clays are found, mainly, as drug vehicles and more recently as carriers of cosmeceuticals and nutraceutical agents. One of the disadvantages in preparing formulations with nanosized synthetic clays is the stability of aqueous suspensions. In fact, a common challenge nanomaterials scientist is to find media to avoid aggregation of nanoparticles. In the present work, the synthesis of synthetic clays is reported as well as the efforts to achieve stable aqueous suspension with carboxylic acids.

The nanomaterials were analyzed by solid state techniques such as powder X-ray diffraction, infrared spectroscopy and scanning electron microscopy. Results indicated that if aggregation is avoided, the solution stability is increased.

Keywords: Layered double hydroxides, synthetic clays, solution.

DFT study of molecular doping, dangling bonds and nonmagnetic doping in silicon nanowires

F. de Santiago*, A. Miranda*, A. Trejo*, E. Carvajal*, L.A. Pérez⁺, M. Cruz-Irisson*

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

⁺Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000, Ciudad de México, México

The electronic properties of silicon nanowires (SiNW) with surface dangling bonds (DB) and non-magnetic and molecular doping were investigated through spin-polarized DFT calculations, searching for half-metallic behavior. The ultra-thin nanowires are oriented along the [1 0 0] crystallographic axis and have a diameter of ~1 nm. The nanowire surface was passivated with H, and the dangling bonds were created in mutually symmetric sites. Doping with B or P was done substitutionally at the center of the nanowire cross-section, while the molecular doping was done at the surface, using ammine (NH3) and tetrafluoro-tetracyano-p-quinodimethane (TCNQ-F4).

Our results show that, while undoped ferromagnetic SiNWs are semiconductors, ferromagnetic SiNWs with B or P are half-metallic, that is, they have metallic bands for one spin channel, and a band gap for the opposite spin channel. The B and P states are deep into the valence and conduction bands, and shift the band structure of the undoped nanowires, causing some of the bands to cross the Fermi level. A similar behavior was observed with molecular doping, in which ammine and TCNQ-F4 showed the same trends as P and B, respectively: ammine acted as donor and TCNQ-F4 acted as acceptor. These results are useful in the study of the effect of non-magnetic doping on the spin-splitting due to surface dangling bonds on semiconductor nanowires. This type of nanostructured materials can be used to manufacture spintronic devices, like spin transistors.

Keywords: Nanostructures, Spintronics, Semiconductors.

Ag^0 NPs supported on SiO$_2$ microspheres for wound healing induction after infliction of surgical skin incisiones

FJ Gálvez-Gastelum[1], C Velásquez-Ordoñez[2], I Yañez-Sánchez[2], T Franco-Ávila[1], F Rojas-Gonzalez[3], MA García-Sánchez[3], JJ Sánchez-Mondragón[4], ML Ojeda-Martínez.[2]

[1]Pathology Laboratory, Department of Microbiology and Pathology, CUCS, Universidad de Guadalajara, C.P. 44340.
[2]Nanoscience and Nanotechnology Research Center, Department of Natural and Exact Sciences, CUValles, Universidad de Guadalajara.
[3]Deptartment of Chemistry, Universidad Autónoma Metropolitana-Iztapalapa, P.O. Box 55-534, México D.F. 09340
[4]National Institute of Astrophysics, Optics and Electronics (INAOE) Luis Enrique Erro No. 1, Tonantzintla, Puebla, México C.P. 72840

Background: Nanomedicine is a discipline whose goal is the application of nanostructures for treating human diseases such as skin wound healing. Objective: The analysis of the remedial effects of silica microspheres, either pristine or doped with adhered silver nanoparticles (Ag0NPs) in surgical wounds. Methods: Silica microspheres, either pristine or doped with Ag0NPs, were created after the hydrolysis/condensation of tetraethoxysilane, according to the Stöber methodology; these substrates were characterized through spectroscopic and microscopic techniques. The wound healing activity was tested and monitored on Wistar rats during 12 days. Finally, a skin biopsy samples were analyzed through hematoxylin-eosin and Masson-trichrome stainings or by immunohistochemical localization of fibroblastic and proliferative cell markers. Results: Silica microspheres of 300 nm in size, carrying Ag0NPs of about 1.6-3 nm were synthesized and employed for skin tissue repairing.

The animals that received treatment with pristine or Ag-doped silica nanosystems showed similar recovery patterns; nevertheless, the animals treated with Ag doped microspheres exhibited additional features such as an enlarged presence of hair follicles, insignificant inflammatory infiltrate and an epithelial thickness of a lesser extent. Similarly, in the same group an important presence of blood microvessels and α-SMA+ and PCNA+ cells, were observed. Conclusion: Silica microspheres coated with Ag0NPs induce significantly better skin wound reparation effects through the modulation of inflammatory, fibrogenic, and proliferative mechanisms.

Keywords: SiO2-microspheres, wound healing, Ag-nanoparticles.

Thermal Stability and Magnetic Properties of Magnetite Hexagonal Nanoflakes Coated with Carbon Layers

Marisol Reyes-Reyes[1], Román López-Sandoval[2],*, José Antonio Ávila-Niño[1,2] and Hector Silva-Pereyra[2]

[1]Instituto de Investigación en Comunicación Óptica, Universidad Autónoma de San Luis Potosí, Álvaro Obregón 64, San Luis Potosí 78000, Mexico.

[2]Advanced Materials Department, IPICYT, Camino a la Presa San José 2055, Col. Lomas 4a sección, San Luis Potosí 78216, Mexico.

*E-mail: sandov@ipicyt.edu.mx

We report a successful technique that provides a one-step process for the synthesis of single-crystalline Fe3O4 hexagonal nanoflakes. The modification on the surface of magnetite nanostructures is performed through carbon coating during the synthesis process via the use of ferrocene, mainly as the iron source, alcohols, as the carbon and oxygen source, mixed with deionized (DI) water for increasing the oxidative environment in the reaction mixture. It is reported that an important parameter for the thickness and kind of coating layer on the iron oxide nanostructures is the type of alcohol used during the synthesis process. Those synthesized using methanol showed lower thermal stability in comparison with those synthesized isopropanol or ethanol. Finally, the magnetic properties between them are similar and differences are related to different carbon fractions and kind of carbon coating on the hexagonal nanoflakes.

Ab initio study of the electronic properties of Ge nanostructures for applications to lithium batteries

A. N. Sosa-Camposeco, A. Trejo,M. Cruz-Irisson

Instituto Politécnico Nacional-ESIME Culhuacán Av. Santa Anna 1000, C. P. 04430 D. F, México

In the recent years there have been multiple advances on the synthesis of Ge nanostructures which have ushered multiple applications such as in infrared detectors, solar cells, field effect transistors among others. One of the most interesting emerging applications of Ge nanostrucutres is as anodes on Li-ion batteries, which would dramatically increase their charge capacity and durability.

The most promising nanostructures to this end are the porous Germanium (pGe) and Germanium nanowires (GeNWs), however the theoretical characterization of these materials, particularly pGe, for this applications is still rare, and would prove useful for the development of the new generation of Li batteries. In this work the effect of surface Li on the electronic properties of pGe was investigated by means of the density functional theory and the supercell scheme [1,2], where the porous structures are modeled by removing atoms of a 32-atom Ge supercell along the [001] direction.

The surface dangling bonds were passivated with H. To model the effects of surface Li the H atoms were gradually replaced with Li atoms until achieving a total coverage of the pore surface. The calculations show that as the Li concentration increases on the surface the electronic band gap decreases by effects of trap like states on the band gap energy, those states increase the overall electron conductivity favoring the electron conduction on these nanostructures which would be beneficial for its use on Li-ion batteries.

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Effects by doping and surface Lithium termination on the electronic band gap of porous silicon: A theoretical approach

I. González-Cortés, A. Trejo, M. Cruz-Irisson

Instituto Politécnico Nacional-ESIME Culhuacán Av. Santa Anna 1000, C. P. 04430 D. F, México

Actually portable technologies such as tablets and phones have become an integral part of common life, for these technologies to continue to thrive and develop it is necessary the research of new materials for Li ion batteries, which have higher charge capacities and do not degrade after numerous charge/discharge cycles. One of the most interesting materials for this end is the porous Silicon (pSi) overcoming some of the limitations of bulk Si such as the dramatic volume expansion (of about 300%) which leads to a subsequent fracture of the material and loss of charge capacity.

There are plenty of experimental investigations on this matter however the theoretical characterization of pSi and its interaction with Li is still scarce. In this work the effects of Li as a dopant and as surface passivation are studied using the Density Functional Theory and the supercell scheme [1,2]. The porous structures were modelled by removing atoms on the [001] direction of an otherwise perfect Si crystal, and passivating the surface with H atoms.

To analyze the effects of Li doping on the nanostructures some Li interstitial atoms were added to the structure on various positions, while the effects of surface terminations was studied by replacing H atoms with Li atoms on the surface. Results show that for the interstitials the effects on the electronic band gap of pSi are akin to that of an N-type doping by shifting the Fermi level to the top of the conduction band with some crossings of the fermi level thus indicating certain degree of metallicity. For the Li surface termination the effects are less dramatic since only some extra states appear on the band gap energy, as the Li concentration increases the band gap energy decreases approaching to a metallic behavior. These results could be of importance for the development of new anode materials since the lower band gap and metallic behavior would be favorable for the electron conduction along the porous structures.

Keywords: Lithium passivation, DFT,Porous Silicon.

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Low temperature-short time SPS processes to produce fine-grained high-coercivity barium hexaferrite ceramics

G. Vázquez-Victorio[1], S. Nowak[2], G. Franceschin[2], S. Ammar[2] and R. Valenzuela[1]

[1]Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Ciudad de México, 04510, México

[2]laboratoire ITODYS, Université de Paris-Diderot, Sorbonne Paris Cité, CNRS-UMR 7086, Paris, 75205, France

In spite of the development of many new materials with improved properties, barium hexaferrite (BaFe12O19, or BFO) remains an important material for permanent magnet technology, as shown by the large number of recent publications and its large fraction of world market. A variety of preparation methods is currently investigated aiming to improve the coercivity and decrease the preparation time and temperature of BFO. In this work, we present a systematic study of a method combining the synthesis of nanoparticles by soft chemistry (hydrolysis in a polyol medium), followed by a consolidation by spark plasma sintering (SPS). The polyol method leads to nanoscaled precursors while the SPS technique allows an effective consolidation to high densities (>95% of the theoretical density) at very low temperatures (290-800°C), for very short periods of time (5-10 min). A remarkable advantage of SPS technique is that grain size remains within the nanometric range. We present the best combination of parameters of polyol (reagents and conditions) and SPS (temperature and pressure profiles) leading to a coercive field of 4.9 kOe and a magnetization of 67 emu/g at room temperature.

Keywords: Barium hexaferrite, Ceramics, SPS processes.

Characterization of carbon nanotubes oxidized to form composites

N. Calzada Dorantes[1], R. Cruz Silva[2]

[1]Centro de Investigación en Ingeniería y Ciencias Aplicadas, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Col. Chamilpa, C.P. 62209, Cuernavaca, Mor. México. 2Aqua Center of Innovation Shinshu University, Faculty of Engineering; 4-17-1 Wakasato, Nagano, 380-8553- Japan.

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

KEYWORDS: Carbon nanotubes´degree of oxidation, Composites, Characterization.

Optical Properties of Bimetallic Au_nAg_m (n+m=20, n:m=1:0, 3:1, 1:1, 1:3, 0:1) Clusters from Relativistic DFT Calculations

Bertha Molina[1], Alonso E. Viladomat[1], Jorge R. Soto[1], and Jorge J. Castro[2]

[1]Departamento de Física, Facultad de Ciencias, Universidad Nacional Autónoma de México, Apdo. Postal 70-646, 04510, México, D.F., México.

[2]Departamento de Física, CINVESTAV del IPN, Apdo. Postal 14-740, 07000, México, D.F., México.

In recent years the Au-Ag bimetallic nanoparticles have attracted very much attention because of the possibility of tuning their optical and electronic properties in function of gold or silver proportio. In general, from a theoretical point of view, searching for the lowest energy bimetallic structures represents a challenging problem, since a variety of skeletal geometric structures and homotopic distributions are obtained. In particular, the study of Au-Ag systems introduces an additional component to consider due to relativistic effects present in the gold atom. In this work we use the scalar relativistic approach ZORA-DFT to predict local minima in the potential energy surface of bimetallic Au_nAg_m, (n + m = 20) clusters and their ions in selected proportions (n:m=1:0, 3:1, 1:1,1:3, 0:1) in the gas-phase, and subsequently we obtained their UV-Vis spectra from TD-DFT calculations. The results were analyzed in function of the charge and the gold and silver n:m proportions present in the bimetallic clusters.

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Keywords: Optical properties, Au-Ag clusters, DFT.

Ligand effects on the optical and chiroptical properties of the thiolated Au18 cluster

A. Tlahuice-Flores[1]

[1]Universidad Autónoma de Nuevo León, CICFIM-Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL 66450, México.

The effect of chiral and achiral ligands protecting the inner Au_9 core of the $Au_{18}(SR)_{14}$ cluster is studied based on density functional theory (DFT) and its corrected long range interactions (DFT-D) approach. It was found that electronic properties (energy levels) depend on the specific ligands which induce distinct distortions on the Au-S framework. However, the substitution of the $S\text{-}c\text{-}C_6H_{11}$ as SCH_3 ligands may be considered as correct given the obtained resemblance on their displayed bonding, optical and chiroptical properties. A further comparison of CD and UV spectra displayed by Au_{18} cluster protected by chiral and achiral ligands attests that more intense profiles are featured by ligands including phenyl rings and/or oxygen atoms. In such manner that Au18 cluster protected by either chiral meta-mercaptobenzoic acid (m-MBA) or achiral SPh ligands displays more intense UV and CD signals.

Keywords: Thiolated gold clusters, Circular dichroism, UV.

Nanoencapsulation of Iron Oxide Nanoparticles as a Theranostic Vector

Perla Yazmín Sauceda-Oloño[1], Jesús Armando Lucero-Acuña[2], Patricia Guerrero-German[2], Paul Zavala-Rivera[2]

[1]Departamento de Física, Posgrado en Nanotecnología, Universidad de Sonora, 83000, México

[2]Departamento de Ingeniería Química y Metalurgia, Universidad de Sonora, 83000, México

With the recent advances on the nanotechnology science, nanoencapsulation is rapidly growing. Nanocapsules are nanostructured materials composed of a core and a protective layer [1]. The core is typically solid or liquid, and the protective layer is usually a non-toxic polymer membrane, which makes the delivery of the drug controllable. Today researchers are interested in novel drug delivery systems that are able to release drugs in a specific area without affecting other non-contaminated areas, preventing overdoses and leveraging the effect of the drug and its use in the diagnosis of the diseases as marker or contrast agent at the same time [1], [2], [3].

Recently, the most commonly used polymers for the nanocapsules synthesis is chitosan [4], [5], [6], due to its properties such as low toxicity, biocompatibility, biodegradability and relatively low production cost from abundant natural sources [7]. Also the use of iron oxide nanoparticles (ION), in particular the magnetic nanoparticles have been increased its interest in the use as a multiuse bionanomaterial. The different applications are due to its ability to behave superparamagnetically [6], [8], the resonance plasmons behavior that leads to the production of thermal effects [9] and its use as a contrast agent in MRI [6].

In this work, we show the nanoencapsulation of hydrophobic IONs within an oleic acid nanoemulsions using sodium dodecyl sulfate (SDS) as surfactant coated with chitosan and its characterization. As a result of our work, nanocapsules of 220 nm in size with a Z potential of +32 mV were obtained. Due to the properties of toxicity, biocompatibility, and biodegradability, exhibited by the materials used for the

nanocapsules synthesis, is believed that they could be a good alternative to the state-of-the-art ones. Due to the possibilities of use the nanocapsules with the iron oxide nanoparticles within as contrast agents, thermo-therapies and delivery vectors for bioactive ingredients.

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Thiolated Au_{18} Cluster: Preferred Ag Sites for Doping, Structures, and Optical and Chiroptical Properties

Bertha Molina[1] and Alfredo Tlahuice-Flores[2]

[1]Departamento de Física, Facultad de Ciencias, Universidad Nacional Autónoma de México, Apdo. Postal 70-646, 04510, México, D.F., México.

[2] CICFIM-Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL 66450, México.

Recently, the X-ray determined structure of the thiolated Au18 cluster has been reported. In this work, we addressed a study of structures and chiroptical properties of thiolated Au_{18} cluster doped with up to ten Ag atoms, which have been calculated by Time Dependent Density Functional Theory (TD-DFT). The number of Ag atoms was steadily varied and more stable isomers showed optical and Circular Dichroism (CD) spectra distinct fromthat found for the parent Au18 cluster. Doping with more than four Ag atoms results in enhancement of the oscillator strength of the HOMO–LUMO peak and it is expected that this feature can be exploited for photoluminescence applications.

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Keywords: Chiroptical properties, Au_{18} cluster, Ag doping.

Methods for generating modulated amplitude voltage pulses for switching PFM

E. A. Murillo-Bracamontes[1], J.J. Gervacio-Arciniega[1], E Cruz-Valeriano[2], C. I. Enriquez-Flores[2], E. León-Sarabia[2], D. E. Bojorquez-Valenzuela, J. M. Yañez-Limon[2], J. M. Siqueiros[1], M. P. Cruz[1].

[1]Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, AP 14, Ensenada 22860, B. C., México.

[2]CINVESTAV Unidad Querétaro, Lib. Norponiente 2000, Real de Juriquilla, 76230 Querétaro, Qro., México.

Email: emurillo@cnyn.unam.mx

Over the last years, piezoresponse force microscopy (PFM) has become the leading technique to straightforwardly map and manipulate domains in ferroelectric materials at nanoscale level [1][2]. In PFM operation, ferroelectric domain imaging is achieved by using the basic experimental setup of atomic force microscopy (AFM) in which a conductive tip is brought into contact with the surface of the sample while a sinusoidal voltage is applied [3]. A lock-in amplifier is then used to detect variations of amplitude and phase of the piezoresponse to the applied voltage. Switching PFM (S-PFM) is utilized to study the dynamic properties of ferroelectric domains. In this technique, a sinusoidal waveform is added to amplitude modulated voltage pulses at a frequency near the cantilever tip-sample resonance to enhance the output signal which is detected by a lock-in amplifier. Each pulse of the amplitude modulated voltage consists of two states: an on-state where a DC voltage level is applied and a zero voltage level referred as off-state. Previous research articles report the use of this kind of pulses [4][5], however, as far as we know there are no reports on how these DC pulses are generated. This information is important to be able to externally implement this technique in an atomic force microscope. Different ways to generate the pulses are presented in this work, such as using an arbitrary function generator, a DAQ system and a low cost method by using a microcontroller with D/A converter. A previously characterized PZT thin film was used to measure and compare the local hysteresis loops obtained by the different methods to generate the amplitude modulated pulses.

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Keywords: Piezoresponse force microscopy, PFM switching spectroscopy, hysteresis loop.

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Synthesis and characterization of copper substituted nickel ferrite by solid-state reaction and Pechini method

Tomás C. Hernández García[1], Luis Ernesto Padilla Villalobos[1]

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

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

Ferrites are unique magnetic materials, their applications are found in almost all fields, are highly sensitive to the synthesis method, heat treatment, stoichiometry of the constituent metals etc. In this work, the nickel-copper ferrite with the general formula Ni0.5Cu0.5Fe2O4 have been prepared using solid-state reaction and Pechini type method. Nickel nitrate, copper nitrate and ferric nitrate were used as precursors reactants for both methods. Citric acid was used as the polymerization agent and the metal nitrate- to -citric acid taken as ratio 1:5 for the situation Pechini method. X-ray diffraction (XRD), thermo gravimetric analysis (TGA), differential thermal analysis (DTA) and scanning electron microscopy (SEM), were used to characterize the obtained powders of each synthesis. XRD patterns suggests that Cu substituted Ni ferrite with chemical composition Ni0.5Cu0.5Fe2O4 shows cubic spinel structure. The DTA/TGA was performed at 0°C-800°C in order to determine the temperature range for growth of the ferrite. SEM images showed agglomerated spheroidal particles.

Keywords: Ni–Cu ferrites, Solid state reaction, Pechini method.

Target type effect on PL properties of SRO films grown by Sputtering

A. Coyopol[1], T. Díaz-Becerril[1], G. García-Salgado[1], E. Rosendo-Andrés[1], G. Escalante[1], and A. Morales-Sánchez[2]

[1]CIDS-ICUAP, BUAP, Ciudad Universitaria, Ed. 103 D, Col. San Manuel, C.P. 72570, Puebla, México.

[2]Centro de Investigación en Materiales Avanzados SC, Unidad Monterrey-PIIT, 66600 Apodaca, Nuevo León, México.

*E-mail: acoyopol@gmail.com

The interest in developing optoelectronic devices integrated in the same silicon chip, has motivated the study of non-stoichiometric silicon oxides (SiOx, x <2). In this work we report optical and structural properties of SRO films grown by Co-sputtering (Silicon and SiO2) by using 3 different targets of Silicon; type n, p and intrinsic. In all cases, RF powers in the range of 20W to 70W were applied to Silicon target and 100W fixed to SiO2 target. The samples were deposited at 100 °C on Si substrates (100) and subsequently samples were annealed at 1100°C. The samples were characterized by infrared spectroscopy (FTIR), photoluminescence (PL), and XPS. By FTIR and XPS measurements was determined the stoichiometric and composition of SRO films. Two bands of FL in the range of 400 to 1100 nm are observed in all samples, a band with peak maximum at730 nm, unchanged in position with the growth temperature is associated with defects Si=O, on the other hand, a second band (430) associate to ODC defects. The emission properties were compared, being the SRO films obtained with the p-type target, the emission spectra with greater intensity, suggesting that some radiative defects are benefiting.

Strategies to discern ferroelectricity in piezoresponse force microscopy

J.J. Gervacio-Arciniega[1], E. A. Murillo-Bracamontes[1], E Cruz-Valeriano[2], C. I. Enriquez-Flores[2], E. León-Sarabia[2], J. M. Siqueiros[1], M. P. Cruz[1]

[1]Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, AP 14, Ensenada 22860, B. C., México.
[2]CINVESTAV Unidad Querétaro, Lib. Norponiente 2000, Real de Juriquilla, 76230 Querétaro, Qro., México.

E-mail: gervacio@cnyn.unam.mx

In the last few years piezoresponse force microscopy (PFM) has become the leading technique to obtain ferroelectric information at the nanoscale. PFM hysteresis loops and switching images have been taken as a ferroelectric signature in several works, however similar PFM measurements in non-ferroelectric systems such as glass or silicon have been also obtained, for this reason several strategies have been proposed to differentiate the electromechanical mechanism arising from spontaneous polarization [1-3].

However, the implementation of some of these methodologies result complicated because PFM configuration is not the only one used to check up ferroelectricity. In this work a review of strategies to dissern ferroelectricity by using only the PFM set up is show. For this purpose, a KNN ceramic with ferroelectric and non-ferroelectric phases were used.

The methodologies consist in analyze the PFM images, verify the time of induced polarization retention, compare the first and second harmonics, measure the linear behavior and obtain the hysteresis loops with different ac bias. Using these strategies allow to check ferroelectricity in materials with low piezoelectric response, with several structural phases and in new systems.

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Keywords: Piezoresponse force microscopy, electromechanical, ferroelectricity.

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Characterization of a simple chemical process using the Tsallis' entropy

E. Guerrero-Muñoz*, N. Flores-Gallegos.

Benemérita Universidad de Guadalajara, Centro Universitario de los Valles, Carretera Guadalajara – Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México.

E-mail: ejrgm1991@gmail.com

The entropy is a concept widely used in many disciplines, and exists numerous definitions of it, according to the area of usage, from the thermodynamics to information theory. During many years, the Boltzmann's entropy has been used, as an essential tool to describe in a macroscopic way some physical process using statistical probabilities, however, this tool could not be completely effective to describe complex systems that are non-extensive. In 1988, C. Tsallis proposed a generalization of the Boltzmann's entropy [1], Tsallis' entropy has a dependency of a parameter q, generally called "non-extensive parameter"; such parameter is real and unique for each system and must be calculated for a specific system. This entropy has been used in several areas of the science and technology, such as Mathematics, Physic, Chemistry, Biology, Astrophysics, Economics, among others [2]. In this work, we applied this concept to describe a chemical reaction. Our results show that this q parameter may be related to the variation of some physical properties as the electron energy, the structural properties, and the normal modes of vibration, and there are specific intervals of "q" where this changes may be appreciated, thus it is possible to associate such physical changes to a linear (extensive) and non-linear (non-extensive) behavior.

Keywords: non-extensive, entropy, statistical mechanics, Tsallis' entropy

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Synthesis and Characterization of TiO_2:Pt thin films obtained by Dip-Coating Technical

J.C.Solis-Cortazar, L.Rojas-Blanco, G.Pérez-Hernández, C.Ricardez- Jiménez, M.González-Solano Erik R.Morales.

Universidad Juárez Autónoma de Tabasco, Avenida Universidad S/N, Col. Magisterial, C.P: 86040, Villahermosa, Tabasco, México.

* E-mail: eriking10@hotmail.com

Thin films of TiO_2 and TiO_2:Pt were deposited by sol-gel dip coating technique. The sol was prepared with different concentrations of Pt: 0, 0.2, 0.5, and 1 wt%. The films were characterized for its optical, morphological and electrical properties-The electrical resistivity in the dark and light were measured. The results from XRD analysis showed that the as-deposited films are amorphous and after annealing at 550oC in air for 1 hour, the films changed to anatase phase. The crystalline size was in the range of 16-20 nm. The resistivity of the films was observed to decrease considerably with the incorporation of Pt, however, no change in band gap was observed due to the incorporation of Pt. The incorporation of Pt was confirmed with the TEM analysis of TiO_2: Pt films. The surface roughness of TiO_2 and TiO_2:Pt films were estimated at 3.37 and 2.87 nm respectively.

Keywords: Thin Film, TiO_2:Pt, Dip-Coating.

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

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

[1]Instituto de Energías Renovables, Universidad nacional Autónoma de México, Temixco, Morelos, C.P. 62580, México.

[2]Centro Universitario de los Valles. Universidad de Guadalajara Carretera Guadalajara - Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México.

[3]Instituto de Fısica, BUAP, Av. San Claudio y Blvd. 18 Sur Col. San Manuel, Ciudad Universitaria, C.P. 72570 Puebla, Mexico.

*E-mail: xm@ier.unam.mx

The kesterite compound Cu2ZnSn(S,Se)4 (CZTSSe) has become a promising material for solar cell applications due to its p-type conductivity, an absorption coefficient higher than 104 cm-1 and a band-gap value between 1.0 - 1.5 eV depending on Se/(S+Se) ratio. In this work we are reporting the development of CZTSSe thin films through a vacuum-free, low-cost method and the material characterization using different experimental tools to understand the properties and optimize the processing of this promising material for photovoltaic applications. Nanoparticles of the precursor materials ZnS, SnS and CuS were synthesized by solid-state chemical reaction.

Then, Cu2ZnSnS4 thin films are deposited by doctor blade using a paste of these three binary compounds mixed in appropriate proportions, and submitted to a thermal treatment under Se atmosphere at different temperatures and pressures. The impact of temperature and pressure on structural, compositional, optical, and opto-electronic properties are discussed in order to optimize the physical properties CZTSSe. By increasing temperature from 450°C to 600°C, improvements in Cu2ZnSn(S,Se)4 crystalline quality as well as a better Se incorporation are found for all chamber pressures. Besides, as an interesting result, it was observed that the kesterite band-gap can be tailored as a function of thermal annealing temperature and chamber pressure.

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Keywords: $Cu_2ZnSn(S,Se)4$, Thermal Annealing effect.

Silver nanoparticles for biosensing applications: a new methodology

Loreta Cortés Espinosa[1], Víctor Rentería Tapia[1]*, Cesar Rosas Aceves[1]

Centro Universitario de los Valles, Universidad de Guadalajara, Ameca, Jalisco, c.p. 46600, México.

*E-mail: victor.renteria@profesores.valles.udg.mx

It is well known that silver nanoparticles are sensitive to the dielectric properties of their local environment and an important application of this effect is the sensing of biomolecules. However, the colorimetric changes produced by this methodology, generally cannot produce a dramatic change in the UV-Vis spectrum, because the refractive index of the medium is similar to the biomolecule in solution. In this work is shown a simple method in order to increase the sensitivity depending on the change of shape of anisotropic silver nanoparticles in epoxy resin in presence of antibodies. The sensing properties were evaluated by the means of the analysis of spectral absorbance measured with a UV-Vis-NIR spectrophotometer. Besides, morphological changes were observed by AFM due to this interaction molecular. The optical absorption spectra exhibited splitting bands due to elongated particles with longitudinal mode centred at 750 nm. The advantage of these optical properties is that can use in systems biological optically turbid (such as blood). The results are discussed in terms of changes of the physical properties of the resin in presence of the antibodies and the silver nanoparticles.

Decane desorption on graphene layers by Sodium Alpha-Olefin Sulfonate/Cocoamidopropyl Betaine mixture. A computational simulation study

José Guillermo Méndez Bermúdez*, Héctor Domínguez Castro**, Carlos G. Aranda Bravo**.

* Departamento de Ciencias Naturales y Exactas. Centro Universitario de los Valles, Universidad de Guadalajara. Carretera Guadalajara – Ameca Km. 45.5 C.P. 46600. Ameca, Jalisco, México.

** Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México. Circuito Exterior, Ciudad Universitraria, Coyoacán C.P. 04519, Ciudad de México, México.

Email presenting author: jgmendez88@gmail.com

We study the desorption of decane absorbed on graphene layers by a mixture of a Sodium Alpha-Olefin Sulfonate (AOS)/Cocoamidopropyl Betaine (BET) by a molecular simulation.

We prepared three different systems of a decane + graphene + water + surfactant (AOS, BET and AOS/BET mixture). In each case we varying the molar concentrations at room temperature. AOS and BET promoted the decane removal by the formation of a third layer of decane. On removal process the AOS has less effect than BET. In the case of the AOS/BET mixture it was found a maximum removal at a ratio concentration of 0.24/0.76. To reach this conclusion we calculated density profiles of decanes and both surfactants and the orientation probabilities of the decane layer next to the surface.

Keywords: graphene layers, surfactants, desorption.

Black paint based on silver nanoparticles in resin for solar energy harvesting

Enrique Barrera[1], Federico González[1], Celso Velásquez[2], María Luisa Ojeda[2], Marciano Sánchez[2] and Víctor Rentería[2*]

[1]Departamento de Ingeniería de Procesos e Hidráulica, Universidad Autónoma Metropolitana–Iztapalapa, Ciudad de México, 09340, México.

[2]Departamento de Ciencias Naturales y Exactas, Centro Universitario de los Valles–Universidad de Guadalajara, Ameca, Jalisco, 46600, México.

E-mail: retv61@yahoo.com.mx

We show in this work a novel, simple and inexpensive method to prepare a black pigment based on silver nanoparticles in resin. They exhibited broadband light absorption and large scattering intensity over the UV-Vis spectrum. This optical property is ideal for the solar thermal energy harvesting. Then, a selective absorber based on silver nanoparticles deposited on copper by the dip coating method was prepared. The samples showed reduced reflectance in the UV-VIS-NIR region and the solar optical properties were estimated. The synthesis of the silver nanoparticles, their optical and morphological properties, the preparation of the coatings and the solar optical properties are reported and discussed. The selectivity is susceptible to improvements and the method of deposition is suitable in large area coatings. To our knowledge this is the first study of a selective absorber based on silver nanoparticles in polymer deposited on copper.

Optical properties of Germanium nanoparticles synthesized by ion implantation

Alejandra López Suárez[1], Thania Andrea Briano Veloz[1], Betsabeé Marel Monroy Peláez[2] and Guillermo Rodríguez Santana[2]

[1]Instituto de Física, UNAM. México

[2]Instituto de Investigaciones en Materiales, UNAM. México

E-mail-: chipi72@gmail.com

Nanostructured semiconductor devices are expected to play an essential role in the development of the next generation of solar cell technology. Among the more promising materials that have been studied, the Si and Ge holds great interest; nevertheless the Ge is a better candidate due its favorable band gap and better transport properties. In order to synthesize the Ge nanoparticles, high purity silica glass plates were implanted with 2 MeV Ge ions, using fluences of 8E16 to 1.6E17 ions/cm2. After implantation the samples were thermally annealed in a reducing atmosphere (50%N2+50%H2) at 600, 700, 800, 900 and 1000ºC. The thermal treatment is used to promote the nucleation of the Ge nanoparticles from the supersaturated solution, as well as to passivate the defects formed during implantation. The Ge samples were characterized by means of Rutherford Backscattering Spectrometry (RBS) and Photoluminescence (PL) spectroscopy. In this work we study the relationship between the implantation fluence and the annealing temperature with the photoluminescence response of the Ge devices.

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Nanocristals de celulosa obtenidos de deshechos agroindustriales

Belkis Coromoto Sulbarán Rangel, Victor Hugo Romero Arellano, Carlos Guzmán González, Marianelly Esquivel Alfaro, Alberto Missael Ponce Camacho

[1]CU Tonalá, Av. Nuevo Periférico No. 555 Ejido San José Tatepozco, C.P. 45425, Tonalá, Jalisco, México.

E-mail: belkis.sulbaran@cutonala.udg.mx

Los nanomateriales se obtienen de las transformaciones físicas y químicas de diferentes materias primas. La materia prima para la síntesis de nanomateriales es diversa, depende de las propiedades y aplicación final que se quiera obtener. Por tanto, una gran cantidad de estudios se desarrollan con el objetivo de probar diferentes fuentes y materias primas. Uno de los enfoques más novedosos es sintetizar nanomateriales a partir de residuos agroforestales o marinos. En este sentido, el estudio que se plantea es desarrollar materiales nano estructurados con polímeros naturales proveniente de un residuo agroindustrial como el bagazo de agave. La planta Agave tequilana Weber var. azul tiene gran importancia agroindustrial en la región de Jalisco y estados circunvecinos de México, ya que es la materia prima para producir el tequila. Para producir un litro de tequila se requieren 8 kg de agave y se generan 3.2 kg de bagazo de agave que se considera residuo. El manejo de estos residuos representa un problema muy grande y hasta el momento se ha utilizado como composta y para la producción de productos de bajo valor económico. El bagazo de agave tequilero se compone (% en peso) de celulosa 42%, hemicelulosas 20%, lignina 15% y extraíbles 23%. La celulosa es un polímero que en su forma cristalina a nivel nanométrico ofrece una excelente resistencia, capacidad adecuada de adsorción de iones de metales pesados entre otras propiedades, esto hace que sea un material versátil para diversas aplicaciones desde biomédicas hasta industriales.

TiO_2-Pectin paste, formulation and evaluation for sensitized solar cells applications

V. H. Romero[1], J. M. Flores Gómez[1], T. López Luke[2], M. O. Vázquez Lepe[3], B. C. Sulbarán Rangel[1], C. A. Guzmán González[1], E. De la Rosa Cruz[2]

[1]CUTonalá, Av. Nuevo Periférico No. 555 Ejido San José Tatepozco, C.P. 45425, Tonalá, Jalisco, México.

[2]Centro de Investigaciones en Optica, A.P. 1-948, León, Gto. 37150 México

[3]Centro Universitario de Ciencias exactas e Ingenierías de la Universidad de Guadalajara, Departamento de Ingeniería de Proyectos, Jalisco 44430, México

E-mail: vicromare@gmail.com

Currently in development sensitized solar cells, TiO2 is a semiconductor widely studied for its excellent physical and chemical and electrical properties. The implementation of this material within the architecture of the cell is one of the most significant factors for the performance of the Solar cell. One of the main strategies is to deposit the TiO2 in paste, as this ensures control of film thickness and its homogeneity. In the present study the formulation and evaluation of TiO2 paste using pectin as binder medium is presented. The results reveal photoconversion efficiencies of 2.8%.

Qualitative study to determine removal of cationic and anionic compounds with nanoparticles of layered double hydroxides

Alma Elia Medina Espinoza

Centro Universitario de Ciencias Exactas e Ingeniería, Univerdad de Guadalajara.

E-mail: alma_ej5@hotmail.com

The structure of layered double hydroxides HDLs is explained with the structure of magnesium hydroxide, Mg(OH)2, also called brucite. Brucite contains Mg2+ cations in the middle of the layers octahedrally coordinated by OH groups. LDHs are part of a family of synthetic clays with chemical and thermal stability; Their synthesis is simple and inexpensive and these compounds are attractive for their diverse functionality and adsorption capacity as well as for their biocompatibility. This paper compares qualitatively the removal capacity of a cationic dye (methylene blue) and two anionic compounds (methyl orange and red 40). X-ray diffraction, infrared spectroscopy and UV-visible spectroscopy were used to analyze the compounds in order to observe and evaluate the structure produced after reaction with the anionic and cationic compounds.

Keywords: layered double hydroxides, clays, intercalation.

Synthesis of nanomaterials based on anionic clays and lanthanides

Cecilia Sánchez Jiménez[1], Gregorio Guadalupe Carbajal Arízaga[2]

[1]Maestría en Ciencias en Química, Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421. C.P. 44430. Guadalajara, Jalisco, México.

[2]Departamento de Química, Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421. C.P. 44430. Guadalajara, Jalisco, México.

E-mail: celisan2905@hotmail.com

One of the tasks entreprised by materials scientists is the search of alternative materials for pharmaceutical industries to transport and give stability to drugs. A relevant family of materials is composed by layered double hydroxides (LDH), also known as synthetic clays, which are layered structures with divalent and trivalent cations. The presence of trivalent cations in the layered units produce an excess of charge which is stabilized by anions located in the interlayer region. The importance of LDHs increases since they present a wide range of properties and the ability to be tuned. In this project, a LDH composed with Zn(II) and Al(III) cations stabilized with interlayer nitrate was modified with different amounts of dysprosium and gadolinium cations in order to achieve the isomorphic substitution of aluminum cations. The inclusion of these lanthanide cations add properties to the LDHs such as fluorescence and then they could be used as probe in fluorescence microscopy with the simultaneous ability to transport drugs or any other biologically active molecule.

The analytical techniques used in this project were X-ray diffraction to assess crystallinity and dimensions of the interlayer spaces of the compounds and infrared spectroscopy to study molecular changes, especially those related hydroxyl in the layers and the interlayer anions.

Keywords: Clay; Probe; Fluorescence.

Nanotechnologies and water issues in Mexico

Domingo Rafael Castañeda Olvera[1]

[1]Universidad Tecnológica Fidel Velázquez, Av. Emiliano Zapata S/N, Nicolas Rómero, Estado de México,

E-mail: rafaelcastaneda10@yahoo.com.mx

Nanotechnologies represent a knowledge platform where technological power can do more efficient water treatment methods. Through this investigation we follow NT's technological route from research and development to its comercialization as water in Mexico; it has given us a view from the sector, its productive entrance and prospective social impact. This investigation focuses on generating a general view about nanotechnological applications for water in Mexico, we focused on the analysis of several areas: bibliometric analysis (publications), registration of academic groups or research lines, patents and enterprises. We are looking forward to contributing with the emerging debate about nanotechnological applications in the water sector in Mexico.

Synthesis oxide-hydroxide and gallium oxide for functionalization with organic compounds and determining the energy bandgap width

Waldo Isaías Quezada Martínez[1], Gregorio Guadalupe Carbajal[1]

[1]Centro Universitario de Ciencias Exactas e Ingenierías (CUCEI), Departamento de Química, Blvd. Marcelino García Barragán No. 1421, C.P. 44430, Guadalajara, Jalisco, México.

E-mail: vicsek8@hotmail.com

The functionalization of galium oxyhydroxide and gallium hydroxide with organic compounds and the influence on the band gap was studied through the analysis of UV-vis spectra taking as reference the non-functionalized particles.Gallium oxyhydroxide was precipitated from a solution with 0.01M of Ga(III) cations with two alkaline solutions, namely 1.0 M NaOH or 14% NH4OH. The solid produced was separated by decantation and dried and analyzed by X-ray driffraction. The obtained profile matched with the structure of a galium oxyhydroxide.This oxyhydroxide was subjected to functionalization by immersion/incubation in solutions with adipic acid, phenylphosphonic acid, sodium dodecyl sulphate and urea. All these compounds coated the gallium oxyhydroxide particles. All the compounds were analyzed by UV-vis spectroscopy and the data were handled trhough the Tauc equation to determine the band gap energy. All the functionalizing compounds produced a change in the band gap energy.Once the organic molecules over the surface of gallium oxyhydroxide particles seems to modify the band gap energy, a further calcining of the oxyhydroxide in a tubular quartz furnace at 700 °C for 5 hours was conducted in order to produce gallium oxide, which is a more stable compound and this is currently being functionalized with the same organic compounds. Preliminary result are not enough to conclude whether the band gap in this compound is influenced.

Layered double hydroxides containing magnesium and aluminum cations

Alexandra Arelí Viruete González[1]. José Guadalupe Quiñones Galván[2]. Gregorio Guadalupe Carbajal Arízaga[3].

[1]Maestría en Ciencias en Química, Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421. C.P. 44430. Guadalajara, Jalisco, México.

[2]Departamento de Física, Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421. C.P. 44430. Guadalajara, Jalisco, México.

[3]Departamento de Química, Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421. C.P. 44430. Guadalajara, Jalisco, México.

E-mail: alexa_aleli26@hotmail.com

Layered double hydroxides (LDHs) are a family of synthetic materials with a similar structure that is exhibited by its natural analogue known as hydrotalcite. This structure is formed by layers with magnesium cations at the center, which are octahedrally coordinated by six hydroxide groups. This structure results from the isomorphic substitution of a divalent cation (M+2) by a trivalent cation (M3+), thus generating a positive charge residue in the layers, which is compensated by the additional presence of interlaminar anions. These anions are easily exchanged in solution.

Currently, LDHs are considered the inorganic synthetic nanomaterials with more biocompatibility. Therefore, they have a wide range of biomedical applications for disease diagnosis and therapy. The LDH particles with minimal or null cytotoxicity are composed by magnesium and aluminum cations. If such composition were modified with with trivalent cations such as gadolinium (Gd) or dysprosium (Dy), new properties would arise like luminescence and paramagnetism, thus opening opportunities to design of biomedical materials including probes detectable by optical microscopy or nuclear magnetic resonance, contrast agents along with the ability to transport drugs.

Therefore, this work has studied the synthesis to prepare LDHs from Mg(NO3)2 y Al(NO3)3 in 3:1 molar ratio and different percentages of Gd and Dy. In addition, the characterization was performed by techniques such as powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy, energy dispersive X-ray spectroscopy (SEM-EDX), and photoluminescence (PL). As a result, the LDHs with Mg and Al in 3:1 molar ratio with 25, 50 and 75% of Dy, and the LDH with 50% of Gd, was successfully synthesized. Thus, they would serve to design of biomedical materials.

Keywords: Layered double hydroxides, cytotoxicity and biomedical applications.

Synthesis and characterization of CNT-NaTNT nanocomposite synthetized by hydrothermal method.

Gabriel Correa Chávez[1], Hiram Joazet Ojeda Galván[2], Diego Eduardo Góngora Pantoja[3], Ángel Gabriel Rodríguez Vázquez[2], Brent Edward Handy[3], Alejandra Londono Calderon[4].

[1]Facultad de Ciencias (FC-UASLP), Av. Chapultepec 1570, Privadas del Pedregal, 78295, San Luis Potosí, SLP, MEX.

[2]Coordinación para la Innovación y la Aplicación de la Ciencia y la Tecnología (CIACyT-UASLP), Sierra Leona 550, Lomas 2da. Sección, 78210, San Luis Potosí, SLP, MEX.

[3]Facultad de Ciencias Químicas (FCQ-UASLP), Av. Manuel Nava 6, Zona Universitaria, 78290, San Luis Potosí, SLP, MEX.

[4]Department of Physics and Astronomy, University of Texas at San Antonio, One UTSA Circle, 78249, San Antonio, TX, USA.

E-mail: 203gcc@gmail.com

Titanium dioxide (TiO2) is a metallic oxide semiconductor very popular and with many potential applications for being inexpensive, non-toxic, hydrophilic, biocompatible, chemically stable and photoreactive, being the last property improved in tubular nanostructures because of the formation of plus active sites in a bigger surface area. Sodium-titanate nanotubes (NaTNT), its reactive capacity and its geometry are strongly influenced by the different parameters involved in the synthesis, as pH, temperature, synthesis time, washing conditions and sodium content. On the other hand, carbon nanotubes (CNT) have been extensively studied for their mechanical, electrical and optical properties, as high strength and significant elasticity.

The carbon nanotubes - sodium titanate nanotubes nanocomposite (CNT-NaTNT) was synthetized via alkaline hydrothermal method from TiO2 and NaOH, following the method described by Kasuga but adding single wall carbon nanotubes (SWCNT). As result of synthesis, an upper interface and a lower interface are formed. Through Raman spectroscopy, FTIR, EDX analysis, UV-vis, X-ray diffraction, HRTEM and SEM it was found a different carbon content among interfaces and a chemical interaction between NaTNT and SWCNT is suggested trough a Ti-O-C bond attributable to vibrations around 1050-1130 cm-1 according to FTIR data, while Raman characterization shows a stretch band around 1430-1480 cm-1 which not correspond to NaTNT or CNT. Morphologically, it was observed a little variation of internal, external diameter and layer width between the interfaces and the NaTNTs synthetized by Kasuga´s method without CNT.

Keywords: titanate nanotubes, carbon nanotubes, Raman spectroscopy.

Synthesis of layered double hydroxides and the study of their properties for the enzymatic immobilization

Potenciano Minero Martin T.[1], Carbajal Arizaga Gregorio G.[2], Velázquez Juarez Gilberto[2].

[1]Licenciatura en Ingeniaría en Nanotecnología, Universidad de Guadalajara, Av. Nuevo Periférico Oriente 555, Ejido San José Tatepozco, 45425 Tonalá, Jalisco, México. e-mail: tlahuis@msn.com

[2]Departamento de Química, Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421. C. P. 44430. Guadalajara, Jalisco, México.

E-mail: tlahuis@msn.com

Layered double hydroxides (LDH) are stratified crystalline compounds that are comprised of layers of divalent and trivalent metallic cations stabilized by an excess of negative electrostatic charge of the anions in the interlayer. The aim of this research was to synthesize LDH by precipitation of metallic salts (zinc and aluminum). To these compounds were added a salt of copper varying the molar ratio during synthesis. The resultant materials presented a powder form and were analyzed by X-ray Diffraction (XRD), Infrared Spectroscopy (IR) and Scanning Electron Microscopy (SEM). XRD gave information relative to the quality of the crystalline structure and also it was made a comparison with the diffraction cards of the database from The International Centre for Diffraction Data (ICDD). IR reveled signals of –OH of stretching vibrations of the layers, and also vibrations produced by interlayer nitrate ions, that confirmed the successful synthesis of the LDH structure.

Images obtained by SEM allowed to observe and characterize the surface and their morphological aspects. HDL particles presented platelet shape with thicknesses in the nanometer regime.

The structure, composition and morphology indicated that the LDH particles can be used in the next stage for the immobilization of enzymes.

Key words: Layered double hydroxides; X-ray Diffraction; Infrared Spectroscopy; Scanning Electron Microscopy; Enzymatic immobilization.

Novel and facile transfer of gold nanoparticles into organic solvents using amphiphilic molecules

L. L. Valadez-Martínez[1], J. L. Pichardo-Molina[2], M.M. Martínez-Garcia[2], P. Cardoso-Avila[2]

[1]Universidad Iberoamericana León, Blvd. Jorge Vértiz Campero, Fracciones Cañada de Alfaro, 37238 León, Mexico

[2]Centro de Investigaciones en Óptica (CIO), Loma del Bosque 115, Lomas del Campestre, 37150 León, Mexico

E-mail: uislvm@gmail.com

Gold nanoparticles (NP's) were synthetized into water and subsequently transferred to different organic solvents using 1-dodecanotiol (DDT) and PEG-thiol. compounds selection was based on their amphiphilicity and gold affinity. The transferred methodology requires control of several parameters such as pH, temperature and stirring along with resting times. Nevertheless, the method ensures quickness and allows the appreciation of the NP's migration between the phases due to their characteristic color. Gold NP's into oil phase were obtained when a simple decantation was performed and then cleaned by centrifugation. During the experimentation, nanorods and nanospheres were utilized, achieving transfer into hexane, chloroform and toluene. Characterization was accomplished by UV-VIS spectrometry and scanning microscopy, making possible to observe a high concentration of the transferred NP's with an intact morphology and recovered with the compounds. Having stable colloidal NP's in the oil phase generates great advantages since it allows the improvement in the handling of these, the functionalization with organic molecules and it also opens the possibility of working onto several technological areas like coatings or health materials. In summary, with this novel method, a new way to transfer the NP's it is obtained without compromising the solution stability, enabling a wide range of applications due to its compatibility with different solvents.

Keywords: Phase transferr, Gold nanoparticles, Anphiphilyc compounds.

Photochemical Synthesis of Flat Silver Nanoparticles

P.E. Cardoso-Avila[1], M.M. Martinez García[1], A. Martinez Hernandez[2], J.L. Pichardo-Molina[1]

[1]Laboratorio de Espectroscopia Biomédica y Nanomateriales, Centro de investigaciones en Óptica, A.C., León, México.

[2]Universidad Tecnológica de Tulancingo.

E-mail: pecardoso@cio.mx

Flat Silver Nanoparticles (FS-NPs) were obtained by means of a photochemical transformation process. Small spherical NPs synthetized by chemical reduction show an excellent colloidal stability, as they can be stored for months without aggregation or any change in morphology. But as soon as the spherical silver NPs (plasmon band around 400nm) are irradiated with green and red LEDs to promote the photochemical process. The use of these out-of-resonance light sources allowed us to tune the plasmon band in the red region of the visible spectra. UV-Vis spectroscopy was used to study the growth kinetics and the optical characterization of these colloids. On the other hand SEM and DLS allowed us to determine the morphology and size distribution. We have developed a fast and low cost photochemical method to synthetize flat silver NPs with a plasmon band in the red region of the visible spectra while maintaining a small size.

Biological response of HeLa cell uptake: The case of gold nanoparticles with different organic coatings

P.E. Cardoso-Avila[1], J.L. Pichardo-Molina[1], L.L. Flores-Villavicencio[2], M. Sabanero-Lopez[2].

[1]Centro de Investigaciones en Óptica A.C. León, Gto. Mexico.

[2]Departamento de Biología, DCNE, Universidad de Guanajuato. Guanajuato, Gto. México.

E-mail: pecardoso@cio.mx

Drug delivering, therapies, imaging, biosensors and biomarkers are some the most notable applications of nanoparticles in biology and medicine. However, their toxicity, genotoxicity and biological characteristics are not completely clear. Therefore it is important to get more knowledge about their possible consequences on the use of this kind of materials. In this work we carried out and in-vitro study of the cytotoxicity of silica-capped gold nanorods and gold nanospheres coated with three different organic molecules: 4-aminothiophenol (4-ATP), cysteamine, and bovine serum albumin (BSA). Transmission electron microscopy allowed us to access the average sizes of the silica-capped gold nanorods (22±4 nm long, 9±1nm wide and 10±5nm silica shell), the 4-ATP- (34±5nm), Cysteamine- (24±4nm) and Cysteamine-BSA– capped gold nanoparticles (GNPs) (25±5nm). The GNPs functionalization with the biomolecules was confirmed by Raman spectroscopy.

The human cervix cancer cell line (HeLa) was selected, and cells were incubated with the GNPs at the time of subcultivation (0hrs) and when the monolayer cells were 70% confluent (24hrs). Cytotoxicity of GNPs has been assessed by cell viability, metabolic activity, cytoskeleton and genomic DNA integrity assays. Our results confirmed that the porous silica coated gold nanorods still preserves the Hexadecyltrimethylammonium bromide (CTAB) toxicity (Au concentration 2.47x10-4M), because the metabolic activity was reduced to 73%. On the other hand the GNPs coated with organic molecules not showed any toxicity damage at Au concentrations of 3.14x10-4M for the 4ATP-capped and 2.77x10-4M for the cysteamine- and cysteamine-BSA-capped GNPs.

Cytoskeleton integrity analysis indicated that the cellular uptake of gold nanoparticles did not cause any damage to the F-actin filaments.

Key words: Gold nanoparticles, Cytotoxicity, HeLa cells.

Novel and facile transfer of gold nanoparticles into organic solvents using amphiphilic molecules

L. L. Valadez-Martínez[1], M.M. Martínez-Garcia[2], P.E. Cardoso-Avila[2], J. L. Pichardo-Molina[2]

[1]Universidad Iberoamericana León, Blvd. Jorge Vértiz Campero, Fracciones Cañada de Alfaro, 37238 León, Mexico

[2]Laboratorio de Espectroscopia Biomédica y Nanomateriales, Centro de Investigaciones en Óptica (CIO), Loma del Bosque 115, Lomas del Campestre, 37150 León, Mexico

E-mail: uislvm@gmail.com

Gold Nanoparticles (NPs), synthesized in water medium, were transferred to different organic solvents with the use of dodecanethiol and thiolated poly(ethylene glycol). The choice of these compounds was done due to their amphiphilicity and their high affinity to gold. It was possible to transfer the NPs to chloroform, hexane and toluene. The transfer method requires controlling pH, temperature and the stirring and rest times. This is a fast method that allows seeing the migration to the organic solvent by the naked eye. The NPs were purified by centrifugation in order to remove the surfactant excess and to obtain them in the organic solvents. UV-Vis spectroscopy showed that the plasmonic properties were preserved once the NPs were transferred to the organic media. Furthermore, the morphology and size were not affected by the medium transfer as the scanning electron microscopies showed. By having the NPs in organic solvents it is easier to deposit NPs monolayers in different surfaces even if these surfaces are functionalized or not.

Keywords: Gold nanoparticles, Phase transfer, Amphiphilicity.

Comparative effects on rat primary astrocytes and C6 rat glioma cells cultures after 24 hours exposure to silver nanoparticles (AgNPs)

S. Salazar-García[a], A. S. Silva-Ramírez[a], M. A. Ramirez-Lee[a], E. Rosas-Hernandez[a], E. Rangel-López[b], C. G. Castillo[c], A. Santamaría[b], G. A. Martinez-Castañon[d], C. Gonzalez[a]

[a]Universidad Autonoma de San Luis Potosi, Facultad de Ciencias Quimicas, San Luis Potosi, Mexico.

[b]Laboratorio de Aminoácidos Excitadores, Instituto Nacional de Neurologia y Neurocirugia Manuel Velasco Suárez, Mexico.

[c]Universidad Autonoma de San Luis Potosi, Facultad de Medicina, San Luis Potosi, Mexico.

[d]Universidad Autonoma de San Luis Potosi, Facultad de Estomatologia, San Luis Potosi, Mexico.

E-mail: samuelsg_9@hotmail.com

The aim of this work was to compare the effects of 24 hours exposure of rat primary astrocytes and C6 rat glioma cells to 7.8 nm AgNPs. Glioblastoma multiforme (GBM) is the most aggressive primary brain tumor and current treatments lead to diverse side-effects; for this reason, it is imperative to investigate new approaches, including those alternatives provided by nanotechnology, like nanomaterials (NMs) such as silver nanoparticles. Herein, we found that C6 rat glioma cells, but no primary astrocytes, decreased cell viability after AgNPs treatment; however, both cell types diminished their proliferation.

The decrease of glioma C6 cells proliferation was related with necrosis, while in primary astrocytes the decreased proliferation was associated with the induction of apoptosis. The ionic control (AgNO3) exerted a different profile than AgNPs; the bulk form did not modify the basal effect in each determination whereas cisplatin, a well-known antitumoral drug used as a comparative control, promoted cytotoxicity in both cell types at specific concentrations.

Our findings prompt the need to determine the fine molecular and cellular mechanisms involved in the differential biological responses to AgNPs in order to develop new tools or alternatives based on nanotechnology that may contribute to the understanding, impact and use of NMs in specific targets, like glioblastoma cells.

Keywords: Silver nanoparticles, glioma, primary astrocytes.

Concave gold nanocubes for SERS: exploring the size effect on the enhancement factor

M.M. Martinez Garcia[1], P.E. Cardoso-Avila[1], J.L. Pichardo-Molina[1]

[1]Laboratorio de Espectroscopia Biomedica y Nanomateriales, Centro de investigaciones en Óptica, A.C., Leon, Mexico.

E-mail: monsemtzgca@cio.mx

The morphology and nanoparticle size are key factors for its use in a variety of applications, such as surface enhanced Raman spectroscopy (SERS). In this work, concave gold nanocubes (CGNC) were synthesized in a two-step method and a series of nanoparticle sizes ranging from 40nm to 95nm were obtained. The nanoparticle solutions were deposited over an electropolished aluminum substrate by drop casting and left to dry in room conditions. The molecule 4-Aminothiophenol was used as analyte, in order to determine the size of CGNC that presented the best SERS enhancement factor.

Keywords: SERS, concave gold nanocubes, Raman.

Study of a photonic crystal with a chessboard lattice that include dispersive metamaterial inclusions

Héctor Pérez Aguilar, Alberto Mendoza Suárez

Facultad de Ciencias Físico Matemáticas, Universidad Michoacana de San Nicolás de Hidalgo, Av. Francisco J. Mújica S/N, C.P. 58030, Michoacán, México

E-mail: hiperezag@yahoo.com

The photonic structure of a two-dimensional square lattice with square columns rotated by 45° is theoretically studied. For a filling factor tends to 0.5, the lattice reduces to a chessboard. This kind of photonic crystal has been studied in the case of dielectric inclusions [1,2]. Wide photonic band gaps can be obtained for this geometry and certain values of parameters. In this work we study the properties of a photonic crystal with a chessboard lattice when it is formed with dispersive metamaterial inclusions. The numerical technique used to solve the model equations is based on integral equations methods [3]. The results obtained allow concluding that exist electromagnetic surface modes, with TE polarized light, propagating on the metamaterial surfaces.

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Keywords: Photonic crystal, Electromagnetic surface mode, Metamaterial.

Surface plasmons in systems that include dispersive metamaterials

Hugo Enrique Alva Medrano, Alberto Mendoza Suárez, Héctor Pérez Aguilar

Facultad de Ciencias Físico Matemáticas, Universidad Michoacana de San Nicolás de Hidalgo, Av. Francisco J. Mújica S/N, C.P. 58030, Michoacán, México.

E-mail: hugoalva9@gmail.com

The study of plasmons on surfaces of metamaterials is of current interest from theoretical and applied point of view. In this work we show a numerical study of the presence of surface modes and plasmons in electromagnetic systems formed by photonic crystals waveguides that include layers of dispersive metamaterials. The waveguide model assumes perfectly conducting surfaces. The periodicity required in order to a photonic crystal in the waveguide is performed in several ways; for example, with sinusoidal conductive surfaces and with flat surfaces that surround a periodic arrangement of conductive cylinders. Some conductive surfaces are coated with layers of metamaterials, because it is known that in the interface between a metamaterial and vacuum appear surface plasmons. The numerical techniques used are based on integral equations methods [1]. The results obtained for periodic systems allow concluding that exist surface plasmons with TM polarized light and surface modes for TE polarization.

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Keywords: Photonic crystal waveguide, Surface plasmon, Metamaterial.

Experimental and numerical study of the angular dependence of the reflective optical properties of two-dimensional photonic structures with square and hexagonal periodicity

Victor Castillo Gallardo[(a)], Miguel Ángel Téllez Villaseñor[(a)], José Guadalupe Murillo Ramírez[(b)], Héctor Pérez Aguilar[(a)], Alberto Mendoza Suárez[(a)]

[(a)]Facultad de Ciencias Físico Matemáticas, Universidad Michoacana de San Nicolás de Hidalgo, Av. Francisco J. Mújica S/N, C.P. 58030, Michoacán, México.

[(b)]Centro de Investigación en Materiales Avanzados, Miguel de Cervantes 120, C.P. 31136, Chihuahua, Chihuahua, México.

E-mail: victor1_1@hotmail.com

In this work we present an experimental and numerical study of the angular dependence of the reflective optical properties of two-dimensional photonic structures with square and hexagonal periodicity, built on a silicon substrate. The work is motivated largely by the need for a new alternative development in telecommunications technology that is purely photonic. The structures that have circular and square inclusions were manufactured with the technique of Focused Ion Beam (FIB). This manufacturing technique was easy to use and has advantages over other techniques; because the structure can be machined in several sessions and we may induce structural defects in the photonic structure. The numerical analysis of the reflective optical properties was through the technique known as Integral Equation Method This method allows studying both infinite and finite systems. For infinite systems the band structure is obtained and in the case of finite systems, the propagation of electromagnetic waves through the system. When performing the numerical simulations, prohibited bands were obtained by increasing the filling fraction of the square or hexagonal unit cell. Finally, we show the numerical analysis about the wave propagation through photonic structures with similar features to those machined. One of the results was that when considering inclusions in a dielectric plate, considerably improving optical reflectance.

Keywords: Photonic structures, Focused Ion Beam, Integral Equation Method.

Modification of carbon nanostructures using a conductive polymer for application in biofuel cells

N. E. Hernández Loredo[1], R. A. Escalona Villalpando[2], L. G. Arriaga Hurtado[2]

[1]Facultad de Ciencia de la Universidad Autónoma de San Luis Potosí, Av. Salvador Nava S/N, San Luis Potosí, S.L.P., MÉXICO. C.P. 78290.

[2]Centro de Investigación y Desarrollo Tecnológico en Electroquímica, Parque Tecnológico Querétaro s/n Sanfandila, Pedro Escobedo, Querétaro, MÉXICO. C.P. 76703.

E-mail: minna@live.com.mx

The use of modified carbon structures by conducting polymers has been an important field of application as supports in the fuel bioceldas (BFC) to obtain high energy densities. In this work, different papers carbon conductive were prepared from the modification of carbon nanofibers (CNF) with polypyrrole (PPy) polymerizing in situ comparing two catalysts; ferric chloride and hydrogen peroxide. Furthermore, a variation where chitosan (CS) was added to obtain a better consistency of aggregation of the CNF. The CNF were filtered and dried on filter paper to obtain a conductive paper and finally compressed at 3600 lb. The study of the different carbon paper (CP-Py) derived from both catalysts with and without CS was performed by an electrochemical half-cell study immobilizing enzymes lactate oxidase LOx / FcMe2-LPEI and lacasa Lc / An-MWCNT. The electrodes PC-Py modified with H2O2 had a higher energy density in lactate oxidation by LOx / FcMe2-LPEI; similar result was obtained with the same carbon paper but immobilizing Lc / W-MWCNT in reaction reduction oxygen. Both electrodes have a high potential for use in a full BFC using lactate as fuel.

Keywords: conductive paper, nanofiber, biofuel cell.

Fabrication of ZnO/Ag2O composites and its application as photocatalyst in the degradation of indigo blue

Ma. De Lourdes Ruiz Peralta[1], Karla de Lázaro Gasca[1], Ismael Angel Nieto[1], J.H. Camacho García[1], and Lizeth Rojas Blanco[2].

[1]Benemérita Universidad Autónoma de Puebla, Adpo. Postal J-48, Puebla, Pue. 72570, México.

[2]Universidad Juárez Autónoma del Estado de Tabasco Carretera Cunduacán-Jalpa KM. 1. Col. La Esmeralda CP. 86690 .

E-maul: lavig_124@hotmail.com

Discharge of dye waste-water has caused environmental problems, promoting new methods to treat discharge of textile industries [1]; advances oxidation process has emerge as an alternative; TiO2, and ZnO are the most reported materials with a potential application as photocatalyst, in some cases, has been modified in order to improve the photo catalytic properties, and developed different alternatives to enhance the catalysis efficiency. Ag2O is a p-type semiconductor with a narrow band gap on 1.37 Ev , highly efficient visible- light photocatalyst and has been used as sensitizer to tune the light response [2].

In this work, ZnO/Ag2O mesoporous heterostructures has been synthetized and applied as photocatalyst in the degradation of indigo blue, a dye used in jeans industry, the ZnO/Ag2O heterostructure was sensitized in two steps: first ZnO by solvothermal technique, and finally the Ag2O nanoparticles. The samples were characterized by DRX, scanning electron microscopy (SEM), diffuse reflectance spectroscopy, and, micro-Raman, techniques. Finally, ZnO/Ag2O was applied in the descomposition of indigo blue under visible irradiation.

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Highly reproducible Perovskite based solar cell with an average efficiency of 9% and best cell efficiency of 9.9 % using single step anti-solvent method

Siraj Sidhik, Diego Esparza, Tzarara Lopez Luke, Elder De La Rosa*

*Centro de Investigaciones en Óptica, A.P. 1-948 León, Gto. 37150, Mexico

E-mail: desparza@cio.mx

Perovskite solar cells have turned out to be one of the most promising photovoltaic technologies with their rapid increase in efficiency and simple fabrication process. The single step method used for depositing the perovskite pigment onto the mesoporous metal oxide layer uses a mixture of PbI2 and CH3NH3I with a common solvent. The uncontrolled precipitation of perovskite layer produces large morphological variations that hamper the performance of photovoltaic devices. The poor morphology is the result of irregular evaporation of solvent used for dissolving the perovskite precursors. Here, some of the initial results employing the modified anti-solvent method for the formation of perovskite pigment on the mesoporous metal oxide layer is proposed. A non-polar anti-solvent is used during the deposition process to completely wash away the solvent, thus solving the rapid or irregular evaporation problem. Highly homogenous and crystalline nature of perovskite layer has been observed with this modified method, when compared to the widely used single step process. This modified technique happens to be highly reproducible and provides an efficiency of approximately 10 %. Further improvement in the efficiency is expected with the optimization of different layers and the work for it is in progress. This anti-solvent method would open up immense opportunities for the fabrication of solution based photovoltaic devices with high power conversion efficiencies and stability.

Synthesis and Characterization of Ag Nanoparticles by Bioreduction with Henequén

Luisa Briones-Gómez[1], Pedro Márquez Aguilar[1],Jorge Ascencio Gutiérrez[2]

[1]Centro de Investigación en Ingeniería y Ciencias Aplicada, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Col. Chamilpa, Cuernavaca Mor.

[2]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Av. Universidad 1001, Col. Chamilpa, Cuernavaca Mor.

E-mail: brilugo.89@gmail.com, luisa.brionesgom@uaem.edu.mx

Small particles of Ag have been synthesized by a bioreduction method using as a reducing agent Henequén biomass. The controlling parameter was the pH of the solution where they were grown in [1]. High Resolution Transmission Electron Microscope, TEM and Uv-vis have been used to characterize the morphology and structural properties of such small particles in the range of 1-4 nanometers.

Keywords: Ag Nanoparticles, Bio-Synthesis, Henequén

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Fabrication and caracterization of hemicelulose hydrogels with carbon nanotubes scaffolds for osteoblastic cell culture in Tissue Engineering

Claudia Judith Castorena Alejandro, José Manuel Gutiérrez Hernández, Diana María Escobar García, Amaury Pozos Guillén, Héctor Flores, Guillermo Toríz, Francisco Javier González[1]

[1]Facultad de ciencias de la Universidad Autónoma de San Luis Potosí

E-mail: claudiacastorena95@gmail.com

Hemicellulose hydrogels has a huge potential for being biocompatible with many tissues or cell lineage for their chemical and structural composition. This hydrogels have been a great focus of interest on biomaterials sciences for a long time. Likewise, despite Carbon Nanotubes (CNT's) are reported as toxic materials to living organisms because of their accumulation in some tissues and organs, has been proved that carbon nanoestructures, in combination with other biomaterials, give improved properties to the biomaterials like physical or mechanical ones. This becomes a unique, important new material in biomedical applications, specially their use as drugs carriers vehicles, extracellular matrices or scaffolds in tissue engineering. These lasts ones are made by an affordable easy procedure to be subjected to a culture of osteoblasts. Osteoblastic cells are the main way in the formation mechanism of bone tissue and their susceptibility to nanomaterials are similar on in vitro experiments than in vivo, so to assess whether a material is suitable or not for their use in cell culture, we make cytotoxicity, proliferation and adhesion tests to the proposed material through microbiological techniques.

Key words: Biomaterials, carbon nanotubes, tissue engineering, osteoblasts, scaffolds.

Self-Assembled ZnO Nanostructures Incorporated in a MIS Diode Architecture

R. J. Aranda-García[1], A. Escobedo-Morales[2], D. Valdivia-Montes[2] and J. A. Luna-López[1]

[1]Instituto de Ciencias, Centro de Investigaciones en Dispositivos Semiconductores, Benemérita Universidad Autónoma de Puebla, 72570 Puebla, Pue., Mexico.

[2]Facultad de Ingeniería Química, Benemérita Universidad Autónoma de Puebla, 72570 Puebla, Pue., Mexico.

E-mail: alejandro.escobedo@correo.buap.mx

Because of its physical properties, ZnO is considered a potential semiconductor for fabricating electronic and optoelectronic devices. In this regard, several growth techniques have been developed to ensure the required control for manufacturing commercial devices based in this compound. On the pathway for improving the performance of the current devices, low-dimensional ZnO structures seem to be a promising alternative.

Here, we report the fabrication of a metal-insulator-semiconductor (MIS) diode architecture based on ZnO nanostructures grown on anodized aluminum (ZnO/Al2O3/Al) by chemical routes. Specifically, while the ZnO nanostructures were obtained through a low-temperature hydrothermal route, the Al2O3/Al substrate was obtained by electropolishing and anodizing methods. The used electrochemical techniques for obtaining the substrate involve soft reaction conditions, short reaction times and low-cost. The obtained ZnO/Al2O3/Al architecture was studied by x-ray diffraction (XRD), scanning electron microscopy/energy-dispersive x-ray spectroscopy (SEM/EDS), micro-Raman spectroscopy (μRS) and electrical measurements. The voltage-time plot acquired during the anodizing process indicates the formation of an insulating barrier (Al2O3) on the metallic substrate (Al). The SEM analysis reveals that the semiconductor layer grown on the insulator film is nanostructured in nature, constituted by self-assembled leave-like structures with an average thickness of 50 nm. According with the Raman spectrum, these ZnO nanostructures are well-crystalline. The formation of Al2O3 and ZnO phases was further confirmed by means of XRD. Finally, the characteristic rectifying response of a metal-oxide-semiconductor junction is observed in the I-V and C-V curves of the obtained architecture, indicating that it is possible to build a MIS diode based on ZnO nanostructures using chemical routes.

Keywords: ZnO, Nanostructures, MIS diode.

An easy method based on spray pyrolysis deposition to obtain thin films

Mora Herrera David, Salazar Villanueva Martín.

Facultad de Ingeniería, Benemérita Universidad Autónoma de Puebla. Ciudad Universitaria, CP. 72570 Puebla, México.

E-mail: davidmoraherrera@outlook.com

Materials in thin film form such as optoelectronic devices, flat panel displays, narrow band coating, electrodes in solar cells, sensors etc. have attracted the attention due to their wide range of applications both in industry and in research. Techniques that are simple and economical have attracted attention for commercial and other reasons. The chemical spray pyrolysis technique offers an extremely easy way to prepare thin films and with dopants. The deposition rate and thickness of the film can easily be controlled. It also offers an opportunity to have reactions at low temperatures. The versatile nature of this technique lies in the way various parameters that include effect of precursors, dopants, substrates temperature, solution concentrations and so on can easily be controlled. Various types of metal oxide can be prepared, such as ZnO, ZnO: F ≡ FZO, SnO2, SnO2: F ≡ FTO, etc. and from simple metallic oxide to binary and ternary oxide compounds, like SnO2: ZnO.

In this work, the metal oxides: ZnO, ZnO: F ≡ FZO, SnO2, SnO2: F ≡ FTO and SnO2: ZnO on the structural, electric and optical properties has been investigated, for applications in Dye-sensitised solar cells (DSSC) and demonstrate that cheap, easy to use and friendly environment technologies are the key to Mexico diversify its renewable energy sources.

Keywords: Thin films, Spray Pyrolysis, Metal Oxides, Dye-sensitised solar cells (DSSC).

Study of thermal annealing effect under different pressures on the material properties of Cu2ZnSn(S,Se)4 thin films

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

[1]Instituto de Energías Renovables, Universidad nacional Autónoma de México, Temixco, Morelos, C.P. 62580, México.

[2]Centro Universitario de los Valles. Universidad de Guadalajara Carretera Guadalajara - Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México.

[3]Instituto de Fısica, BUAP, Av. San Claudio y Blvd. 18 Sur Col. San Manuel, Ciudad Universitaria, C.P. 72570 Puebla, Mexico.

E-mail: xm@ier.unam.mx, isaacms88@gmail.com

The kesterite compound Cu2ZnSn(S,Se)4 (CZTSSe) has become a promising material for solar cell applications due to its p-type conductivity, an absorption coefficient higher than 104 cm-1 and a band-gap value between 1.0 - 1.5 eV depending on Se/(S+Se) ratio. In this work we are reporting the development of CZTSSe thin films through a vacuum-free, low-cost method and the material characterization using different experimental tools to understand the properties and optimize the processing of this promising material for photovoltaic applications. Nanoparticles of the precursor materials ZnS, SnS and CuS were synthesized by solid-state chemical reaction. Then, Cu2ZnSnS4 thin films are deposited by doctor blade using a paste of these three binary compounds mixed in appropriate proportions, and submitted to a thermal treatment under Se atmosphere at different temperatures and pressures. The impact of temperature and pressure on structural, compositional, optical, and opto-electronic properties are discussed in order to optimize the physical properties CZTSSe. By increasing temperature from 450°C to 600°C, improvements in Cu2ZnSn(S,Se)4 crystalline quality as well as a better Se incorporation are found for all chamber pressures. Besides, as an interesting result, it was observed that the kesterite band-gap can be tailored as a function of thermal annealing temperature and chamber pressure.

keywords: CZT(S,Se) thin films, doctor blade coating, thermal treatments.

Bolometers based multiwall carbon nanotubes decorated with ZNO

K. G. H Martínez-Reyna[1], M. G. García-Valdivieso[1], H. R. Navarro-Contreras[1], J.J.Velázquez-Salazar[2]

[1]Laboratorio Nacional CIACYT-Universidad Autónoma de San Luis Potosí, Av. Sierra Leona 550, Col. Lomas 2a. Sección, C.P 78210, San Luis Potosí, S.L.P., MÉXICO.

[2]University of Texas at San Antonio (UTSA), 1 UTSA Circle, San Antonio, TX 78249.

E-mail: kghmr@hotmail.com

The objective of this work is to fabricate and study bolometers, based on multiwall carbon nanotubes decorated with ZnO, and characterize them. The multiwall carbon nanotubes (MWCNTs) and ZnO present good thermal and electrical properties. This is the reason to explore MWCNTs/ZnO nanocomposites as energy absorbent material i.e, as Bolometer devices. A Bolometer is a device that absorbs energy, infrared and terahertz radiation, thus increasing its temperature resulting in a decrease in electrical resistance. The figure of merit of the bolometers is the temperature coefficient of resistance (TCR).

In order to obtain MWCNTs/ZnO nanocomposites we dispersed 5mg of MWCNTs in 10 ml of DMF solution into ultrasonic bath sonication. Then we added 50 mg of Zn (acac) and Tiophene as caping agents in a ratio 26.4 µl/ml and the final solution was dispersed by ultrasonic agitation for an hour. The growth of ZnO nanoparticles on the MWCNTs surface has been induced by heating the solute material in a microwave to 160°C, and applied power of 500 W for 3 minutes.

Subsequently gold was evaporated on the MWCNTs to obtain proper ohmic metal contacts in order to characterize the bolometers thus created. The samples morphology and its decoration were characterized by SEM; in the same set up EDS and XRD were performed. The TCR of the constructed bolometers was electrothermally measured.

The results obtained with SEM and EDS show a successfully decorated set of MWCNTs with ZnO nanoparticles. X-ray diffraction confirmed the presence of ZnO, and in SEM, ZnO characteristic granular structures bound to and partially covering the MWCNTs can be observed. We obtained values of TCR=-3.3% K¬-1, this results compare favorably with some of the best reported in the literature.

Key Words: Bolometers, MWCNTs, ZnO nanoparticles.

Synthesis, characterization and evaluation of catalysts to base CoMo/Al2O3 in Hidrodesoxigenación's reactions

Avalos Arroyo Omar Ivan[1], Nuño Hernàndez Claudia[2]

[1]Universidad Tecnológica Fidel Velazquez

[2]Instituto Mexicano del Petroleo

E-mail: omar.ivan01@hotmail.com

The Above mentioned project was realized by the aim of the obtaining formulation of catalytic increased activity (in HDO's schemes), based on sulphurs of Since deposited on alúmina modified by basic agents. Preparation of catalytic materials with high capacity of removal of oxygen and of properties saturantes limited in saturation reactions of aromatic rings.

There is possible the obtaining formulation of catalytic increased activity, applicable to HDO's schemes and based on sulphurs of Since deposited on alúmina, by means of the optimization of the integration of the promoter of cobalt to the cristalitos of sulphur of molybdenum across the employment of organic agents. Likewise, it is possible to diminish the capacity hidrogenante of such materials improved by means of the use of supports of Al2O3 modified with basic agents.

These materials were obtained by method of impregnation to incipient dampness. Likewise, materials were prepared based on Since supported modified by impregnation of organic additives quelantes and not quelantes (citric acid and saccharose, repectivamente), to evaluate the effect of such modifiers on the degree of promotion of the Mo for Co in HDO's reactions, under conditions of hidrogenación of aromatics limited. The obtained materials were characterized by means of the following instrumental technologies:

- Espectroscopia UV-vis for identification of condition of coordination of species of Mo and Co deposited.
- For gas chromatography to be able to determine the % of diminished oxygen
- IR to demonstrate that the metals are in the material

The catalysts prepared based on cobalt - molybdenum, supported on alúmina modified with basic agents and in phase I sulfurate they will be studied in synthetic representative presence of mixtures containing a become oxygenated representative species of the present ones in the lignina.

Keywords: Hidrodesoxigenacion and Catalysts.

Preparation of magnetic nanoparticles coated with carboxymethyl-Inulin

P. Pérez Hernández[1], M. A. Méndez Rojas[1], R. Salazar Salazar[1]

[1]Universidad Tecnológica Fidel Velázquez, Av. Emiliano Zapata S/N, Nicolas Rómero, Estado de México,

E-mail: pao.ph@hotmail.com

Iron oxide nanoparticles as magnetite and maghemite as are attractive for many applications because they can be manipulated using an external magnetic field, there are various methods to synthesize this material and chemically modified.

In this paper we will talk about the crystal polymorph of iron (III) known, magnetite (Fe3O4) because it is a promising candidate for biocompatibility and present biodegradable activity obtained by co-precipitation, which were coated with a new polysaccharide-based polycarboxylate, carboxymethyl inulin (CMI) because increase performance within the body for transport and release of drugs.

The aim of this work was synthesized and coated nanoparticles having variables of concentration, pH, temperature and stirring times.

Polymethylmethacrylate (PMMA) fibers reinforced with carbon nanotubes obtained by de electrospinning technique

R.Y. Ponce Cano[1], L.A Martínez Ara[1], P. Maldonado Altamirano[1], J.A Hernández[1], J. Ortiz López[1], M.A Hernández Pérez[3]

[1]Escuela Superior de Física y Matemáticas - I.P.N., Edificio No. 9 U.P.A.L.M., Lindavista C.P. 07738 México D. F.

[2]Escuela Superior de Ingeniería Química e Industrias Extractivas - I.P.N., Edificio No. 8 U.P.A.L.M., Lindavista C.P. 07738 México D. F.

E-mail: yetzira_16@hotmail.com, ESFM-IPN

In this work we present the results of the manufacture of Polymethylmethacrylate fibers (PMMA) reinforced with carbon nanotubes. The PMMA fibers were obtained by the technique of electrospinning from polymers in solution. The electrospinning technique involves applying a potential difference on the order of 15 kV or more, between a metal needle, which contains the polymer solution, and the collector comprising a metal plate of cooper. Progressively which the increasing of the potential difference between the electrodes the surface tension of the solution is overcomed expelling a fiber which is deposited in a collector. In this work PMMA fibers were obtained using a voltage of 15 kV and a distance of 7 cm between electrodes. Additionally, two type of solvent were used in this case Dimethylacetamide (DMac) and Dimethylformamide (DMF). The incorporation of the nanotubes was conducted by ultrasound treatment of the solutions for two hours to obtain the complete dispersion; the solutions were heated to 80 ° C to obtain a homogeneous solution. For the characterization of the fibers used Scanning Electron Microscopy, Raman and FTIR Spectroscopy were employed. The results of this work, from the mentioned characterization techniques indicate that carbon nanotubes are incorporated in an orderly manner, perpendicular to the cross section within the fibers and PMMA, besides the characteristic functional groups of the Nanotubes Carbon and Polymethylmethacrylate (PMMA) were identified.

Growth of ZnO nanoplates for gas sensor applications

Germán Escalante[1,2], Antonio Coyopol[1] and José Alberto Alvarado[3]

[1]Research Center on Semiconductor Devices - Sciences Institute, Meritorious Autonomous University of Puebla, 72570, Mexico.

[2]Materials Physics Department, Faculty of Physics, University Complutense of Madrid, 28040, Spain.

[3]Department of Materials and Engineering, University of Washington, Seattle, WA 98195-2120, USA

E-mail: german.esnot@gmail.com

Chemical vapor deposition technique has been optimized for the growth of ZnO nanoplates, in order to obtain a single morphology and good reproducibility. Glass substrate was used in order to grow these nanostructures, after this process, aluminum electrodes were deposited to carry out electrical characterization. The gas sensing properties of the nanoplates were studied for different concentrations of CO and analyzed according to operating temperatures. At 200 ppm of CO concentration and 300°C a high sensitivity for these nanoplates was reached.

Keywords: ZnO, nanostructures, sensing properties.

Mechanosynthesis of CuO and ZnO nanoparticles and their antibacterial activity

A. R. Vazquez-Olmos[1], B. Paz-Diaz[1], A. Almaguer-Flores[2]

[1]Centro de Ciencias Aplicadas y Desarrollo Tecnológico, UNAM.

[2]Laboratorio de Genética Molecular. División de Estudios de Posgrado e Investigación de la Facultad de Odontología, UNAM.

E-mail: america.vazquez@ccadet.unam.mx

In this contribution we present the nanoparticles (NPs) obtaining of CuO and ZnO as well as the study of their antibacterial activity. It is well known that copper oxide (CuO) have been used to disinfect liquids, solids and human tissue for centuries. Today it is used as water purifier, an algaecide, a fungicide and a nematocide as well as an antibacterial and antifouling agent [1]. On the other hand ZnO is currently being investigated as an antibacterial agent in both microscale and nanoscale formulations. ZnO exhibits significant antimicrobial activities when particle size is reduced to the nanometer range, then nano-sized ZnO can interact with bacterial surface and/or with the bacterial core where it enters inside the cell, and subsequently exhibits distinct bactericidal mechanisms[2]. In this work, we present a preliminary study of the bactericide activity of CuO and ZnO nanoparticles to Gram (-) Pseudomonas aeruginosa and Gram (+) Staphylococcus epidermidis. CuO and ZnO nanoparticles have been successfully synthesized via an uncomplicated mechanochemical method where protic and aprotic solvents are involved. Their crystalline structures and their average diameters of 22 nm for CuO and 30 nm for ZnO were determined from XRD patterns and by TEM images. The NPs were characterized by UV-visible, Raman, FT-IR and electronic paramagnetic resonance spectroscopies. From our results we suggested that (Vo+) singly ionized oxygen vacancies, Zn2+ vacancies, and Cu2+ions, play an important role in the bactericide activity of these nanoparticles.

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Synthesis of layered double hydroxides and the study of their properties for the enzymatic immobilization

Martin T. Potenciano Minero[1], Gregorio G. Carbajal Arizaga[2], Gilberto Velázquez Juarez[2]

[1]Licenciatura en Ingeniaría en Nanotecnología, Universidad de Guadalajara, Av. Nuevo Periférico Oriente 555, Ejido San José Tatepozco, 45425 Tonalá, Jalisco, México. e-mail: tlahuis@msn.com

[2]Departamento de Química, Universidad de Guadalajara, Boulevard Marcelino García Barragán 1421. C. P. 44430. Guadalajara, Jalisco, México.

Layered double hydroxides (LDH) are stratified crystalline compounds that are comprised of layers of divalent and trivalent metallic cations stabilized by an excess of negative electrostatic charge of the anions in the interlayer. The aim of this research was to synthesize LDH by precipitation of metallic salts (zinc and aluminum). To these compounds were added a salt of copper varying the molar ratio during synthesis. The resultant materials presented a powder form and were analyzed by X-ray Diffraction (XRD), Infrared Spectroscopy (IR) and Scanning Electron Microscopy (SEM). XRD gave information relative to the quality of the crystalline structure and also it was made a comparison with the diffraction cards of the database from The International Centre for Diffraction Data (ICDD). IR reveled signals of –OH of stretching vibrations of the layers, and also vibrations produced by interlayer nitrate ions, that confirmed the successful synthesis of the LDH structure.

Images obtained by SEM allowed to observe and characterize the surface and their morphological aspects. HDL particles presented platelet shape with thicknesses in the nanometer regime.

The structure, composition and morphology indicated that the LDH particles can be used in the next stage for the immobilization of enzymes.

Key words: Layered double hydroxides; X-ray Diffraction; Infrared Spectroscopy; Scanning Electron Microscopy; Enzymatic immobilization.

Synthesis and characterization of nano-particles of carbon from the combustion of paraffin

Lorenza Augusta Cortés Villegas[1], Raul Garibay Alonso[2], Pablo Daniel Astudillo Sanchéz[2], Iván Guillén Escamilla[1]

[1]Departamento de Ciencias Naturales y Exactas, CU Valles, Universidad de Guadalajara, Carretera Guadalajara - Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México.

[2]Departamento de Ingenierías CU Tonalá, Universidad de Guadalajara, Av. Nuevo Periférico No. 555 Ejido San José Tatepozco, C.P. 48525, Tonalá Jalisco, México.

E-mail: lacv13ster@gmail.com

In this work we present the synthesis, characterization and fluorescence of nanoparticles of carbon (NPC) from candle soot, the experimental process took place through the carbon oxidation treatment with HNO3, the NPC in solution were obtained from a reflux process and the size separation is reached through a series of centrifugations at high velocities, the result are particle size between 355 nm and 1200nm. With this NPC in solution we find fluorescence in green color; we obtained stability and solubility of NPSC in solution.

Keywords: nanoparticle, carbon, fluorescence.

Color tunability of the downconversion emission in Y2O3:Eu3+,Tb3+ nanocrystals

E. S. Vargas-Rodríguez[1], V. H. Romero-Arellano[2], J. C. Mixteco-Sánchez[1], H. Desirena-Enríquez[2], L. O. Meza-Espinoza[3]

[1]Departamento de Ciencias Naturales y Exactas, CU Valles, Universidad de Guadalajara, Carretera Guadalajara - Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México.

[2]Departamento de Ingenierías CU Tonalá, Universidad de Guadalajara, Av. Nuevo Periférico No. 555 Ejido San José Tatepozco, C.P. 48525, Tonalá Jalisco, México.

[3]Instituto de Física "Ing. Luis Rivera Terrazas", Av. San Claudio y Blvd. 18 Sur, Col. San Manuel. Edificio 110 'A', Ciudad Universitaria - BUAP C.P. 72570, Puebla.

E-mail: susana137@live.com.mx

The rare earth doped nanophosphorus are not only effective converting ultraviolet light to visible light, these materials also have the capacity to absorb adjacent infrared light and cast fluorescence. Luminescent materials have gotten attention due to its great potential for technological applications. [1] Rare-earth-ions doped yttrium oxides (Y2O3) are important optical materials, which exhibit excellent luminescent efficiency, color purity and chemical and thermal stability [2,3]. Rare earth doped nanophosphorus have great potential in different applications such as biomedicine, solar cells, luminescent tags, photochemical catalysis, detectors and temperature sensors.

The rare-earth ions show abundant emission colors based on their 4f-4f or 5d-4f transition. Eu3+ y Tb3+ show red-orange and green emission respectively. Y2O3: Eu3+, Tb3+ phosphor emits red emissions, green emission and has an excellent chemical stability. This phosphor is the only existing red, green phosphor used in three bands fluorescent lamp. [4]

Luminescence quenching was observed at high dopant concentrations. Strong and effective color-tunable emission is expected to find a wide range of applications in industry. [6]

In this work, we will focus at the Y2O3 nanocrystals that act as a matrix. This material will be doped with different rare earth ions such as Eu3+ and Tb3+. Within this investigation, optical properties of the materials will be analyzed by the absorption, emission, and excitation spectrums. Furthermore, they will be morphologically characterized by X-ray diffraction, Ramman and TEM images.

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Enhancement of visible light photocatalytic activities of TiO_2-chabazite composites in the decolorization of AZO dyes in aqueous solutions

J. Torres-Díaz[1], E. R-Morales[1], G Pérez-Hernández[1], L. Ruiz-Peralta[2], L. Rojas-Blanco[2], R. Ramírez-Bon[3].

[1]Universidad Juárez Autónoma de Tabasco, Avenida Universidad S/N, Col. Magisterial, Villahermosa, Centro, Tabasco 86040, México.

[2]Benemérita Universidad Autónoma de Puebla, Facultad de Ingeniería Química Ciudad Universitaria, Edificio 106H, Av. Sn. Claudio y 18 sur Col. Jardines de San Manuel, CP. 72570 Puebla, Puebla.

[3]Centro de Investigación y Estudios Avanzados del IPN. Unidad Querétaro, Apdo. Postal 1-798, C.P. 76001, Querétaro, Qro., México.

A new class of supported photocatalysts is introduced recently with high activity under visible light for decolorization the dyes using in the textil industry. The composition comprises silicoaluminates (natural zeolite) and Titanium dioxide (TiO2) as the semiconductor. TiO2-Zeolita was synthesized by high energy mill. The composites were characterized by XRD, SEM, EDS, and XPS. The photodegradation activity of the composites was investigated for the removal of dyes under visible light irradiation. The results revealed that the mix was very active under visible light irradiation and the photocatalytic efficiency was more efficient that of unmodified pure TiO2. This novel TiO2-doped zeolite system provides a promising application for the UV and Visible disinfection process in wastewater treatment plants.

Influence of salt fluxes on recycled Al nanocomposites reinforced with TiO_2 nanoparticles produced in liquid state

A. Santos-Beltrán[a], H. Morales-Rodriguez[a], I. Roquillo-Ornelas[a], D. Anaya-Vazquez[a], I. Estrada-Guel[b], V. Gallegos-Orozco[a, c]

[a]Universidad Tecnológica de Chihuahua Sur, Km. 3.5 Carr. Chihuahua a Aldama, C.P. 31313. Chihuahua, Chih. México.

[b]Centro de Investigación en Materiales Avanzados (CIMAV), Miguel de Cervantes No. 120, C.P.31109, Chihuahua, Chih., México.

[c]Instituto Tecnológico de Chihuahua, Av. Tecnológico #2909,C.P 31310,Chihuahua, Chih. México.

E-mail: asantos@utchsur.edu.mx

Aluminum reinforced with hard nanoparticles are very attractive in many applications in the industry, this kind of materials form part of the group of materials named Metal Matrix Nanocomposites (MMNCs). An important characteristic of these kinds of materials is the low contents of reinforcement material required to improve significantly the mechanical properties of the Al matrix. In the present work, nanocomposites based recycled aluminum alloy 6063 swarf with hard nanoparticles of TiO2 were fabricated by combining techniques such as mechanical milling, stir-casting method and the use of different types of salt fluxes additions. Microhardness tests were carried out in order to identify the effect of flux additions on the reinforcement dispersion into the Al matrix. The microstructure of the nanocomposites were characterized by optical microscopy (OM), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and X-ray diffraction (XRD).

Keywords: Recycled Al, Metal Matrix Composite, Mechanical Milling, Nanoparticles Dispersion.

Study of nanostructured NiCrMo base alloy coatings applied via LVOF thermal spray

A. Santos-Beltrán[1], M. Santos-Beltrán[2], V. Orozco-Carmona[2], H. Morales-Rodriguez[1], G. Lerma-Echavarria[1], Luis Sotelo-Rivera[1], V. Gallegos-Orozco[1,3]

[1]Universidad Tecnológica de Chihuahua Sur, Km. 3.5 Carr. Chihuahua a Aldama, C.P. 31313. Chihuahua, Chih. México.

[2]Centro de Investigación en Materiales Avanzados (CIMAV), Miguel de Cervantes No. 120, C.P.31109, Chihuahua, Chih., México.

[3]Instituto Tecnológico de Chihuahua, Av. Tecnológico #2909,C.P 31310,Chihuahua, Chih. México.

The mechanical properties and corrosion behaviour of nanostructured NiCrMo base alloy coatings applied via thermal sprayed by low velocity oxy-fuel (LVOF) technique was evaluated. The nanostructured powder was synthetized via high energy ball milling and was used to provide sliding wear and corrosion protection for stainless steel type 316. The corrosion resistance of stainless steel samples with nanostructured coating synthesized at different milling times were evaluated. As indicated by the results, the coatings possess high corrosion resistance, especially the nanostructured NiCrMo coating fabricated for relatively long ball-milling times. Microhardness was used to test the nanostructured coating prepared at different milling times on stainless steel samples.

The hardness was increased when incorporating nanostructured NiCrMo base alloy coatings on the stainless steel substrate, the high resistance is related with the nanostructured coating fabricated also at long ball-milling times. The less porosity of the nanostructured coating contributed to improve the anti-corrosion and mechanical properties. The nanostructured coating of samples were characterized by optical microscopy (OM), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and X-ray diffraction (XRD).

In order to evaluate microstructural evolution of the powder at different milling times, the X-ray diffraction peak were analysed by using Rietveld refinements method.

Keywords: nanostructured; coating; high energy ball milling.

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