NANO TECH

Puerto Vallarta 2017

November 06th - 10th
Puerto Vallarta, Jalisco, México.

CONGRESS

International Topical Meeting on Nanostructured Materials and Nanotechnology/4th Symposium on Nanomaterials with applications in solar energy, environment and health/DINANO and Mexican Nanoscience & Nanotechnology theme network meetings.

PLENARY SESSIONS, COURSES AND WORKSHOPS

CONACYT
SMF
Symposium on Nanomaterials with applications in solar energy, environment and health.
DINANO SMF
RedNyN
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Malvern PANalytical
JEOL
INTERCOVAMEX

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EDITORS

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

ABSTRACTS BOOK OF THE 13th INTERNATIONAL TOPICAL MEETTING ON NANOSTRUCTURED MATERIALS AND NANOTECHNOLOGY (NANOTECH 2017)

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The Nanoscience Division of Mexican physics society (DINANO) recognizes to companies and institutions which generous sponsorship made possible the Nanotech 2017 congress, and we especially thanks to:

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13th International Topical Meeting on Nanostructured Materials and Nanotechnology (Nanotech 2017)

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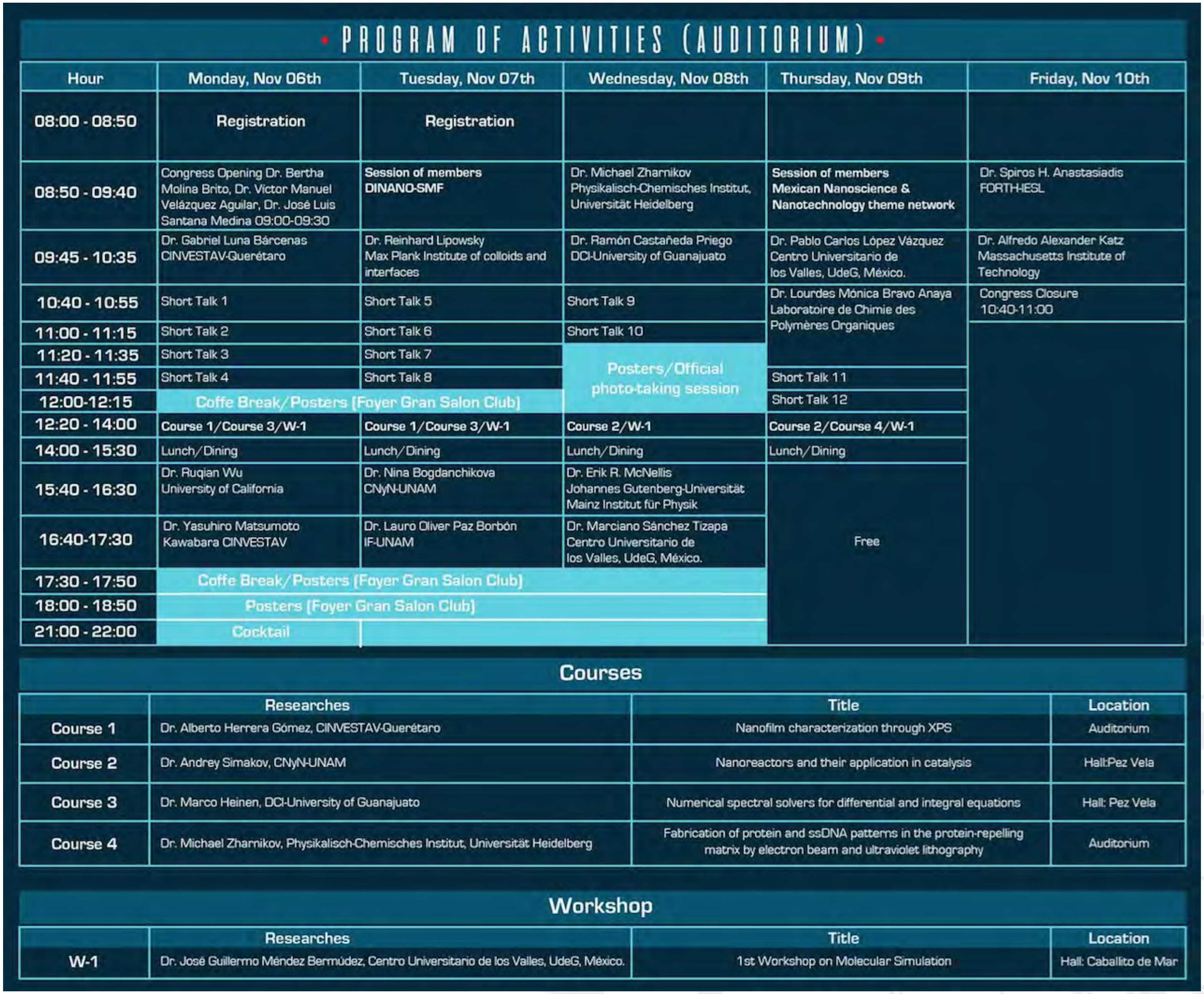


PROGRAM OF ACTIVITIES (AUDITORIUM)

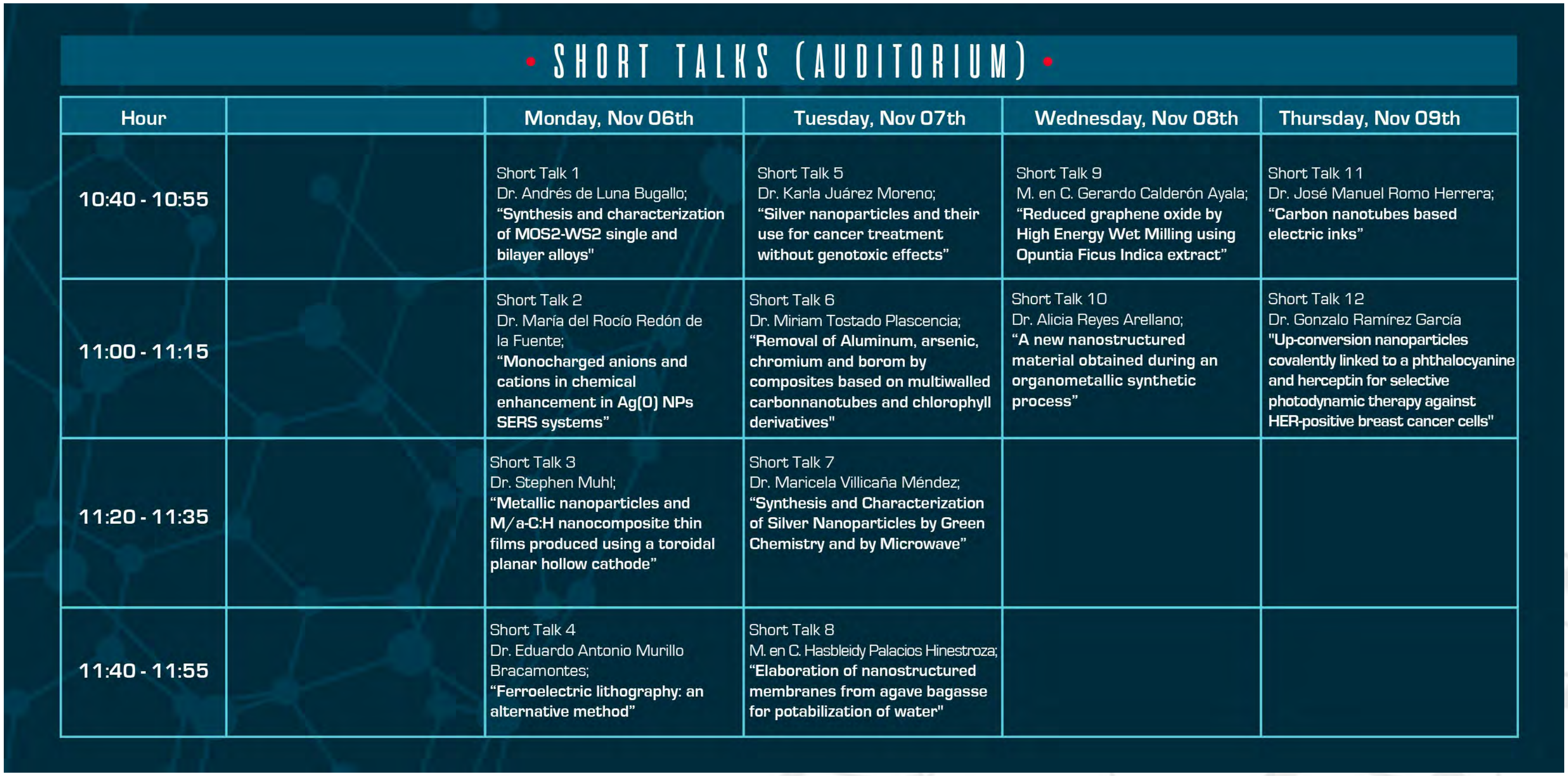
Hour	Monday, Nov 06th	Tuesday, Nov 07th	Wednesday, Nov 08th	Thursday, Nov 09th	Friday, Nov 10th
08:00 - 08:50	Registration	Registration			
08:50 - 09:40	Congress Opening Dr. Bertha Molina Brito, Dr. Víctor Manuel Velázquez Aguilar, Dr. José Luis Santana Medina 09:00-09:30	**Session of members DINANO-SMF**	Dr. Michael Zharnikov Physikalisch-Chemisches Institut, Universität Heidelberg	**Session of members Mexican Nanoscience & Nanotechnology theme network**	Dr. Spiros H. Anastasiadis FORTH-IESL
09:45 - 10:35	Dr. Gabriel Luna Bárcenas CINVESTAV-Querétaro	Dr. Reinhard Lipowsky Max Plank Institute of colloids and interfaces	Dr. Ramón Castañeda Priego DCI-University of Guanajuato	Dr. Pablo Carlos López Vázquez Centro Universitario de los Valles, UdeG, México.	Dr. Alfredo Alexander Katz Massachusetts Institute of Technology
10:40 - 10:55	Short Talk 1	Short Talk 5	Short Talk 9	Dr. Lourdes Mónica Bravo Anaya Laboratoire de Chimie des Polymères Organiques	Congress Closure 10:40-11:00
11:00 - 11:15	Short Talk 2	Short Talk 6	Short Talk 10		
11:20 - 11:35	Short Talk 3	Short Talk 7	Posters/Official photo-taking session		
11:40 - 11:55	Short Talk 4	Short Talk 8		Short Talk 11	
12:00-12:15	Coffe Break/Posters (Foyer Gran Salon Club)			Short Talk 12	
12:20 - 14:00	**Course 1/Course 3/W-1**	**Course 1/Course 3/W-1**	**Course 2/W-1**	**Course 2/Course 4/W-1**	
14:00 - 15:30	Lunch/Dining	Lunch/Dining	Lunch/Dining	Lunch/Dining	
15:40 - 16:30	Dr. Ruqian Wu University of California	Dr. Nina Bogdanchikova CNyN-UNAM	Dr. Erik R. McNellis Johannes Gutenberg-Universität Mainz Institut für Physik	Free	
16:40-17:30	Dr. Yasuhiro Matsumoto Kawabara CINVESTAV	Dr. Lauro Oliver Paz Borbón IF-UNAM	Dr. Marciano Sánchez Tizapa Centro Universitario de los Valles, UdeG, México.		
17:30 - 17:50	Coffe Break/Posters (Foyer Gran Salon Club)				
18:00 - 18:50	Posters (Foyer Gran Salon Club)				
21:00 - 22:00	Cocktail				

Courses

	Researches	Title	Location
Course 1	Dr. Alberto Herrera Gómez, CINVESTAV-Querétaro	Nanofilm characterization through XPS	Auditorium
Course 2	Dr. Andrey Simakov, CNyN-UNAM	Nanoreactors and their application in catalysis	Hall:Pez Vela
Course 3	Dr. Marco Heinen, DCI-University of Guanajuato	Numerical spectral solvers for differential and integral equations	Hall: Pez Vela
Course 4	Dr. Michael Zharnikov, Physikalisch-Chemisches Institut, Universität Heidelberg	Fabrication of protein and ssDNA patterns in the protein-repelling matrix by electron beam and ultraviolet lithography	Auditorium

Workshop

	Researches	Title	Location
W-1	Dr. José Guillermo Méndez Bermúdez, Centro Universitario de los Valles, UdeG, México.	1st Workshop on Molecular Simulation	Hall: Caballito de Mar



• SHORT TALKS (AUDITORIUM) •

Hour		Monday, Nov 06th	Tuesday, Nov 07th	Wednesday, Nov 08th	Thursday, Nov 09th
10:40 - 10:55		Short Talk 1 Dr. Andrés de Luna Bugallo; **“Synthesis and characterization of MOS2-WS2 single and bilayer alloys”**	Short Talk 5 Dr. Karla Juárez Moreno; **“Silver nanoparticles and their use for cancer treatment without genotoxic effects”**	Short Talk 9 M. en C. Gerardo Calderón Ayala; **“Reduced graphene oxide by High Energy Wet Milling using Opuntia Ficus Indica extract”**	Short Talk 11 Dr. José Manuel Romo Herrera; **“Carbon nanotubes based electric inks”**
11:00 - 11:15		Short Talk 2 Dr. María del Rocío Redón de la Fuente; **“Monocharged anions and cations in chemical enhancement in Ag(0) NPs SERS systems”**	Short Talk 6 Dr. Miriam Tostado Plascencia; **“Removal of Aluminum, arsenic, chromium and borom by composites based on multiwalled carbonnanotubes and chlorophyll derivatives"**	Short Talk 10 Dr. Alicia Reyes Arellano; **“A new nanostructured material obtained during an organometallic synthetic process”**	Short Talk 12 Dr. Gonzalo Ramírez García **"Up-conversion nanoparticles covalently linked to a phthalocyanine and herceptin for selective photodynamic therapy against HER-positive breast cancer cells"**
11:20 - 11:35		Short Talk 3 Dr. Stephen Muhl; **“Metallic nanoparticles and M/a-C:H nanocomposite thin films produced using a toroidal planar hollow cathode”**	Short Talk 7 Dr. Maricela Villicaña Méndez; **“Synthesis and Characterization of Silver Nanoparticles by Green Chemistry and by Microwave”**		
11:40 - 11:55		Short Talk 4 Dr. Eduardo Antonio Murillo Bracamontes; **“Ferroelectric lithography: an alternative method”**	Short Talk 8 M. en C. Hasbleidy Palacios Hinestroza; **“Elaboration of nanostructured membranes from agave bagasse for potabilization of water"**		

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INTRODUCTION

Appreciable participants, on behalf of the organizing committee, we take great pleasure in welcoming you to Puerto Vallarta, Mexico, for the 13th International Topical Meeting on Nanostructured Materials and Nanotechnology (NANOTECH2017).

The NANOTECH2017 is the meeting place of the community of scientists dedicated to the nanoscience and nanotechnology areas, and the ideal space for the presentation and discussion of ideas and projects in these fields.

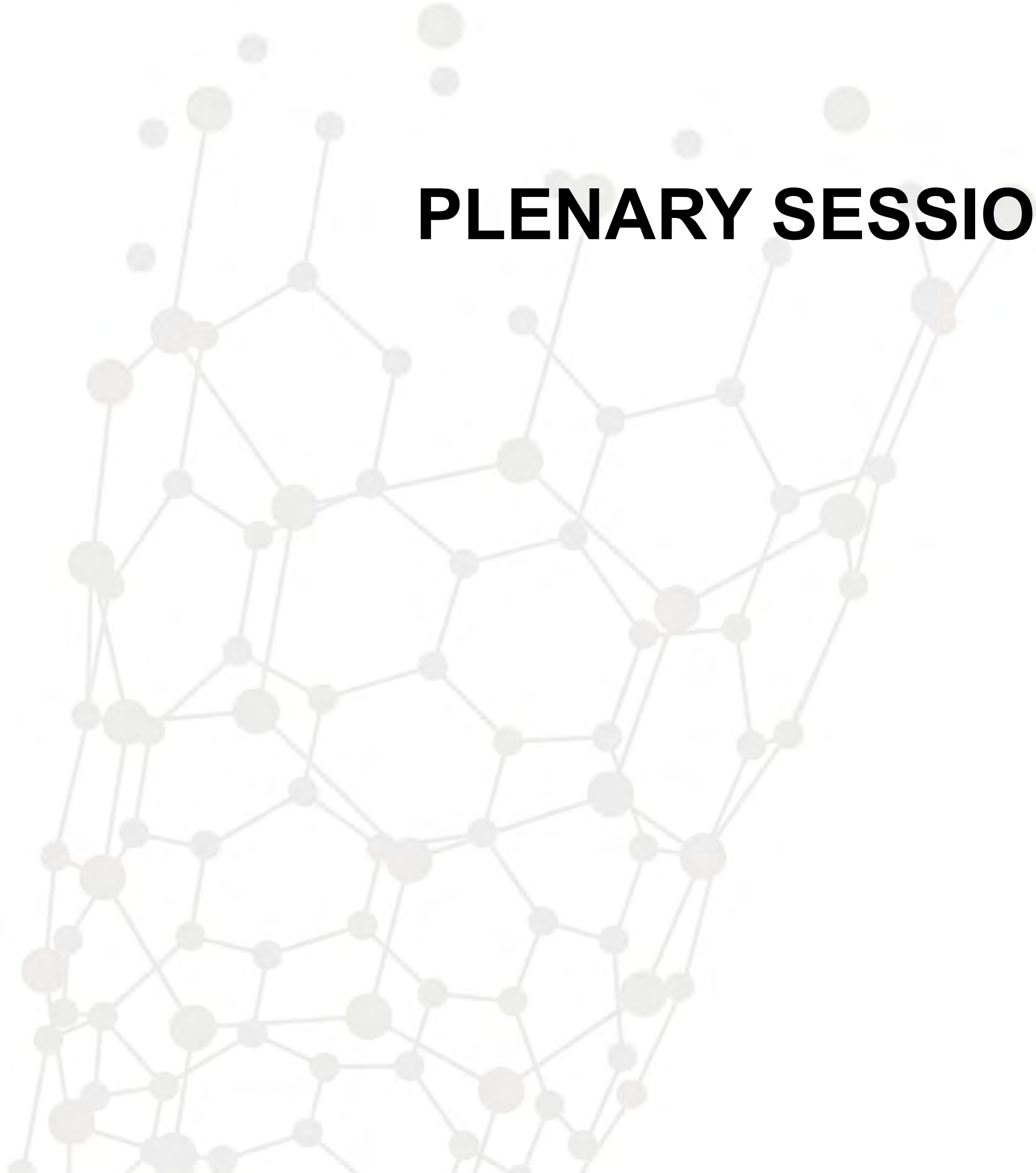
In this edition we have fourteen excellent senior scientists (plenary sessions) sharing their experiences in the resolution of energy, environment and health problems using systems and tools in the nanoscale; twelve short talks complement the oral presentations; three mural sessions (120 posters) allow to broaden the discussion topics into the conference, covering the different lines of research whiting of the areas of nanosciences and nanotechnology. Also, in this occasion we have the first workshop on Molecular Simulation, the activities of the fourth symposium of nanomaterials with applications in solar energy, environment and health, the annual meetings of the Nanosciences Division of the Mexican Physics Society and the CONACyT Mexican Nanoscience and Nanotechnology theme network. Finally, four short courses are available for undergraduate and graduate students.

The NANOTECH events have favored thematic and interdisciplinary discussions and they have promoted collaborations between several academic groups in the country. We invite you to enjoin these opened spaces for the reflection during this forum and encourage you to incorporate young Mexican graduates in nanoscience industry with the goal of increment the impact of this discipline in our country.

We express our sincere thanks to all of you who have contributed to the successful completion of all activities of this congress, 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 13th NANOTECH

PLENARY SESSIONS



Deep Eutectic Solvents: a Green Platform for Advanced Materials Synthesis

Gabriel Luna Bárcenas

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Abstract

The increasing environmental awareness has led to the search of alternative reaction media to alleviate or completely eliminate organic solvents use. Deep eutectic solvents (DESs), a subclass of ionic liquids, have emerged as sustainable solvents for a plethora of chemical reactions. In this talk, DES utilization in free-radical polymerizations will be presented and discussed. Two main fields of application are reported. In the first section, monomers able to undergo free-radical polymerization while taking part of DES, as hydrogen bond donor or ammonium salt, so called DES monomers, are presented. In the second section, the role of DES as solvent where the polymerization takes place, either in the same phase or emulsion, is described. Finally, the properties of the polymers resulting from these particular methods of synthesis are discussed with emphasis on their green aspects and the formation of nanocomposites.

Density Functional Theory Studies of Materials

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Abstract

The development of density functional theory and software packages allows reliable simulations of various material systems, from nanojunctions to topological insulators. In this talk, I will review our recent progresses in studies of 1) sensing properties of nanowires; 2) spintronic and topotronic properties of graphene and topological insulators; and 3) catalytic properties of small entities down to a single atom. The purpose of this general talk is to elucidate the usefulness of theoretical simulations on supercomputers for the establishments of new science and predictions of new materials and properties.

Photovoltaic Systems and Solar Cell Conversion Efficiency Improvements Via Nanotechnology

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Abstract:

An explanation about the general photovoltaic development and situation in the world will be given. Considerations as bulk and thin-film based technologies will be discussed and the possible scheme for solar cell energy conversion improvement by using nanotechnology.

Solar photovoltaic systems (PVS) are becoming one of the important clean and alternative-energy technology in several countries. The PV-systems are safe, reliable with a low-maintenance cost without any on-site pollutant emissions. Nowadays, the utility grid-connected PVS are increasing rapidly in the world and estimated global PV market grew to over 70 GW and about 300 GW cumulatively installed capacity at the end of 2016 [1]. The underlying deployment scenario assumes 3,155 GW of cumulative installed PV capacity by 2050 [2].

We have obtained different nanocrystalline-based thin-films to analyze its light interaction, mostly for the visible range. The obtained photoluminescence from the silicon-based nanoparticles has a bright luminescence in almost all of the visible spectra. The deposited samples are nc-SiOx and nc-SiO_xC_y thin films fabricated by using catalytic chemical vapor deposition method (Cat-CVD). We have used two different precursors as Monomethyl Silane (MMS) and Tetraethyl Orthosilicate (TEOS) for film deposition at relatively low substrate temperatures of 200 to 300° C. In our earlier work, we have obtained the white emission from as-deposited samples by varying the catalyst temperature from 1700 to 1900 °C. By using Scanning electron microscope (SEM) and transmission electron microscope (TEM), it was confirmed the formation of nano-crystals related to the composite of silicon oxide and silicon oxicarbide in the amorphous-SiO_x or a-SiO_xC_y matrix, respectively, without any need of extra annealing treatment. Various morphological and structural analysis has been performed using atomic force microscopy (AFM), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD). Some size distributions of particles were observed and its correlation with their bonding states to silicon, hydrogen and oxygen. Time resolved photoluminescence (TRPL) explains the possible emission mechanism. The decay time of < 2ns obtained from the thin films, remarks the possible contribution of quantum confinement effect (QCE) from the nano-crystals in the SiO_xC_y matrix.

Now we are in the stage to clarify the PL mechanism by means of Density functional theoretical calculations [3] and to explain the possible electronic transitions for the possible application of the nc-Si materials for the optoelectronic devices.

References:

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Nanoparticles and Biomembranes

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Abstract

The endocytosis of nanoparticles by biomembranes is essential for many processes such as biomedical imaging, drug delivery, nanotoxicity, and viral infection. In all cases, the cellular uptake of the nanoparticles starts with the adhesion of the nanoparticles to the membranes, followed by the complete engulfment of these particles. The key parameters for these endocytic processes are particle size and adhesive strength of the particle-membrane interactions as well as bending rigidity and spontaneous curvature of the membranes. [1, 2] In fact, these parameters determine four different regimes for the engulfment of a single nanoparticle. [2] When a vesicle interacts with many nanoparticles, it can exhibit a variety of engulfment patterns consisting of up to three different engulfment regimes. [3, 4] Under certain conditions, the nanoparticles may assemble into membrane nanotubes. [5] Partially engulfed particles ex- perience curvature-induced forces that push the particles towards minima of the membrane curvature. [4] Completely engulfed particles involve a narrow membrane neck that connects the particle-bound membrane with the mother membrane. The formation of these necks is gov- erned by local stability conditions. [2, 6] Our theory provides a quantitative explanation for the nonmonotonic dependence of particle uptake on particle size as observed for clathrin-dependent endocytosis of gold nanoparticles. [2]

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Bionanotecnology for Medicine, Veterinary, Agriculture and Aquaculture

Nina Bogdanchikova[1], Cesar A. Almonaci Hernandez[2], Karla Oyuky Juarez M.[1], Horacio Almanza Reyes[3], Jerico Bello Bello[4] and Ismael Plascencia Lopez[5], Roberto Luna Vazquez Gomez[6], Alexey Pestryakov[7]

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Abstract

In the present work achievements of the International Network of Bionanotecnology of CONACYT (Mexico) will be presented. One of the nanomaterial products developed by our network was successfully applied for the healing of diabetic foot ulcers of 1st, 2nd and 3rd grades of the Wagner classification. For this technology, clinical studies were completed at the ISSSTECALI Hospital in Tijuana and Rosarito General Hospital, both in Baja California, Mexico. Actually, the product is on the market as cosmetic and has cured ulcers of more than 420 patients in Mexico, United States, Spain, Guatemala, Argentina, Peru, Paraguay, Costa Rica, Venezuela, and Costa Rica.

The other achievement consists in discovery of the first non-genotoxic nanotechnological agent which opens up new possibilities for cancer treatment without toxic side effects. It represents a new paradigm in cancer treatment. To bring the results of this discovery to clinical studies and patient treatment, a new National Megaproject of Cancerology is emerging. Actually it is represented by 20 institutions in Mexico, including 3 National Institutes, 1 National Laboratory, 1 International Medicine Program, and 3 abroad research institutions.

In plant biotechnology, micropropagation nanotechnologies have been developed for the disinfection of explants, the sterilization of culture media and bioreactors, the elimination of viruses and plant growth acceleration. This technology is applied for sugar cane, stevia and coffee. The innovative product is in Mexican market and intensive studies for widespread applications are conducted in Mexico, Cuba, Ecuador, France and Brazil.

Application of our nanomaterial products in veterinary and aquaculture: for treatment of Rift valley fever, distemper, white spot syndrome, cow mastitis, usage as a prebiotics and nanoantibiotic, etc., will be also presented.

Computational Simulations of Metal Clusters and Nanoparticles

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Abstract

Transition and noble metal nanoparticles have been the subject of major research efforts with the aim to gain insights on aspects relevant to heterogeneous catalysis. Gaining control at small nm-scale could open new technological possibilities. This has motivated extensive experimental and theoretical studies of mono- and bi- metallic clusters and nanoparticles both in the gas-phase and supported on different type of surfaces, including those of metal oxides. With the constant development of powerful high-performance computing facilities, materials modelling and simulations at the nanoscale has evolved in recent years to a successful field of research, particularly with advances in accurate theoretical approaches based, namely, on Density Functional Theory (DFT) and many-body semi-empirical potentials such as the Gupta potential. In this talk, I will introduce computational methodologies currently used to find minimum energy arrangements of metal clusters - involving a few tens of atoms - as well as of larger nanoparticles. Namely, I will describe a number of global optimization techniques such as Genetic Algorithms, Basin Hopping Monte Carlo, as well as Molecular Dynamics simulations, utilized for an efficient exploration of the particle's configurational space and to gain understanding of the energetics, thermodynamics and reactivity of gas-phase and supported metal clusters and nanoparticles.

Keywords: Global optimization methods; metal clusters, metal nanoparticles, semi-empirical potentials, Density Functional Theory.

Bottom-up Approach to Interface Engineering - Molecular Self-Assembly on Metal Surfaces

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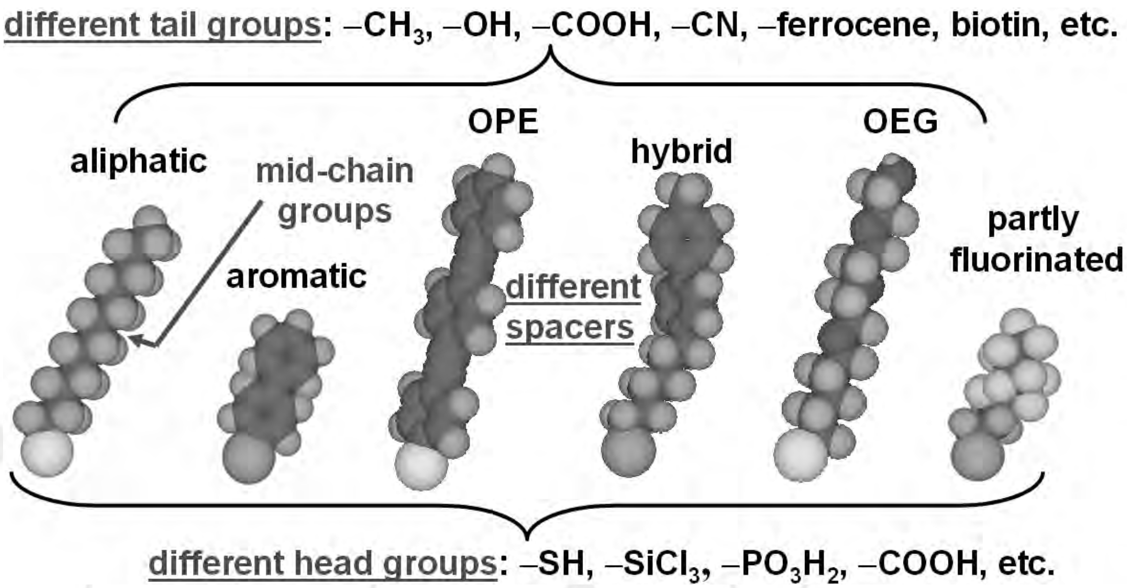
Abstract

Self-assembled monolayers (SAMs) are 2D polycrystalline films of semi-rigid molecules that are chemically anchored to a suitable substrate. Blocking the substrate off the ambient, a SAM gives the surface a new physical and chemical identity, which can be precisely adjusted by the selection of the SAM constituents. These can be flexibly designed by a suitable combination of the individual building blocks, which are a headgroup that makes the anchoring to the substrate, a tail group that is exposed to ambience, and a spacer that separates the head and tail groups. The flexibility of the SAM design and the possibility to prepare these films on almost any substrate result in a variety of applications, such as e.g. tailoring surface properties (wetting, adhesion, lubrication, corrosion, and biocompatibility), sensor fabrication, molecular and organic electronics (injection barrier and growth mode), and conventional and chemical lithography. In most cases, these applications rely on a specific architecture of SAM constituents and SAM as a whole as well as on precise knowledge of the SAM properties. In the overview talk, I will describe the basic properties and architecture of SAMs, address the current state of understanding of the molecular self-assembly, and give representative examples for design of application-relevant SAMs on noble metal and semiconductor substrates. The emphasis will be put on tailoring molecular organisation to achieve specific structural organization of the fabricated films as well as to create a definite chemical identity of the functionalized substrate. This is a prerequisite for well-defined chemical and physical properties of the modified surface. Several examples of application-related molecular design will be given, viz., in the areas of molecular electronics, control of electronic coupling at the interfaces, nanofabrication, chemical lithography, and biofunctionalization.



Typical molecular precursors of self-assembled monolayers. OPE and OEG are abbreviations for oligo(phenyleneethynylene) and oligo(ethylene glycol), respectively.

Linking the Colloidal Cluster Morphology with the Extended Law of Corresponding States

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Abstract

Particle aggregation is an obligatory step for the initiation of the phase separation or the large-scale formation of materials that exhibit a highly heterogeneous structure, such as gels, porous media and glasses. Nevertheless, even though the macroscopic structure of such materials depends strongly on the shape and size of the main building blocks, i.e., the basic units that constitute the supporting structure of any material, the physical mechanisms that lead to the rich cluster morphology is far from being completely understood. In this contribution, we show that it is possible to establish a connection between the cluster morphology in short-ranged attractive colloidal systems and the reduced second virial coefficient, B2. Overall, we observe that small clusters display the same morphology regardless the value of B2, whereas large clusters of two different colloidal systems have the same fractal dimension provided B2 is equal in both systems. Furthermore, weak attractions lead to open clusters, whereas strong attractions produce compact structures. Interestingly, this physical scenario holds at different thermodynamic conditions, namely, at the fluid state and the fluid-crystal coexistence, and close to the gas-liquid phase separation. Hence, our findings allow us to link reversible colloidal aggregation with the extended law of corresponding states.

Multi-Scale Modeling of Molecular Spintronics: the Interplay of Spin-Charge- and Thermal Dynamics

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Abstract

Molecular materials and components offer a range of exciting possibilities and advantages for spintronics. Electronic spins interact with magnetic fields and electronic motion through spin-orbit coupling (SOC). Systematic design of molecular spintronic materials is therefore synonymous with precise tuning of the strength and distribution of fields and SOC throughout the material. Theoretical modeling is an essential tool for achieving this kind of tuning, in particular for understanding the complex interplay between local fields, SOC interactions, electron- and thermal dynamics in the system. In molecular modeling, the ultimate model accurately describes geometric and electronic structure from first-principles theory - without empiricism or adjustable parameters. For materials, it must also describe molecular ensemble effects and macrostructure on a relevant scale. We fulfill these criteria by implementing spin dynamics from first-principles theory on top of a state-of-the-art multi-scale model for thermal- and electron dynamics in soft matter. This tool allows us to simulate a range of phenomena in realistic material models directly comparable to experimentally studied systems, as well as 'zooming in' on single-molecule aspects of spin dynamics. Applications of our methodology thus far include Alq3 - the 'fruit-fly' molecule of molecular spintronics - and several high-mobility chalcogenide organic semi-conductors (e.g. BTBT, the pBTTT polymer etc). In addition to a methodological overview, insights from modeling and concomitant experimental studies of these systems, and an outlook on the near future of this field, will be presented.

Studies of the Electrical Properties of the Interphase $\underline{ITO/In_2S_3}$ by Electrochemical Impedance Spectroscopy and Atomic Force Microscopy

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Abstract

In this work the study of the electrical properties of the interphase Indium Tin Oxide/Indium Sulphide (ITO/In_2S_3), by atomic force microscopy and electrochemical impedance spectroscopy is presented. Thin films (~120 nm) of In_2S_3 were synthesized by electrodeposition. The films were electrodeposited using different complexing agents: 1) sodium citrate; 2) diethylene glycol; and c) acetic acid, the best results were obtained using acetic acid, as thin and uniform films with possibilities of being used as window layer in solar cells were synthesized. The films were characterized by profilometry, X-ray diffraction, energy dispersive X-ray spectroscopy, electrochemical impedance spectroscopy and photoelectrochemical reponse. The mapping of the electrical properties of the materials (electrostatic forces, spreading resistance) was done by atomic force microscopy. The measurement of the mismatch between work functions of ITO and In_2S_3 resulted in ~1 eV, according to previous reports. X-ray diffraction showed a mix of tetragonal and cubic phases, by X-ray spectroscopy it was observed that stoichiometric films were synthesized. Electrochemical impedance spectroscopy probed to be useful as it was the only technique capable of detecting and analyzing thin films of In_2S_3, that no other technique could detect. Mott Schottky characterization and photoelectrochemical response showed the characteristic behavior of an n-type material.

Keywords: indium tin oxide, thin film, indium sulphide, electrochemical impedance spectroscopy, semiconductor, atomic force microscopy, electrostatic forces, spreading resistance.

Novel Nano-Materials Approaches Towards Opto-Electronics and Energy Applications

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Abstract

In spite of often superior properties, in terms of materials and device performance, compound semi- conductors like GaAs and GaN often encounter difficulties in market acceptance, in most cases due to issues of fabrication costs. Nanowires (NWs) constitute a special case due to the opportunities they offer to form highly ideal one-dimensional materials that can be designed into three-dimensional heterostructures via axial as well as radial heterostructures, furthermore with the ability as a technology to add compound semiconductor functionality to a silicon platform. I will structure this presentation into three areas:

(1) The development of high-quality GaN nanowires forming the basis for visible light-emitting diodes [1], primarily with application opportunities in displays, presently with a huge potential market in the areas of micro-LEDs for direct-view displays.

(2) Know-how gained from nitride NW nucleation offers a technology base for realization of relaxed and dislocation-free, c-oriented GaN and InGaN platelets and wafers [2] of significant value for directly driven RGB-emitting LEDs. Many applications areas for nitrides, for optics as well as RF/Power-applications, need higher quality, low dislocation density, wafers.

(3) Opportunities to drastically reduce cost of NW fabrication, based on a dramatically novel growth approach, which we have given the name Aerotaxy [3], by which NWs are grown in an aerosol phase, without use of substrates. I will discuss means by which such NWs may be processed into thin films, thus bridging the many orders of magnitude from discrete NW-devices to square-meter scale applications like for solar cells [4, 5].

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Polyplex Nanoparticles for Gene Therapy: Polysaccharides and Novel Elastinlike Polypeptide-Based Nanovectors Development and Prospects

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Abstract

Nanomedicine is holding tremendous hope in the fields of gene delivery and cancer therapy. One aim of gene therapy is to introduce a normal copy of a given gene to defective cells in order to restore an impaired biological function. Gene transfer principle relies on the use of natural or synthetic DNA complexing agents, referred to as vectors or gene carriers, that are able to compact and protect the genetic material from degradation in biological fluids and to transport it through the target cell membranes for integration into the transcription machinery of a target cell. Nowadays, cationic polymers, which interact electrostatically with negatively charged DNA forming polyplexes, are amongst the most studied non-viral gene delivery vectors. Only few natural polycations possess the characteristics favorable for gene delivery, such as low immunogenicity, biocompatibility and minimal cytotoxicity. Chitosan in particular, which is the most important derivative of chitin, is a polysaccharide that has been identified as a safe and efficient cationic carrier possessing suitable aforementioned characteristics, and the ability to protect DNA from degradation by nucleases. DNA/chitosan electrostatic complex stoichiometry, net charge, dimensions, conformation and thermal stability have been extensively studied. Furthermore, the development of innovative protein polymer nanovectors, resulting from the complexation of positively charged elastin-like polypeptides (ELPs) and DNA was recently proposed. ELPs engineering, which allows controlling several characteristics such as temperature responsiveness, biocompatibility, cell-adhesion functions, among others, is currently explored to design DNA/ELPs nanoparticles and considered as an attractive alternative delivery system for improving the efficiency of gene therapies.

Effects of Confinement on Polymer Structure and Dynamics: The Case of Polymer Nanocomposites[#]

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Abstract

The behavior of polymers restricted in space or close to surfaces/interfaces can be very different from that in the bulk. In this work, we investigate the morphology and thermal properties of hydrophilic polymers in nanohybrids containing either layered silicates or silica nanoparticles. Mixing polymers with layered silicates can lead to intercalated hybrids when the interactions between the constituents are appropriate; these can serve as model systems for the investigation of the static and dynamic properties of macromolecules in nano-confinement. On the other hand, using silica particles of largely different sizes is an attempt to bridge the case of polymers confined within the galleries of layered silicates with that of polymer / single nanoparticle nanocomposites. Confinement is shown to modify the polymer structure, e.g., its crystallinity [1], with the effect being qualitatively different for different types of confinement. The behavior in systems containing different ratios of large-to-small silica nanoparticles is found intermediate between that of PEO/montmorillonite and that of PEO/silica with single-size particles; this behavior can be tuned by varying the ratio of large to small nanoparticles [2]. The dynamics of the confined polymer is probed by dielectric spectroscopy and quasi-elastic neutron scattering [3]. The very local dynamics of the confined chains show similarities with those in the bulk, whereas the segmental dynamics depend very strongly on the polymer/inorganic interactions [4] varying from much faster to much slower or even frozen dynamics [5] as the strength of the interactions increases.

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¥ In collaboration with K. Chrissopoulou, H. Papananou, K. Androulaki, S. Bollas, S. Fotiadou, E. Perivolari, I. Tanis, K. Karatasos, B. Frick, K. Andrikopoulos, G. A. Voyiatzis, M. Labardi, D. Prevosto

Nano-Bio Interactions: A Soft Matter View

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Abstract

Nanomaterials are an emergent platform for multiple applications. Of particular interest are their potential for therapeutics and biological applications. In this seminar I will talk about nano-bio interactions. In particular, I will discuss a new class of nanoparticles that are able to navigate complex biological environments by adapting on-the-fly to different chemical conditions, reminiscent of the behavior of intrinsically disordered proteins. These nanoparticles are amphiphilic by design due to a mixture of hydrophobic and hydrophilic groups on the ligand shell. This property enables the particles to fuse with cell membranes, and cross undetected into internal parts of the cell by transferring to internal membrane structures or protein constructs. They are also able to carry hydrophobic drugs and deliver them to remote regions in the body. The complete pathway of insertion and navigation for these nanoparticles into cells has been recently uncovered and will be presented. The path is reminiscent of the fusion pathway for lipid membranes , and offers much promise not only for applications but for better understanding how nano materials can behave as intrinsic biological entities, and vice versa, what properties of biological systems we can understand with much simpler synthetic nano materials.

Synthesis of Hybrid Templates (PTFE-CNT) Applied to Cellular Growth and Transplantation.

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Abstract

In the present work we synthesized a Hybrid template based on Multiwall Carbon Nanotubes (NTC) and Polytetrafluoroethylene (PTFE) for biomedical applications. Hybrid template synthesis and its functionalization were done by Gas-Face functionalization assisted by microwave irradiation. This process reduce the time of reaction to some minutes.

Digital Fourier Microscopy as a Tool to investigate the Dynamics of Nano and Microparticles in Complex Environments

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Abstract

Nano and microparticles embedded in composites and biomaterials as well as proteins and peptides in biological systems encounter a complex and often crowded environment. Therefore their transport properties, which are of fundamental importance for their dispersions, rheology and information exchange (in biology), are typically anomalous and need to be studied at different length scales due to the complex internal structure of the host system. We present in this talk recent developments in image correlation techniques in Fourier space, which allow a thorough characterization of the dynamics of nano and microparticles over a broad range of length scales and under complex conditions. These techniques can be applied to many different contrast conditions that are available in commercial optical microscopes, including super-resolution and fluorescence/confocal microscopy. To highlight the power of this class of techniques we showcase the study of dynamics of nanoparticles in a porous medium whose structure slowly changes with time [1], and we review other recent applications in different fields.

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Quantum Single-Electron Tunnelling Motor

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Abstract

In Ref [1] the dynamics of a nano-electromechanical rotor driven by a single-electron tunneling has been considered using classical equations of motion for the rotor and a mean field approach. The device is described by a rod that has attached two quantum dots on its extremities. The rod can freely rotate about a fixed axis. The device is located between two Fermionic baths which couple to the rod via tunneling of single electrons to the quantum dots. The baths also provide a static bias voltage that drives the system. In the classical treatment of Ref [1] some interesting phenomena have been observed, like a negative differential conductance. Possible applications of such device are for example signal amplification, current rectification and viscosity measurements.

In the present work we present a quantum derivation of the device and give a full description of the quantum dynamics of the system. Additionally, we discuss similarities and differences to the classical results.

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In Search of an Appropriated Carrier for Cancer Treatment (Cisplatin/Au_{18} Complex)

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Abstract

This talk is related to the study of cisplatin molecule and its interaction with the $Au_{18}(SR)_{14}$ cluster. The aim is to study a protected gold cluster as a carrier for cisplatin which is used during treatment of testicular Cancer with a 90% of success. [1] The idea is to avoid that cisplatin is missed during its transit toward the affected tissues or organs in such manner that the presence of secundary effects migh be reduced. Moreover, the indiscriminated attack to ill and healthy cells can be reduced by improving the cisplatin delivery into the correct organ or tissue. We studied the interaction among one $Au_{18}(SR)_{14}$ cluster and cisplatin molecule(s) and our results indicate that it represents an option for cisplatin delivery given its bio-compatibility and the obtained adsorption energy values. Our calculations based on Density Functional Theory,[2] attests that the $Au_{18}(SR)_{14}$ cluster is able to adsorb an important number of cisplatin units. Further analysis demonstrate that the interaction is strong enought to avoid cisplatin loss. Finally, we provide with electronic and optical and chiroptical properties which can be used as fingerprints to characterize the proposed cisplatin/ $Au_{18}(SR)_{14}$ system.[3]

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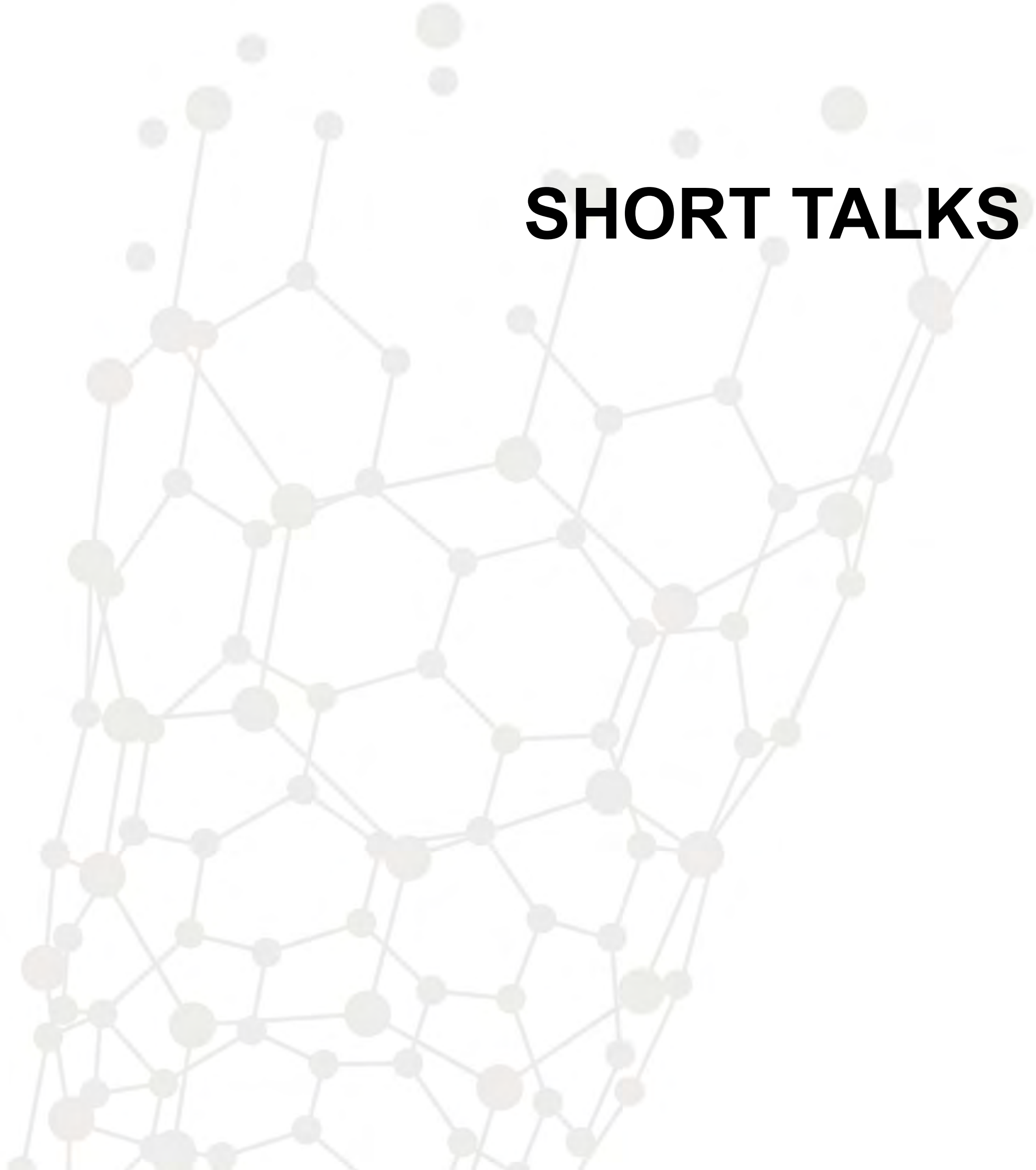

SHORT TALKS

Synthesis and Characterization of MoS_2-WS_2 Single and Bilayer Alloys

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Abstract

Two dimensional materials (2D) have become one of the most exciting fields of material science research. The possibility to achieve and engineer Van der Wall heterostructures and alloys have opened the door for new and exciting research opportunities especially for the development of ultra-fat high efficiency optoelectronic devices.

In this work we present the synthesis and optical characterization of 2D single bilayer MoS_2-WS_2 alloy. The structure was synthetized on a single step APCVD growth using a mixture of MoO2 and WO_2 solid precursors at 1000°C. Micro-Raman spectra recorded at different points of the structures reveals the presence of in-plane and out-plane vibrational modes of both materials. Raman maps revealed the distribution of each material, while MoS_2 predominates in the case of monolayer the content of WS_2 is more important for bilayers.

Photoluminescence (PL) spectra performed on MoS_2-WS_2 monolayer alloy exhibits two broad peaks centered at 1.84 and 1.60eV, however in the case for the bilayer, we observed a redshift of one contribution from 1.60 to 1.51 eV. In order to understand the recombination mechanisms, we studied the intensity dependence of these contributions. In addition, in order to identify each spectral feature, the data was fitted using lorentzian functions. Based on the power dependence law (1), the results indicate that the MoS_2-WS_2 alloys (monolayer and bilayer) PL spectra is composed by multiple contributions such as excitons, trions and defects. Moreover, the peak related to the presence of WS_2 A exciton was found at 1.88eV and a contribution at low energies (~1.6 eV) suggests a strain induced by the substitution of tungsten atoms in MoS_2 crystals (2,3).

Monocharged Anions and Cations in Chemical Enhancement in Ag(0) NPs SERS Systems

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Abstract

It is well known that the electromagnetic mechanism can explain most of the phenomena on the huge enhancement in SERS systems, although it is quite important to take in count the chemical enhancement, since most of the studied molecules interact and/or bind to the surface, thus the study of the molecule-surface interactions, adsorption, surface configuration, etc. have to be analyzed in detail. And, to take care of the chemical reaction as molecule-specific; considering the three types of charge transfer process contributing to the chemical enhancement [1], which further contributes to the total SERS enhancement , type I; when the molecule adsorbs on the metal surface, the change in the electron distribution of molecule even in its electronic ground state may cause different enhancements for different vibrational modes. Type II; mainly related to formation of surface complex, consisting of metal ion (or partially charged metal atom), probed molecule and electrolyte ion and, type III; the photo-driven charge transfer process, this mechanism could also be associated with the excited state of the whole molecule/metal system and with the charge transfer between the molecule and the metal surface or surface ad-clusters. Thus, in the present investigation, we would like to present our findings on the influence of 4 different anions (F^-, Cl^-, Br^-, I^-) and 3 cations (Li^+, Na^+, K^+) on the SERS effect of two different tryazine analytes, using Ag(0) nanoparticles as SERS supports, finding the highest enhancement in SERS when the more polarizable salt, KI, was added.

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Keywords: SERS enhancement, Ag(0) NPs, ions.

Metallic Nanoparticles and M/a-C:H Nanocomposite Thin Films Produced Using a Toroidal Planar Hollow Cathode

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Abstract

Hollow cathodes are very popular for a variety of applications from intense light sources to for thin film deposition. The form of the hollow cathode is such that the loss of electrons to the anode or ground electrodes is reduced and can increase the electron density which in turn produces an increase in the number of ions and hence the plasma density. Another important aspect of the cathode geometry is that almost all of the material that is sputtered from the cathode is re-deposited on the opposite cathode wall. Using these ideas we recently designed, constructed and used a new hollow cathode system based on the planar geometry, similar to a combination of a toroidal electrode and the GHFC; Toroidal Planar Hollow Cathode (TPHC). Here the "hollow cathode" discharge occurs between the upper and lower electrode surfaces and electrons can only leave the discharge via the lower aperture in the electrode. We have studied the plasma density as a function of the applied electrical power and the gas pressure and we have used the system to deposit bismuth and aluminium based thin films and nanoparticles as a function of the experimental parameters. The cathode can be operated from 1 few mili-torr to >5 torr. The material deposition rate mainly is dependent on the plasma power and gas pressure but can be easily controlled by the gas flow. The size of the nanoparticles mainly depends on the gas pressure and plasma power. Nanocomposite coatings have been made by using the plasma plume at the exit of the TPHC to remotely decompose acetylene or methane and deposit a combination of the nanoparticles and an a-C:H film.

Ferroelectric Lithography: an Alternative Method

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Abstract

Over the last years, the leading technique to map and switch domains in ferroelectric materials at nanoscale level has been piezoresponse force microscopy (PFM) [1][2]. In PFM, ferroelectric domain imaging is achieved by using the basic experimental setup of scanning probe microscopy (SPM) 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. For ferroelectric domain switching, a dc voltage, of the correct magnitude and sign, is applied trough the tip into the sample. Ferroelectric lithography using an SPM combines the domain mapping and switching at submicron scale with specific chemical reactions to assemble multicomponents (metal nanoparticles, organic molecules, nanotubes, etc.) into complex structures [4]–[6]. Even though this technique is commercially available, a low cost method to generate ferroelectric templates by automatically detecting the pixel position of the SPM using a data acquisition (DAQ) system and controlling a source-meter as the one that is proposed in this work, could be used. As an example, different templates were written in a PZT sample with the proposed method. .

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Keywords: Piezoresponse force microscopy, PFM switching, ferroelectric lithography.

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Silver Nanoparticles and Their Use for Cancer Treatment Without Genotoxic Effects

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Abstract

Cancer is one of the biggest public health problems in the world. The major challenges of cancer therapy lie in the late detection of cancer, the non-specific administration of drugs and their toxic side effects. Therefore it is urgent to find new antineoplastic agents that cause fewer side effects in healthy cells. In this sense, nanotechnology already has a great potential for biomedical application, where a crucial challenge is to develop biologically safe nanomaterials that have been evaluated through nanotoxicology. One of the most widely used nanomaterials in biomedicine is silver nanoparticles (AgNPs), whose properties as antimicrobial, antiviral and anti-inflammatory agents have already been reported which has allowed them to be used for the treatment and antiseptic coating of medical instruments [1].

Recently, in our research group, we reported a type of AgNPs that exerted a significant cytotoxic effect on 9 different breast, colon, lung, cervix, prostate and melanoma cancer cell lines without causing any obvious genotoxic effect [2]. In addition, we conducted preliminary in vivo studies on a murine model of skin cancer, the results revealed that AgNPs reduce the volume and size of the tumor to the same extent as treatment with the first-line antineoplastic drug. However, we found that in mice with skin cancer that were treated with AgNPs, the genotoxic damage measured by the number of micronuclei in polychromatic erythrocytes was considerably lower than in the antineoplastic drug-treated mice. Therefore, these AgNPs represent the first anti-tumor agent of nanotechnology character that does

not cause a genotoxic effect in the cells and that can be evaluated in future preclinical and clinical tests for the treatment of different types of cancer. In addition, these data allowed us to apply for the registration of a patent before the Mexican Intellectual Property Institute titled: "Pharmaceutical composition of silver nanoparticles and their use in the same in the treatment of cancer without genotoxic effects."

Ackwnoledgments

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Keywords: cancer, silver nanoparticles, nanotoxicology, genotoxicity, biomedicine

A Brief View to the World of Nanomachines

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Abstract

The wold of nanomotors and nanomachines Nanomotors and nanomachines is a cutting edge research area which is being rapidly developing. Nanomotors are nano scale devices capable of convert some form of energy into motion. Special attention has been paid on nanomachines that move in fluids and aqueous media. Multiple designs have been made varying the geometry and propulsion mechanism, using different sources of energy to produce motion like chemical reactions, electric fields, light radiation, magnetic fields and ultrasound. Different advanced capabilities have been added to these tiny devices with potential applications in different fields like transport of micro and nano cargoes, directed drug delivery, sensing, bioremediation, nanosurgery among many others. In this work it is presented an introduction to nanomachines and a small review of the work developed by our group in the field of nanomachines, including potential applications like the aforementioned.

This work is supported by CONACYT Basic Science project 239953.

Removal of Aluminum, Arsenic, Chromium, and Boron by Composites Based on Multiwalled Carbon Nanotubes and Chlorophyll Derivatives

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Abstract

In this research, we present the results of the removal of aluminum, arsenic, chromium and boron by composite materials based on multiwalled carbon nanotubes and chloropyll derivatives such chlorophyllide and pheophorbide. The synthesis of the composites was done following two methods: 1) sonication at room temperature, and 2) stirring at high temperature; in order to compare the removal efficiency of the materials synthesized by both methods. We used pristine, acid functionalized and nitrogen doped multiwalled carbon nanotubes. The procedure for the adsorption tests of heavy metals was done as following: each composite powder was mixed with a solution of known concentration of aluminium, arsenic, chromium or boron for 72 hours with stirring and at room temperature. The concentration of heavy metals was analyzed by atomic adsoprtion spectrometry and ultraviolet-visible spectroscopy, the last one was carried out using erichromocyanine, silver diethyl dithiocarbamate, diphenylcarbazide and curcumin as a complex agents. The results show the differences in the adsorbed quantities of heavy metals depending on two factors: 1) the method of synthesis, and 2) on the characteristics of carbon nanotubes.

Keywords: adsorption tests, removal, heavy metals, boron, carbon nanotubes, protoporpyrin IX

Synthesis and Characterization of Silver Nanoparticles by Green Chemistry and by Microwave

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Abstract

So far, significant advances have been made using wet chemistry strategies to synthesize high quality nanoparticles from a variety of inorganic materials, including gold, silver, iron oxide and semiconductors. The manipulation of the conditions of synthesis allows the rational control of the morphology of the particles and provides the means to adapt the properties of the materials during the synthesis process. Another fundamental aspect of the synthesis of nanoparticles is their stabilization, so that their size and shape can be maintained as a function of time. This paper describes two of the main methods for the synthesis of environmentally friendly nanomaterials. Silver nanoparticles obtained by Green Chemistry and by the use of a microwave reactor, using Silver Nitrate and a dispersant that is Oleyamina for microwaves and for Green Chemistry the reducing agent was extract of guava leaves. The characterization of the nanoparticles by SEM and XRD shows irregular polyhedrons, principal peaks of the Ag with sizes of the order of 134-240 nanometers in a time of 2 to 3 minutes. In addition UV-Vis showed the growth of nucleation as a function of time.

Keywords: Green Chemistry, Microwave, Oleyamine.

Elaboration of Nanostructured Membranes from Agave Bagasse for Potabilization of Water

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Abstract

The development of environmentally friendly technologies, such as those using materials of organic origin, are becoming increasingly important in different areas of knowledge. The area of water treatment is no exception and for this reason in recent years a major effort has been made in the field of nanostructured membrane science and technology for water purification. The aim of this research was to develop a sustainable membrane based technology for the purification of water from agave cellulose nanofibrils. Cellulose extraction was performed from bagasse agave which was delignified and bleached subsequently acetylated with a 6:1 acetic acid CH_3 (COOH) 80% m/m and nitric acid (HNO_3) 65% m/m to 100° C for 15 minutes in an aqueous solution of 1.42% wt. In an ultrafiltration unit Amicon® Ultra at a working pressure of 3.5 psi, membranes with a diameter of 7 cm were obtained. The infrared spectroscopy technique with Fourier transform confirmed the presence of characteristic (O-H, C-H, C-C and C-O-C) groups of cellulose. The X-ray diffraction (XRD) technique allowed to determine the crystallinity of this material. It concludes that nanoscale can improve membrane system because the highly crystalline materials, mechanical properties, strength and specific stiffness and the surface area are favored. The membranes obtained are used in tap water filtracción artificially contaminated to assess retention of pathogenic microorganisms, salts and some heavy metals in the next stage of the project.

Keywords: nanocellulose, membranes, water purification.

Reduced Graphene Oxide by High Energy Wet Milling Using Opuntia Ficus Indica Extract

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Abstract

Green synthesis promote the partial or total substitution of chemical products potentially environment harmful by others more friendly, looking for a new clean product version. We synthesize reduced graphene oxide, using Opuntia Ficus Indica (Ofi) extract and graphite, in an aqueous mixture subjected to High Energy Wet Milling, added with methanol and ascorbic acid, without sulfuric acid and potassium permanganate use. The RGO was identified by Raman spectroscopy. We starts using commercial graphite, in the first step was processed GO, in the last one RGO. The ID/IG relative intensity did changes from 0.22 to 0.91 and then to 1.27. XPS allowed to identify the binding energy between C-C and C-O, C=O and C(O)O bonds. By TEM characterization we studied the structural and morphological properties, it was observed RGO sheets of 0.68 nm thickness and around 100nm length. Our method, using water as solvent and Ofi extract as reductor, represent a green synthesis option to produce RGO due to its low-environmental impact, low-cost production and safety in the process.

Keywords: RGO, Green Synthesis, HEBM, Opuntia Ficus Indica

A New Nanostructured Material Obtained During an Organometallic Synthetic Process

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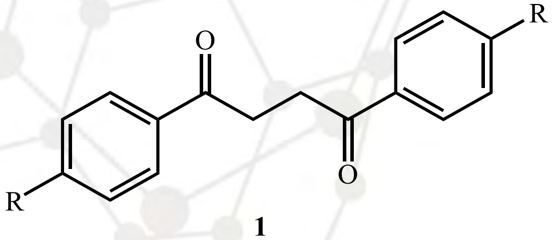
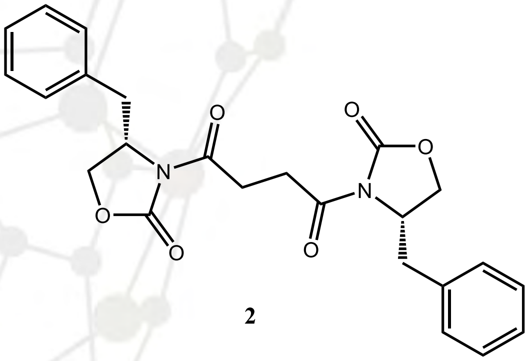
Abstract

Supramolecular materials have attracted the attention of numerous researchers among other factors by their applications in biomedical and technological fields, suffice it to point out the release of drugs, catalysis and the nanomateriales.[1] 1,4-diketones were synthesized by reacting $[Cr(en)_2]^{2+}$ and α-bromo acetophenones[2,3] Figure 1, a procedure applied to the synthesis of dione 2 as well Fig. 2. Gel formation was detected in the mother liquor of this procedure. This is interesting considering that DMF and water were present in large quantities and DMF has a b.p. of 159 °C, therefore the origin of this gel was investigated as well as its characterization was made.



1

Figure 1. Diketones obtained from α-bromo acetophenones mediated by $[Cr(en)_2]^{2+}$



2

Figure 2. 1,4-bis[(S)-4-benzyl-2-oxooxazolidin-3-yl]butane-1,4-dione (2)

As in similar works[4], the gel was analyzed by differential scanning calorimetry (DSC), thermogravimetry (TGA), scanning electron microscopy and energy dispersive spectroscopy (SEM/EDS), transmission electron microscopy (TEM, Fig. 3), scanning electron microscopy (SEM; Fig. 4) and EDS analysis.

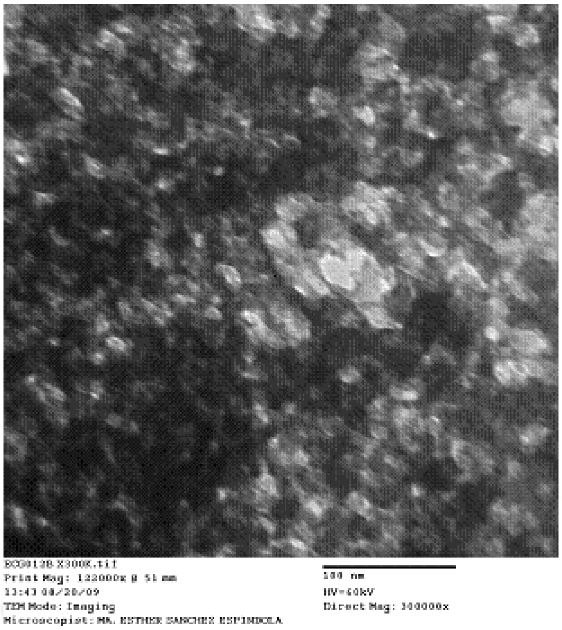


Figure 3. TEM Micrograph of the gel obtained

It was found the gel is a nanostructured material, Figure 3, 4[5]. The material consisted of nanoparticles with an average of 17 nm and fulfills the criteria of a nanogel. In the present work the components of the nanogel and their characterization are presented and discussed.

Keywords: Nanogel, oxooxazolidin dione, TEM

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Carbon Nanotubes Based Electric Inks.

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Abstract

A current trend in the carbon nanotubes (CNTs) field is based in the development of new processing methods to obtain functional materials that can make the most of the nanostructures properties. This is mainly driven by the commercial interest of CNTs based products, making use of their mechanical, electronic or thermic properties [1].

In this work, we made a full study of the electrical conduction properties of inks based in carbon nanotubes, which should be useful to print conductive patterns on flexible substrates by screen-printing techniques.

The obtained inks were designed based in water, while the functional components were either multi-walled carbon nanotubes (MWCNTs) or single-walled carbon nanotubes (SWCNTs), due to their flexibility and high electric conductivity properties.

It is presented a comparative study of the electric conductivity of the inks as a function of the CNTs concentration. Moreover, the study also includes a comparison of the electric conductivity of the inks and an estimation of the production costs for a group of commercial inks. The results to be presented should be very helpful for the application of this type of electric conductive inks.

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Acknowledgments

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Up-Conversion Nanoparticles Covalently Linked to a Phthalocyanine and Herceptin for Selective Photodynamic Therapy Against HER-Positive Breast Cancer Cells

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Abstract

Up-conversion nanoparticles (UCNPs) that convert low-energy light into high-energy light hold promise for enabling biological imaging with enhanced contrast and high spatial resolution because of the absence of natural light-emission in biological samples under infrared excitation at the region of the therapeutic window. In this work we explore the application of the UCNPs as energy transducers for photodynamic therapy (PDT) applications. The light emitted by the UCNPs can represent the source for the excitation of the phthalocyanine (a photosensitizer), which in turn could transfers energy to ground state molecular oxygen to produce cytotoxic singlet oxygen resulting in irreversible photo-damage of the tumor cells. For that, we first synthesize $NaYF_4$:Yb,Er UCNPs and then disperse it in water by means of a ligand exchange reaction, and afterward the amino functionality in the ligand was covalently attached to the -COOH group present in a zinc tetracarboxy phthalocyanine (ZnPc) through an amide bound. The UCNPs-ZnPc composites were then bioconjugated with the anti-HER protein (herceptin). The characterization was carried out in terms of chemical and photophysical properties by appropiated techniques. The nanoconjugates having a diameter of 20 nm were well dispersed and colloidally stable in pH 7.4 phosphate buffer. There was an observed decrease in the fluorescence intensity when they were linked to the ZnPc due to Förster resonance energy transfer. The selectivity of our conjugates against HER-positive breast cancer cells was demonstrated by incubation of the MCF-7 (HER -) and SKBR-3 (HER +) cells with herceptin-attached nanoparticles, and the corresponding analysis under confocal microscope. The free radical production by the nanoconjugates after 975 nm infrared-light irradiation was demonstrated by the XTT assay. The UCNPs-ZnPc-Herceptin conjugates were selectively attached only to the SKBR-3 cells. The presented theranostic nanoconjugated can represent a valuable tool for breast cancer imaging and therapy.

Keywords: Photodynamic therapy, zinc phthalocyanines, HER-receptor.

POSTER SESSION
MONDAY

Optical and Morphological Characterization of ZnSe Nanoparticles Processed by Laser Ablation in Liquid

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Abstract

In this work we present some results and analysis concerning the processing of semiconducting ZnSe nanoparticles obtained by laser ablation of diluted ZnSe powder in acetone. A Nd-YAG pulsed laser was used for ablation, tuned at the first harmonic, 1064 nm, 50 Hz frequency repetition during 60 minutes. The experiment was performed at different power intensities. UV-Vis and Raman spectroscopies were used to characterize the ZnSe particles, whereas scanning and transmision electron microscopy were used to determine the morphology and size of the particles finally, TEM and XRD were used to describe the ZnSe nanoparticles morphology. According to the UV-Vis results it was confirmed a shift of the band edge towards high energy (blue shift) from 2.75 to 3 eV in the sample processed at lower laser power intensity. Raman spectroscopy show the LO phonon at 250 cm-1 and also the so called surface mode at 230 cm-1, for the case of the smaller particles, approximately 20 nm, which was estimated through SEM and TEM pictures. A deep analysis of the results is presented and discussed.

Keywords: semiconducting nanoparticles, nanoparticles synthesis, Raman

Dependence of the Reflective Optical Properties on the Wavelength of Incident Light Beam in a Two-Dimensional Photonic Crystal with Square Periodicity and Optical Micro-Cavities

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Abstract

A Si-ZnO hybrid photonic crystal with square periodicity fabricated by the focused ion beam milling technique (FIB) and studied in this work revealed its ability to selectively enhance the reflectance, at normal incidence, in the border of VIS-NIR range. This ability is connected to the coupling of light beam and the arrangement of embedded micro-cavities in the photonic crystal. The results found suggest the presence of a photonic band gap around the border of VIS-NIR range in the hybrid photonic structure studied.

Keywords: Photonic crystals, Optical properties, Focused Ion Beam.

Dependence of Reflective Optical Properties on the Wavelength of Incident Light Beam in a Two-Dimensional Photonic Crystal with Triangular Periodicity Including an Arrangement of Optical Micro-Cavities

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Abstract

A Si-ZnO hybrid photonic crystal with triangular periodicity including an arrangement of optical micro-cavities fabricated by the focused ion beam milling technique (FIB) was optically characterized by measuring its reflectance at normal incidence in the VIS-NIR ranges. It was found that the photonic structure has the ability to selectively enhance the reflectance, in the border of VIS-NIR range. This was attributed to the coupling of light beam and the arrangement of embedded micro-cavities in the photonic crystal due to this effect it is not present in a similar photonic structure without the arrangement of micro-cavities.

Keywords: Photonic crystals, Optical properties, Focused Ion Beam.

Non-resonant Enhancement Mechanism in SERS Effect Due to CuO Quantum Dots Embedded in Synthetic Zeolite F_9-Na_X

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Abstract

Metallic oxide nanostructures have been studied in the last years because of their excellent biological and electronic properties. Catalytic and bactericide activities are, for example, common properties of metallic oxides like Fe_3O_4, Al_2O_3, Ag_2O and CuO. The later one, has been used to study vibrational properties of another organic e inorganic compounds. In addition, exist reports of the utilization of Cu2O to enhance the vibrational activities of the organic molecules as 4-mercaptopyridine (C_5H_5NS). The main contribution to total enhancement is attribute to charge transfer resonance (CT). Another mechanism to contribute to the total enhancement for molecules on surface prepared with semiconductor nanoparticles, has been reported to be the non-resonant mechanism. This mechanism is consequence of the chemical bonding effect due to interactions between the surface and the molecule. We show in this work the SERS effect due to interaction between synthetic zeolite F_9-Na_X and CuO embedded quantum dots. This phenomenon was predicted theoretically using the functional density theory (DFT) and the computational pack Gaussian 09.

Keywords: quantum dots, zeolite F_9-Na_X, SERS effect and non-resonant interactions

Comparative Study Between Cobalt Ferrite Films Grown by Pulsed Laser Deposition and Spin Coating Method: Structural and Magnetic Properties

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Abstract

Cobalt ferrite ($CoFe_2O_4$) is a ferrimagnetic oxide with inverse spinel-type structure, and it is an insulator magnetic oxide due to high cubic magnetocrystalline anisotropy and negative magnetostriction. Moreover, the electronic insulating properties and the high Curie temperature allow it to use as a material for spintronics. In this way structural, morphological, and magnetic properties of cobalt ferrite oxide (CFO) films are presented. CFO films were grown by nano pulsed laser deposition (PLD) and spin coating (SC) method. Amorphous quartz and (100)-oriented silicon substrates were employed in both deposit methods. A preferential orientation on (004) planes were observed in films grown by PLD, with a large distribution average grain size of 30 nm due to splashing effect. The films obtained by spin-coating method have a better microstructural distribution with average grain size of 50 nm and low ruggedness. The ratio Raman in bands A1g/ T2g show a good chemical stability in films obtained by PLD while changes in stoichiometry is observed for films grown by SC. The coercive field was increased in films with regard to bulk, obtaining the coercive fields of 1.5 and 3.25 KOe for films grown by PLD and SC, respectively; being originated by the oxygen vacancies, pinning sites, lattice strains, and monodomain particles.

Acknowledgements

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Optical and Structural Study of GaN Films Grown by Pulsed Laser Deposition in Nitrogen Atmosphere

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Abstract

Results about processing and characterization of gallium nitride (GaN) films grown by pulsed laser deposition technique are presented. The films were grown on sapphire (0001) and silicon (111) substrates, under the following conditions: substrate temperature 850°C, time deposition of 20 minutes, pressure of 4.2×10^{-6} torr. A Nd: YAG laser was used with 1064 nm wavelengt, repetition frequency of 50 Hz and power of 2.8 W. To characterize GaN films, diffraction X rays, UV-Vis, photoluminescence and Raman spectroscopy were used. To study the GaN films structural properties, X-ray diffraction was used obtaining peaks around 34.5º corresponding to hexagonal phase of GaN. To study the optical properties, UV-Vis spectroscopy absorption and photoluminescence were used. From the UV-Vis spectroscopy a band-gap value of 3.2 eV was obtained. Photoluminescence at room temperature was observed, and Raman spectrum signal was obtained in 712 cm^{-1} corresponding to GaN in its wurtzite structure.

Keywords: GaN, PLD, Raman

Synthesis and Characterization of $CsPbX_3$ Perovskite Nanocrystals

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Abstract

Organometal halide perovskite has been a point of attraction due to its excellent performance in solar energy conversion and Light Emitting Diodes (LEDs). In this work, organometal halide perovskite quantum dots (PQDs) based on cesium lead halide ($CsPbX_3$, where X=Cl,Br,I) were synthetized using hot injection method. The emission spectra corresponding to $CsPbX_3$ QDs in the visible region is obtained by changing the halogen composition (Cl for blue emission (~450 nm), Br for green emission (~515 nm) and I for red emission (~650 nm)) or by varying the size of nanocrystals. The perovskite nanocrystals are having a size of ~10 nm with uniform cubical morphology. The nanocrystals present high photoluminescence quantum yield of ~80% and have interesting properties which can be utilized in LEDs and solar cell application. The quantum yield (QY) decreases due to the inestability of perovskite nanocrystals. The photostability study indicates that the QY is decreased due to agglomeration of uniform cubical morphology leading to the increase in size of nanocrystals to ~100 nm. The stability of perovskite nanocrystals depend specifically on the ligands of nanoparticles and the optical properties and applications are affected by the size of nanocrystals.

Aknowledgment: CEMIE-Sol 27 and 28

Reference:

Siraj Sidhik, D. Esparza, et. al Journal of Power Sources 365, 169-178

Refractive Index and Bandgap Variation in Al_2O_3-ZnO Ultrathin Multilayers Prepared by Atomic Layer Deposition

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Abstract

This research focuses on the study of the refractive index and bandgap behavior in ultrathin multilayer films of Al_2O_3-ZnO bilayers grown via atomic layer deposition (ALD) technique. Multilayer configuration stack consists in alternate layers of constant thickness Al_2O_3 (2 nm) and varying thickness ZnO films in order to obtain a total thickness of ~100 nm. A set of 10 samples based on bilayers with various 2:X thickness ratios were prepared, where X refers to the ZnO layer thickness. X is proportional to the number of cycles (N) of the ZnO precursor, varying from 1 to 100. The sample morphology was studied via Atomic Force Microscopy and the results show that the surface roughness of the multilayers varies from 0.2 to 1.2 nm, as the ZnO layer thickness increases. In all cases, the roughness values remain below 2% of the total thickness of the multilayer. Thickness and optical properties (n(λ), k(λ) and Eg), of each multilayer sample were studied via spectroscopic ellipsometry (SE). Cross-sectional mode scanning electron microscope images verified the multilayer total thickness and corroborated the accuracy of the optical model. The refractive index varies significantly from values close to the Al2O3 refractive index when the bilayer thickness is small, up to values corresponding closely to ZnO for thicker bilayers. The refractive index, as a function of bilayer thickness, varies between 1.63 and 2.3, for λ~ 370 nm, showing high sensitivity. In addition, the optical bandgap energy, Eg, determined using the Tauc model, decreases when the bilayer thickness increases, with a maximum variation of ΔEg ~1.6 eV. These results reveal that the refractive index and optical bandgap can be modulated systematically as a function of the bilayer thickness. Such behavior is of great importance for optoelectronics applications.

Keywords: Tunable refractive index; Optical bandgap modulation; Ultrathin multilayers.

Angular Behavior of Ferromagnetic Resonance on Yttrium Iron Garnet Films Synthesized by the Polymeric Precursor Method

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Abstract

Yttrium iron garnet (YIG:$Y_3Fe_5O_{12}$) films were obtained by depositing the polymeric precursors onto silica substrates, and it was followed by thermal annealing. Structural studies as: X-ray diffraction (XRD), atomic force microscopy (AFM) and Raman spectroscopy show the formation of nanocrsrystalline YIG films with average particle size of 30 nm for annealing temperatures of 800°C. Films annealed at lower temperatures (450°C, 600°C and 700°C) were amorphous with a short-range ordering around tetrahedral Fe(III) sites as is detected by Raman spectroscopy. Vibrant sample magnetometry (VSM) measurements indicate that the amorphous films are magnetically disordered, whereas the crystalline ones presented hysteresis loops characteristic of soft magnetic materials. Ferromagnetic resonance (FMR) spectra in amorphous films showed two absorption modes, one is associated to the weak magnetic ordering around Fe (III) sites and the second with the amorphous paramagnetic matrix. Crystalline films have a complex angular FMR behavior, where the absorption modes are function of the magnetic field angle. These absorption modes are due to existence of magnetostatic microwaves modes (long wavelength spinwaves), and they are induced by the interaction between dynamical microwave magnetization of the YIG films with the dipolar fields induced by the topographical features on their surface.

Acknowledgements: The authors acknowledge the financial support of PAPIIT IG100517.

Keywords: Yttrium iron garnet (YIG), Ferromagnetic Resonance (FMR), magnetic properties

Synthesis and Characterization of Nanocomposites of Fe_3O_4-C

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Abstract

Compared with other transition metal oxides such as Co_3O_4, Mn_3O_4, NiO, RuO_2, or SnO, the Fe_3O_4 crystals are favorable because of the low cost, high electronic conductivity and environmental benignity. As a result, Fe_3O_4 nanocrystals with distinguished magnetic and electrochemical properties have been widely used in various fields, such as information storage, magnetic resonance imaging, supercapacitors and rechargeable lithium-ion batteries.

Coating with carbon is one of the methods for maintaining the chemical stability of the degradation over a long period of the magnetic particles. In the case of Fe_3O_4 it helps maintain its chemical stability and protect it from oxidation under environmental conditions, without altering its properties. It also plays an important role in improving the electronic conductivity of electrode materials, and serves as a protective barrier to effectively release the volume expansion of the internal active materials during the charge-discharge process. The compatibility of materials with carbon makes it suitable for various applications, both pharmacological and energy storage. From Fe3O4 nanoparticles, a Fe_3O_4-C nanocomposite was synthesized through a green moist chemical pathway under hydrothermal conditions.

Keywords: stability, conductivity.

Localization of Electromagnetic Waves in Aperiodically Modulated One-Dimensional Photonic Crystals

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Abstract

Using the transfer matrix theory [1] and the rational approximation [2], we present a numerical study of the localization of electromagnetic waves in three different structures calculating the inverse participation ratio (IPR) [3] as a function of parameter D (modulation parameter). The structures are one-dimensional photonic crystals having a periodic index profile formed with dielectric non-magnetic bi-layer units AB: slab A with width and refractive index da, na, and slab B with refractive index nb and modulated width db = d*(1 + D*Sg) where d is the basic slab's width, D is the modulation parameter and Sg represents consecutive generations of Fibonacci, Thue-Morse and Cantor sequences formed following the Fibonacci sustitutional rule: 1 -> 1,0; 0 -> 1; the Thue-Morse sustitutional rule: 1 -> 1,0; 0 -> 0,1; and the Cantor sustitutional rule: 1 -> 1,0,1; 0 -> 000. Our results show that light localization can be controlled with a small number of layers and a proper choose of Sg and modulation parameter D. The new structures we propose can be constructed with the available technologies at a nanometric scale [4], and can be considered for novel applications where the light localization with a small number of slabs is important as in the design of multifrequency photonic quasicrystal lasers, optical cavities, etc..

Acknowledgements

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Keywords: aperiodically modulated, inverse participation ratio.

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CdS Films Deposition by the Successive Ionic Layer Adsorption and Reaction Method Towards the Fabrication of the Cascade System CdS/CdSe

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Abstract

During the ongoing work we produced the precipitation of a thin film of CdS on conductive glass by the successive ionic layer adsorption and reaction method (SILAR). By varying the number of cycles (from 3 to 18) of the process we modify the morphology of the produced film. The film was characterized by XRD, SEM, EDS and UV-Vis absorption technics. XRD patterns present the peaks indicative of a hexagonal crystalline structure. A clear and homogenous morphology of semi spherical particles, equally spaced among each other, was observed on SEM images. Whereas results of UV absorption showed very low but consistent absorption ranges, the band gap energy value varied closely to 2.50 eV, which is higher than the characteristic band gap of the bulk material (2.42 eV). The best results regarding morphology and crystallinity grade were obtained at 10 SILAR cycles, room temperature and with vigorous rinsing between each SILAR step. We are currently performing tests for the deposition of a CdSe film by Chemical Bath Deposition (CBD) on the CdS existing layer for the goal of constructing a cascade system of CdS/CdSe in order to evaluate the system for the production of a highly efficient solar cell.

Keywords: SILAR, CdS/CdSe, CBD

Detection of Verwey transition in Fe_3O_4 Nanopowders by Means of Microwave Absorption Measurements

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Abstract

Fe_3O_4 nanopowders are researched by means of ferromagnetic resonance (FMR), magnetically modulated microwave absorption spectroscopy (MAMMAS) and low-field microwave absorption (LFMA); in 85-300 K temperature range at X-band (8.8-9.8 GHz). For FMR spectra, an evolution of the experimental parameters, the resonant field (Hres) and the linewidth (Hpp), as a temperature function is clearly observed, and it is associated with Verwey transition around Tv=137 K. Also, MAMMAS response is used to give further information on this material, showing distinctive features associated with magnetic transition. Additionally, LFMA spectra showed a lineal component of positive slope and a hysteresis loop around zero magnetic field; where the disappearance of the lineal component and a minimum in area of the hysteresis loop is observed around Verwey transition.

Keywords: Fe_3O_4; nanopowders; Verwey transition; Microwave absorption.

Ferroelectric and No-Ferroelectric Contributions in Piezoresponse Force Microscopy

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Abstract

In recent years, the study of ferroelectric materials has been popularized due to its applications, among others, in the microelectronic field [1]. Nowadays, the most common technique to study this kind of materials at nanoscale level is Piezoresponse Force Microscopy (PFM) owing to its high image resolution and its affordable implementation [2]. PFM is a technique based on Scanning Probe Microscopy (SPM) which consists of the application of an alternating electric field to the sample by a conductive tip which is in contact mode [3]. Recently, ferroelectric alike characteristics were found in materials which certainly are not ferroelectric materials [4]. Because of this, the present work shows a methodology to discern the ferroelectric from the non-ferroelectric response. Two materials were studied: sodium-potassium niobate (KNN) and soda-lime glass. To achieve this goal, four tests were performed: the acquisition of the hysteresis loop with different AC voltages, the comparison between the resonance amplitude of the tip -sample system versus the applied AC voltage and the obtainment of the first and second harmonic for both materials. Lastly, the switching retention study was performed in concentric squares for the KNN sample.

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Keyword: Piezoresponse Force Microscopy (PFM), Ferroelectric materials, Atomic Force Microscopy.

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Pseudo Jahn-Teller Effect and Buckling in Phosphorene

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Abstract

Phosphorene, the monolayer of black phosphorus, promises to have unique features that make it an outstanding 2D material: unusual mechanical properties as negative Poisson's ratio, high optical and UV absorption, a charge carrier effective mass anisotropy, etc. Unlike graphene, phosphorene presents a variety of phases, being black and blue phosphorene its most stable allotropic forms (stirrup and chair configurations) [1]. It has been recently proposed, by analyzing the distortions of the benzene-like unit of phosphorene, that the pseudo Jahn-Teller (PJT) effect is the responsible for the buckling in phosphorene [2]. In this work, we evaluate the vibronic parameters that model the puckering distortions of hexa-phosphobenzene (P6H6), through DFT and TD-DFT calculations of the APES (adiabatic potential energy surfaces) corresponding to the ground and excited states of the hexagonal molecular system. The ground state instability is explained as coming from a multilevel coupling between this and some excited states satisfying the Jahn-Teller theorem, under the linear coupling model. Similar studies, for the hexagonal unit of stanene, have shown the relevance of this phenomenon [3].

We are thankful with the computer facilities of the Dirección General de Cómputo y de Tecnologías de Información y Comunicación (DGTIC-UNAM) through the project LANCAD-UNAM-DGTIC-159

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Keywords: phosphorene, pseudo Jahn-Teller, DFT

Atomic Force Acoustic Microscopy for Local Characterization of Mechanical Properties of Nitinol

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Abstract

Currently, there is a demand for new materials that satisfy specific characteristics needed for a variety of applications. The aim of science and technology is to study and develop these new materials. Areas such as nanotechnology have promoted development and have presented materials with unique properties, however, due to their dimensions the study and analysis of such properties represents a challenge [1]. Determining the stiffness of a material at nanoscale level is not an exception. New techniques were developed to solve this limitation, such as nanoindentation or Scanning Probe Microscopy (SPM) [2]. This work shows a study performed with Atomic Force Acoustic Microscopy (AFAM). The goal was to prove the effectiveness of the method to detect local stiffness changes. The measures were conducted on a sample of Nitinol, and qualitative results were obtained. A direct current was applied to the wire to take it to its transition temperature and promote a change in its crystalline phase. The AFAM was implemented by using an Atomic Force Microscopy (AFM) in contact mode, a lock -in amplifier for comparing changes in the phase and the amplitude and a DAQ system (Data Acquisition System). It was demonstrated that a low-cost platform for AFAM characterization is possible. Resonance spectrums and acoustic images were obtained; these results qualitatively describe the stiffness of the material.

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Keyword: Atomic Force Acoustic Microscopy (AFAM), Stiffness, Nitinol

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Ferromagnetic Resonance in Amorphous CoFeMoSiB Thin Film

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Abstract

Thin films were deposited by means of dc magnetron sputtering on a glass substrate; with a $3x10^{-2}$ mbar Argon pressure and sputtering power of 0.834 Watts. In all thin films, X-ray Diffraction (XRD) patterns show an amorphous structure. Soft ferromagnetic properties were determined by magnetization measurements, the amorphous thin films have 17 G in coercive field, suggesting a magneto-elastic contribution due to deposition method and the interface between substrate and film. Ferromagnetic resonance (FMR) study showed a broad absorption mode, which suggests an increase in magnetic anisotropy field associated with the magneto-elastic contributions originated by deposit method.

Keywords: Thin films, Ferromagnetic amorphous, Electric behavior.

Acknowledgements.

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Growth and Characterization of II-VI Semiconductors by PLD

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Abstract

Abstract: ZnTe, CdTe and CdS powder (99.99%) were used to get solid targets whith 2.5 cm of diameter. The films (with around 800 nm thickness) were grown over sapphire, quartz and corning glass substrates by PLD. The substrates were heated to 350°C inside of a vacuum chamber with a pressure of 10^{-6}Torr. A pulsed laser Nd:YAG with a wavelength of 1064 nm, 50Hz and 2.4W of power was used to generate a plasma in the system. In order to get the characteristics of the samples were used UV-Vis absorption, XR-D, SEM and PL techniques. The transmittance spectra were analyzed to calculate the band-gap energy of the samples, obtaining 2.2eV for ZnTe, 1.53eV for CdTe and 2.31eV for CdS. By X-RD we could observe a cubic lattice in CdTe and ZnTe with a preferential orientation in the (111) direction in both cases and hexagonal lattice for the CdS with a preferential orientation in the (002) direction. By Scanning Electron Microscopy (SEM) the material was characterized finding a uniformly distribution in the substrate surface without Pinholes presence. The films show photoluminescence signal at room temperature.

Keywords: PLD, II-IV Semiconductors.

Structural and Magnetic Properties of Pt-Co_n (n = 5, 10, 15) Clusters

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Abstract

Transition metal clusters possess many exceptional properties and have been the subject of nu- merous studies by experimental and theoretical groups due to their application in different areas of nanotechnology such as heterogeneous catalysis, magnetic recording media, medicine and biochemistry. In particular, magnetic bimetallic Pt–Co nanoalloy systems have received in- creasing attention due to their superior catalytic activity in hydrogen oxidation reactions and oxygen reduction reactions. Interestingly the Pt–Co system offers better catalytic performance and selectivity than its pure counterparts. Inspired in experimental works, we present a theo- retical study of the structural and magnetic properties for the Pt-Co$_n$ (n = 5, 10, 15) clusters. As a first step, we perform an exhaustive conformational search of the stable clusters using the Bilatu code. Bilatu includes a suite of automated programs oriented to search the global mini- mum in atomic and molecular clusters [1-3]. In this code the total energy is evaluated using DFT methods just as it is implemented in the electronic structure codes: Gaussian, NWChem, etc. Each geometry optimization was followed by harmonic frequency computations in order to confirm the structural stability. For further determination of the total spin in the lowest total energy state all possible spin multiplicities were tried. Our results for the average magnetization per atom are in agreement with experimental and theoretical reports for similar clusters. We are grateful to LANCAD (DGTIC, UNAM), HCP Kukulcan (CONACyT, INFRA-2012-01- 188147), and HPC Juchiman (CONACyT, U0003-2015-7-26609) by the generous allocation of computational resources.

Keywords: Pt–Co clusters, structural optimization, magnetic properties.

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Conversión Fotocatalítica de CO_2, Usando Materiales Metal-Orgánicos Amino Nano Estructurados (NH_2-Nano MOFs)

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Abstract

Recently, it has been shown that MOFs have good properties as semiconductors for use in photocatalytic reactions. In this work, Nano-Mil-101(Fe) and Nano-NH_2-Mil-101 (Fe) was synthesized by solvothermal/sonochemical method at different reaction times. After, synthesized materials were characterized using X-ray diffraction, UV-Visible, Infrared and Raman spectroscopies and N_2 adsorption-desorption at liquid N_2 at 77 K. The materials obtained were evaluated in a continuous system. The reaction products were determinate by gas chromatography. The results of the characterization showed that the incorporation of amino group in the MOF not show change in its structure. The presence of amino group in MOF increases its catalytic activity that than Nano-Mil-101 (Fe). The results of catalytic activity obtained showed that these materials are very active and selective to methanol.

Keywords: Photocataliysis, MOF, UIO-66

Manufacture of Aluminum Alloys with Carbon Nanotubes Decorated with Gold

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Abstract

In recent years the interest in the development of new materials in this case has been increased, since these more advanced materials can perform their work better than conventional materials (K. Morsi, A. Esawi., 2006).

In the present work the behavior of the addition of carbon nanotubes is analyzed by incorporating nano gold particles to increase both their electrical and mechanical properties. Aluminum alloys were made with carbon nanotubes using low energy grinding at a speed of 140 rpm and during a 24 hour grinding period, starting from 98% aluminum, alloys with 0.35, 0.5 and 1.0% of nanotubes were made. Carbon, the grinding was performed to obtain a good homogenization since the distribution affects the behavior of the properties (Amirhossein Javadi, 2013), in addition to the particle reduction

And finally the incorporation of carbon nanotubes by adding nano gold particles by reduction with sodium borohydride by means of the ultrasonic tip. The obtained alloys were characterized by Scanning Electron Microscopy (SEM), X-Ray Diffraction Analysis. Performed hardness tests and finally electrical conductivity tests were performed.

Synthesis and Characterization of Nanotori by Low Temperature Treatment of Multiwall Carbon Nanotubes and its Tribological Properties

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Abstract

The synthesis and study of carbon nanotori is relatively new due to his discoverment a few years ago. In this work, we present a new method of obtention of this nanoparticle, creating some defects on the surface of multi wall carbon nanotubes. To create these defects, we have made a chemical treatment of carbons nanotubes at low temperatures to add some radical groups to the surface, creating non-lineal defects that causes de rolling of carbon nanotubes, to create a toroidal nanoparticle like a donut, with self-assembly properties. The materials used to this synthesis was multi wall carbon nanotubes doped with COOH radical groups to accelerate the rolling process, Sulphuric Acid, Nitric Acid, Distilled Water, Potassium Permanganate and Hydrochloric Acid. Particles obtained shown uniform size, bidimensional growth due to the self-assembly property, and a characteristic angle of 126º. We have considered its application for water based lubricants, dispersing Carbon Nanotori in distilled water at varying concentrations. Nanolubricants showed excellent stability even without the use of dispersing agents. We have tested it at extreme pressures with excellent results. This material has been characterized by Scanning Electron Microscopy, Transmission Electron Microscopy, FTIR, Raman Spectroscopy and T-02 four-ball tribotester, according to the ITeE-PIB Polish test method for testing lubricants under scuffing conditions.

Keywords: Nanotori, Carbon Nanotubes, Nanolubricants, Extreme Pressures.

$CdS_{1-x}Se_x$ Thin Films Preparation by Chemical Bath Deposition and Laser Ablation

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Abstract

$CdS_{1-x}Se_x$ thin films were deposited via Chemical Bath Deposition (CBD) and Laser Ablation (LA) technics on glass substrates. CBD films were grown at 75°C during 120 min; the Se/S atomic ratio of the bath was modified in order to modulate the composition x. Laser Ablation films were deposited with a Nd-YAG laser emitting at 355 nm. The employed targets were prepared with fixed composition of 0.2 and 0.8. Morphology and structural properties of the films were studied using X-Ray Diffraction, Scanning Electron Microscopy, Energy Dispersive X-Ray Spectroscopy and UV-Vis absorption technics. CBD films composition strongly change from 0.19 to 0.77 by modifying Se/S atomic ratio from 0.1 to 1.7. These films are constituted by semispherical clusters (50-150 nm in diameter) of elongated particles, the density and homogeneity decrease in function of x. Crystalline structure of ternary solid solution also changes with x; hexagonal phase is observed for x=0.2 CBD films but x=0.7 films present cubic structure. However, crystal size is almost constant around 6 nm. The band gap value of these films decreases from 2.23 to 1.94 eV as Se content increases. Films prepared by LA are dense and homogeneous. Their crystalline quality, and crystal size are higher than those of CBD films with the same x, hexagonal phase is observed to these films. Band gap value goes from 1.7 to 1.98 eV.

Keywords: $CdS_{1-x}Se_x$ thin films, Chemical Bath Deposition, Laser Ablation

Electrical Behavior in Ferromagnetic Amorphous Thin Films

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Abstract

Electrical measurements were carried out in thin amorphous films with CoFeBSi nominal composition. The films have thickness of 250 nm, 125 nm, 62.5nm and 31.25 nm and they were obtained by means of magnetron sputtering. The four-probes technique is used to determine DC electrical properties with 4200 SCS Keithley system. All films show ohm-type behavior; however, their electrical resistance have an anomalous increment, where Mohms values are in thinner film. The anomalous increment of the electrical resistance in metallic films can be associated with amorphous order in magnetic structure.

Keywords: Thin films, Ferromagnetic amorphous, Electric behavior.

Acknowledgements.

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Cluster Al_{13}: a Pseudohalogen Like Astatine

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Abstract

The question whether Al_{13} behaves as a superatom, mimicking a halogen atom in its reaction properties, has generated great interest and significant amount of research due to the possibility of being part of the building blocks of tailored materials with specific characteristics. Seeking elucidate this question, Han and Jung1 performed an analysis about the adsorption of the halogen atoms (F-I) on Al_{13}, assuming that all the halogens are atop adsorbed, assigning therefore a unique electronegativity for Al_{13} cluster as if it mimicked an atom. Motivated by their results, in this work we carried out DFT calculations to analyze the adsorption of the X halogen and alkali atoms (X=Li-Rb, F-At) on Al_{13}, on bridge, hollow and atop sites. We show that the adsorption processes presents an inherent regioselectivity, which invalidates the possibility to assign an electronegativity to the cluster similar to atom. In order to further investigate the pseudohalogen characteristic of Al_{13}, we study its capability to mimic interhalogen and alkali metal halides formation, and analyze the charge transfer and the bonding characteristics by studying the Hirschfeld population analysis as a function of the Mülliken electronegativity and the electron localization function (ELF). Our analysis shows that the neutral Al_{13} endohedral cluster displays, in general, pseudohalogen properties consistent with the jellium superatom model when compared with At. We discuss the possible applications of exploiting the At-like behavior of Al_{13}.

Acknowledgements.

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

Keywords: Al_{13}, Astatine, Pseudohalogen

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Simple Synthesis and Characterization of $ZnMn_2O_4$ Nanoparticles

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Abstract

Manganese spinel oxides have attracted much attention due to their excellent physical and chemical properties, which have allowed them to be applied in many technologies. Among these oxides, zinc manganite ($ZnMn_2O_4$) is an interesting material that has been mainly used as an anode material for lithium-ion batteries due to its low cost, environmental friendliness and low oxidation potentials. This work presents the synthesis and characterization of $ZnMn_2O_4$ nanoparticles. The nanoparticles were synthesized by means of a simple microwave-assisted colloidal method, using as starting reagents zinc nitrate, manganese nitrate and dodecylamine. A brown-color solution was obtained after mixing the starting reagents with ethanol. The solvent evaporation was made by applying microwave radiation at low power (~ 300 W) and subsequently, the material was dried at 200 °C for 8 h in air. Further a calcination temperature of 500 °C produced the pure phase of $ZnMn_2O_4$. The $ZnMn_2O_4$ powders were characterized by X-ray diffraction (XRD), thermal gravimetric analysis (TGA), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Raman and UV-vis. The $ZnMn_2O_4$ nanoparticles were identified by TEM with average particle size of ~ 60 nm, and five vibrational modes typical of zinc manganite were registered.

Functionalization of Graphene Oxide with Embedded Silver Nanoparticles

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Abstract

At present, Graphene has been an attractive material in the areas of solar energy and health, some researches are focused on this material due to the possibility to improve some of their properties such as the optical and electronical properties, which in combination with silver nanoparticles a new variety of promising applications.

In order to perform the sample, we exfoliate graphite with sulfuric acid, phosphoric acid, potassium permanganate and hydrogen peroxide. After that process, we obtain graphene oxide (GO), which was functionalized with spherical-like silver nanoparticles. In this case, those nanoparticles used were about 3 to 10 nm of diameter.

The sample obtained were characterized by the use of FTIR, UV-Vis and Raman spectroscopy. We found in the FT-IR spectra some absorption signals at different wavelengths associated with the vibrations of the GO functional groups, the inelastic dispersion of light by the material have a series of characteristic bands in the range of 800 to 3200 $cm^{-1,}$ containing the bands G, DY 2D. Also, in the Raman spectroscopy we observe a change in the intensity for GO. Finally, UV-Vis spectrum shows the surface plasmas around 410 nm which could be attributed to the presence of the silver nanoparticle in the GO.

Angular Dependence of the Reflective Optical Properties of a Two -Dimensional Si-ZnO Photonic Crystal

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Abstract

In this work we present an experimental study of the angular dependence of the reflective optical properties of a two-dimensional photonic structure, built on silicon substrate coated with a ZnO thin film, employing the focused ion beam milling technique (FIB). The photonic device describes a regular square lattice with a lattice constant a = 1.05 μm and air columns of radius r = 0.63a. The silicon substrate was prepared with a double purpose zinc oxide thin film coating. First, to protect the Si substrate from erosion during the photonic crystal fabrication with FIB and, second, to determine its influence on the optical properties of the photonic crystal fabricated. Optical characterization on the photonic structure was performed before and after ZnO thin film was removed from Si substrate to be able in identify the participation of the thin film on the photonic hetero-structure. The photonic crystal was optically characterized measuring reflectance at normal incidence for visible (VIS) and near infrared (NIR) ranges. Results obtained in this work revealed that polycrystalline ZnO thin film coating increase the reflectance of the photonic crystal fabricated on Si substrate compared to measurements on the photonic device in bare Si.

Keywords: Photonic crystals, Optical properties, Focused Ion Beam.

The World of Nanomotors and Nanomachines

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Abstract

Nanomotors and nanomachines is a cutting edge research area which is being rapidly developing. Nanomotors are nano scale devices capable of convert some form of energy into motion. Special attention has been paid on nanomachines that move in fluids and aqueous media. Multiple designs have been made varying the geometry and propulsion mechanism, using different sources of energy to produce motion like chemical reactions, electric fields, light radiation, magnetic fields and ultrasound. Different advanced capabilities have been added to these tiny devices with potential applications in different fields like transport of micro and nano cargoes, directed drug delivery, sensing, bioremediation, nanosurgery among many others. In this work it is presented an introduction to nanomachines and a small review of the work developed by our group in the field of nanomachines, including potential applications like the aforementioned.

This work is supported by CONACYT Basic Science project 239953.

The Effect of Dispersion Forces in the Structure and Photoinduced Charge Separation in Organic Photovoltaics

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Abstract

The use of π-conjugated polymers as electron donors and fullerene derivatives as electron acceptors in bulk heterojunctions represents a potential alternative to silicon-based solar cells. The understanding of the elementary processes that determine the power conversion efficiency plays a key role in the manufacturing of commercially competitive organic photovoltaic devices. In this oral session, the electron transfer parameters that directly affect the photoinduced charge separation in organic solar cells are quantum chemically analyzed in detail. This work is therefore important since charge separation in bulk heterojunctions of oligomers and fullerenes can be more properly described at structures that include van der Waals interactions.

Keywords: organic photovoltaics; Marcus theory, electron transfer

Hierarchical Nanostructures of Platinum Synthesized Using Bicontinuous Microemulsion Reaction Method and Their Electrochemical Characterization

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Abstract

Platinum (Pt) is a noble metal with potential applications as catalyst due to its intrinsic activity and properties. Platinum nanostructures (Pt-NS) composed of numerous active sites or improved surface area are highly advantageous for practical catalytic and electrocatalytic applications. However, the synthesis of nanomaterials with specific shape and morphology is a major challenge. In overcoming this, we proposed the use of bicontinuous microemulsion. Pt-NS were synthesized in this work by chemical reduction of oil and water soluble Pt precursors, respectively. The characteristics of the products obtained were studied by SEM, TEM and XRD. Cyclic voltammetry was used for electrochemical inspection and to obtain critical data regarding the surface activity of the Pt-NS. Nanomaterials made from oil-soluble Pt precursor had an average size of 8.84 nm. Agglomeration of nanoneedles was observed in nanostructure fabricated using Pt water soluble precursor. The electrochemically active surface area (ECSA) was determined from charge associated with the underpotential reduction of hydrogen. The interconnected polycrystalline hierarchical Pt-NS made from oil-soluble precursor had the highest ECSA (33.68 m2g-1), while 26.65 and 21.29 m2 g-1 respectively, were obtained for nanostructure synthesized using platinum water soluble precursor. A mechanism of formation of the PtNS is proposed. Broadly, this report presents a novel knowledge to the study of Pt-NS as electrocatalysts.

Fast Randomization of Block Copolymer Micelles: Dynamics, Relaxation and Mechanisms

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Abstract

Amphiphilic block copolymers self-assemble in water as micelle aggregates with diverse morphologies[1]. Because of the core surface tension, block copolymers micelles exhibit a slow to frozen kinetic[2]. Their dynamic is dominated by two processes; an individual one which involves insertion-expulsion of copolymer chains and collective ones which involve fusion and fission of proper micelles[3]. Fusion and fission are crucial for controlling the behaviour of amphiphilic aggregates particularly in drug delivery and for the synthesis of controlled nano-objects[1]. The insertion-expulsion at equilibrium was reported to be highly sensitive to chain polydipersity and leads to a logarithmic type decay[4]. This was accounted for by the dependence of the activation energy on the core chain length N. This dependence of activation energy on the length of the core forming block is also predicted to affect to the same extent the fusion and fission processes[3]. We have addresses this issue by investigating the fusion and fission kinetics at equilibrium in triblock copolymer micelles PEOxPPOyPEOx, with various x and y. These results establish that the collective fusion and fission mechanisms are highly sensitive to the average molecular weight of the copolymer. On the other hand and contrarily to the insertion-expulsion kinetics, fusion and fission exhibit a single exponential behavior even in highly polydispersed copolymers.

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Keywords: dynamic, copolymer micelles, amphiphilic copolymers

Pt-Co/TiO$_2$ As Catalyst for 2,5-Dimethylfuran (DMF) from 5-Hydroxymethylfurfural (HMF); a Theoretical and Experimental Study

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Abstract

Substitution of the fossil fuels for alternative energy sources is a great priority for the energy security of our region because the petroleum is now unavailable; these sources could in short time be substituted for alternative energy sources as biofuels obtained from biomass. Developments of biofuels are being accelerated because our government is not in a position to direct deep extractions of petroleum and also because our region has a wide variety of agricultural materials considered as waste that can be transformed to biofuels. Therefore, production of 2,5-Dimethylfuran (DMF) like an ideal substitute of conventional gasoline should be achieved because it has energy content like that of gasoline. Using noble metals limits their application as catalysts in the production of DMF due to their high price and low abundance in nature and also their catalytic efficiency is not always the highest found. One option is using bimetallic catalysts where a non-noble metal contributes with their properties and permit to keep the catalytic activity of noble metal. For that, we have developed a material kind Pt-Co/TiO$_2$ with low amount of Pt to produce DMF. Characterization with XRD, electron microscopy SEM and HRTEM confirmed a nanostructured material with low proportion of Pt (1wt%). Through theoretical calculations from first principles the interaction between 5-Hydroxymethylfurfural (HMF) and Pt-Co/TiO$_2$ was studied. Catalyst activity was proved as well and conversion efficiency of HMF was to up 80%.

Keywords: Biofuels, Bimetallic catalysts, First principles.

Characterization of Materials Used to Build a Dye Sensitisized Solar Cell Using the Colorant Protoporphyrin IX

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Abstract

The conversion of solar radiation into electricity has been done using photovoltaic devices in order to avoid environmental issues as global warming. A cheaper variant of the solar cells are the dye sensitized solar cells. Organic dyes have a broad absorption band, and when are coupled with nanocrystalline oxide films it is possible to collect a larger fraction of sunlight [1].In this work we describe the use of the protoporphyrin IX in a dye sensitisized cell. The synthesis of titanium oxide was done by Sol-Gel technique and this material was used as the working electrode, on the other hand, reduced graphene oxide was used as the counterelectrode. The synthesis of the graphene oxide was carried out by the modified Hummer method and the reduction was done by sonication. We are reporting the preliminar results of the characterization of the materials used to build the solar cell. The materials were characterized by X-ray diffraction, Raman, ultraviolet-visible, infrared spectroscopy. X-ray diffraction and Raman showed the presence of anatase phase for the titanium dioxide. Raman spectroscopy showed the characteristic signals of graphene oxide. The band gap calculation of titanium dioxide by ultraviolet-visible spectroscopy resulted in ~3 eV, and infrared spectroscopy of the protoporphyrin resulted in strong signals of hydroxil groups, double bond C=O, and C-N bonds, characteristic of this compound.

Keywords: graphene, titanium dioxide, dye sensitized solar cells, charge transport

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Synthesis and Functionalization of Colloidally Stable ZrO_2:Yb,Er-SiO_2 Core-Shell Up-Converting Nanoparticles for Optical Imaging

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Abstract

Recent advancement in science has allowed a greater availability of advanced tools for optical imaging. Recently, the conversion of near infrared radiations into visible light using non-linear optical processes, termed as up-conversion, has become very attractive in the medical field for applications like cell tracking and optical imaging. This work reports the synthesis, surface modification, and the structural and optical characterization of ZrO_2:Yb^{3+},Er^{3+} nanocrystals. We have synthesized nanocrystals by different methods, and the co-precipitation and solvothermal ones using Pluronic as a surfactant produces the best results. The STEM analysis indicates the formation of nanoparticles (NPs) with sizes ranging from 20 to 30 nm depending on the concentration of surfactant introduced during the co-precipitation step. The NPs demonstrated a strong red luminescence with an emission band ranging from 630 to 700 nm with an excitation of 975 nm. This emission band is included at the tissue transparent-window, which is necessary for optical imaging applications. For the same purpose, luminescent NPs preferably have to form a stable colloidal solution under physiological conditions. However, common nanomaterials with strong up-conversion emission are hydrophobic in nature, or trends to be agglomerated. In order to incorporate the colloidal properties into NPs, they were coated with a SiO_2 shell, and then covalently coated with hydroxyl and 3-aminopropyl triethoxysilane groups. The luminescence intensity was enhanced by the presence of the SiO_2 shell respect to the non-modified ZrO_2:Yb^{3+},Er^{3+} NPs. This enhancement in luminescence intensity could be associated to the presence of structural defects at the NP surface, and by the direct interaction between the NP matrix and the water, which induces the luminescence quenching. The described results demonstrate that ZrO_2:Yb^{3+},Er^{3+} nanocrystals can be successfully functionalized with different molecules and with further biomolecules to develop platforms for biolabeling and bioimaging applications.

Keywords: Up-conversion nanoparticles, colloidal stability, biomedical applications.

Aknowledgment: CEMIE-Sol 27 and 28, PEI (230785) 2016

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Optimization of CdS Quantum Dot Sensitized Solar Cells by Solvent intermixing

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Abstract

In this work the optimization of a quantum dot sensitized solar cell of CdS with the architecture FTO/TiO_2/CdS/ZnS was carried out. The cell was made by the Succesive Ionic Layer Adsorption Reaction (SILAR) method. The effect of the use of different solvents as rinses in the SILAR process was determined. We conclude that the alchohol / water mixture is more efficient in the sensitization of the photoelectrode achieving efficiencies of 3.3% compared to the typical method with only alcohol or water use where efficiencies of 2.7% are obtained. This is demonstrated from the optoelectronic characterization with the curves J-V, IPCE and impedance.

Aknowledgment

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Keywords: QDSSC, CdS, SILAR

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Inverted Structure of Perovskite Solar Cell Under Ambient and Controlled Atmosphere

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Abstract

Organic-inorganic inverted structure perovskite solar cells have been analyzed. This structure use the organic part to electron and hole transport materials and the perovskite to photoactive light absorption. Commonly the method of depositing the perovskite film is the anti-solvent method, this method is used in the conventional configuration FTO/TiO_2/$CH_3NH_3Pb_{I3}$/Spiro-ometad/Ag, however this method is a few used in the inverted structure. In this work, we use the anti-solvent method to fabricate the perovskite film in the configuration ITO/ PEDOT:PSS/$CH_3NH_3Pb_{I3}$/PCBM/Ag, showing that the use of these method enhance the size grain of the perovskite films and the quality of the crystal depend of the atmosphere of deposition. If the perovskite films are deposited under ambient condition then the efficiency is about ~7% and under controlled atmosphere (in a glovebox with nitrogen) increases the efficiency until ~9. These result indicated that the quality of the perovskite film in these configuration depend of the conditions of deposition. Further improvement in the efficiency is expected with the optimization of different layers and the work for it is in progress.

Aknowledgment: CEMIE-Sol 27 and 28

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POSTER SESSION TUESDAY

Synthesis and Characterization of Hematite Nanoparticles for Arsenite Removal in Aqueous Medium

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Abstract

Arsenic is one of the most widespread inorganic pollutants worldwide and represents a significant potential risk to human health and the biosphere. It is well known that arsenic is highly toxic and carcinogenic; at present, there are reports of diverse countries with arsenic concentrations in drinking water higher than those proposed by the World Health Organization (10 μg/L). Nanomaterials and nanotechnologies inspire new possible solutions to major environmental issues nowadays. It has been reported that adsorption strategies using nanoparticles as hematite proved to be very efficient for the removal of arsenic in drinking water. However, the adsorption mechanism is not yet clear. In order to shed light on this subject, we attempt to study the interactions between arsenic species and α-Fe_2O_3 nanoparticles in an aqueous medium. The iron oxide nanoparticles were prepared using a solvothermal method. As-synthesized hematite nanoparticles were put in contact with As_2O_3 solutions at room temperature at pH 4 and 7. The nanoparticles were characterized by FTIR, XRD, UV-vis, XRF and XPS. The results showed that synthesized nanoparticles had an average diameter of the crystallite of 30 nm. The presence of arsenic on particles surface was confirmed, which is more remarkable when pH= 7 conditions are employed. On the other hand, after adsorption experiment, it was evident from FTIR and XPS that once arsenic species interact with the nanoparticles, they form mono and bidentate surface complexes.

Keyword: nanoparticles, hematite, adsorption, arsenic

Evaluation of the pH Effect on DNA/Chitosan Complexes Formation

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Abstract

Gene therapy is considered as an alternative to controlled release of genetic material (DNA and RNA) to target cells. Currently, cationic polymers are the most studied non-viral vectors for gene transfer. The complexes formed between these vectors and DNA need to be able to be injected in the body to enter the organism, to interact with the membrane of the cell, to escape the endosomes and to reach the nucleus of cell. Moreover, non-viral cationic polymers do not generate immune reactions, contrary to viral vectors. In this study, chitosan was selected as non-viral vector. Chitosan is biocompatible and biodegradable polysaccharide with a low toxicity. This polysaccharide has been widely studied and has been shown to be able to form polyplexes with DNA due to its high charge density. Polyplexes resulting from the compaction between DNA negatively charged molecules and chitosan positively charged polysaccharides, can interact with negatively charged cytoplasmic membranes, enabling their cellular internalization through adsorptive endocytosis. The protonation behavior of polycations such as chitosan is one interesting feature controlling endosomal escape of polyplexes, since it determines the density of cationic charges that affect the interaction with cell membranes. In this work, the pH effect on DNA/chitosan complexes formation was firstly studied using a series of chitosan solutions at different initial pHs (3.6, 5.0, 5.5 and 6.0) and a DNA solution at a constant pH. Then, the influence of DNA solution pH in DNA/chitosan complexes formation was also studied by using a chitosan solution with 100 % protonation (pH=3.5). The evolution of the nanoparticles **ζ**-potential and size was studied through electrophoretic mobility and dynamic light scattering (DLS) measurements, respectively. A morphological study of the obtained nanoparticles at the different selected pHs was performed using Atomic Force Microscopy (AFM). It is shown that the stability of DNA/chitosan complexes can be tuned depending on pH and the degree of protonation of chitosan.

Keywords: pH, chitosan, DNA, nanoparticles, compaction, AFM

DNA/Chitosan Complexes Stability Study

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Abstract

Nowadays, gene therapy is considered as one of the most promising therapeutic approaches, due to the possibility to treat disorders at the nucleic acid level through the genetic manipulation. The success of this therapy and the efficient gene transfer relies in the appropriate gene delivery system. Polysaccharides have been widely accepted as non-viral vectors for gene delivery purposes du to their ability to efficiently condensate DNA, interact with cells and protect DNA against nuclease degradation. Furthermore, they present low toxicity and have high biocompatibility. Chitosan is a biodegradable polycationic polymer with low immunogenicity. It is considered a good candidate for gene delivery due to its positively charged structure, which allows the compaction with negatively charged DNA. DNA/chitosan complexes stability is important for reaching the target cell for replication, to avoid DNA degradation and allow decompaction of DNA. DNA/chitosan complexes are formed due to electrostatic interactions between DNA phosphate group and chitosan protonated amine groups. In this work, the formation of DNA/chitosan complexes was carried out through different methods, one of them is the progressive addition of chitosan to the DNA solution and the other one is the formation of a complex at a specific charge ratio by mixing both solutions. DNA/chitosan complexes stability was studied with DNA solutions having different ionic concentrations, at different temperatures, two chitosan molecular weights (MW) and different ($[NH_3^+]/[P^-]$) ratios (from the relation of charges between chitosan and DNA). Complex formation was evaluated in terms of the particle ζ−potential, obtained from electrophoretic mobility measurements, complexes size (RH), obtained from dynamic light scattering (DLS) and morphology, observed from Atomic Force Microscopy (AFM) measurements. It is shown, that complexes prepared at the different studied conditions are stable in size and charge during at least 10 days, suggesting strong electrostatic interactions between both molecules, giving to the nanoparticles a high stability.

Keywords: DNA, chitosan, stability, time, temperature, ionic concentration.

Amphiphilic Block Copolymer micelles Surface Modification with Chitosan for Drug Delivery Applications

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Abstract

Nowadays, nanoparticles are developed to mimic or alter biological processes so their use in medicine could give solutions to problems associated with solubility, bioavailability and/or immunocompatibility of many medicines. Amphiphilic block copolymers are macromolecules composed of a hydrophobic block and a hydrophilic block. In water, they aggregate into micelles, in which the hydrophobic part forms the heart and the hydrophilic segments form the corona. These materials are of great interest because of their applications in drug delivery. Generally they are spherical and with a narrow distribution of particle sizes. Moreover, polysaccharides such as chitosan, which is a biocompatible, antibacterial and environmentally friendly polyelectrolyte, have been proposed for several applications as the development of biodegradable films, biomedical devices and microcapsule implants for controlled release in drug delivery. In this work, a physicochemical characterization of amphiphilic triblock copolymers Pluronic P104 (PEO27–PPO61–PEO27), P103 (PEO17-PPO60-PEO17), P123 (PEO19-PPO69-PEO19) and F127 (PEO100-PPO65-PEO100) was firstly performed in the concentration range from 0.5 to 2.0 wt% and the temperature range from 16 to 60 °C. Dynamic light scattering (DLS), electrophoretic mobility and viscosity measurements were used to determine the particle size, the ζ-potential and the viscosity of the triblock copolymer solutions, respectively. After identifying the conditions at which these copolymers form spherical and elongated micelles in water, surface modifications of the triblock copolymer micelles were performed with the addition of the polysaccharide chitosan and were followed through DLS and ζ-potential measurements. These modifications on micelles characteristics could improve the storage stability of hydrophilic drugs in micelles

core and could prevent their release before reaching the specific target and receiving the adequate stimuli to achieve an efficient and controlled drug delivery.

Au Nanoparticles Synthesis Assisted by Marine Algae

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Abstract

Nanoparticles (NPs) of noble metals, such as gold, silver or copper, have attracted tremendous attention during the last decade due to their exciting optical properties. The understanding of the extreme confinement of light at the nanoscale has facilitated the development of a wide range of applications [1]. However, a “green” synthesis alternative involving the use of aqueous media, environmental friendly reducing agents and the replacement of alkytrimethylammonium halides by biocompatibles agents is urgently needed.

A viable alternative is to explore the algae biomass, which are made of a good amount of polysaccharides. Particularly, the Phaeophycae classs, such as Egregia menziesii contain metabolites which have good properties to be applied in biomedicine.

In this work we present an eco-friendly green synthesis method in aqueous media by using an extract from the alga Egregia sp, which plays a double role as the reducing agent and as the stabilizing capping agent of the NPs giving stability to the Au colloid. A detailed analysis of the role of the alga extract in the Au NPs growth under our scenario is presented. Moreover, the optimized parameters to obtain narrow size distribution of Au NPs are elucidated.

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Acknowledgments

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Aparicio for technical assistance. We are also thankful to Ignacio Beamonte for providing us the marine algae.

Optimization of Nanofiltration Using Artificial Neural Networks

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Abstract

Membrane systems have been widely used in various processes such as in the field of pharmaceutical chemistry, fine chemicals and food production. These devices are associated with expensive and unwieldy processes. Therefore, a lot of studies were developed with the aim of improving the efficiency and control of these processes using filtration. Evolutionary algorithms are stochastic optimization methods that have been developed as a combination of rules and randomness that seeks to imitate different natural phenomena as animal behavior or physical laws. An important feature of evolutionary methods is that their operation is based on the analysis of candidate solutions that are randomly initialized, while every step of optimization is developed better solutions to regions in space of the task. Different operators derived from the analogy of every evolutionary approach is applied to each candidate solution to ensure that each step, such solutions to better approximate that required to meet an objective function solution. One way to find the optimized parameters is to obtain a mathematical model. This model can be obtained using a technique called artificial neural networks which is a computational representation of a set of neural units or artificial neurons that mimic the way a biological brain learns and solves problems based on previous experiences. Accordingly in this study it is proposed to use these methods to optimize the design for manufacturing nanostructured cellulose membranes, with optimization are expected to find the most suitable conditions for manufacturing in order to find that are low cost and potential for various applications.

Keyword: cellulose acetate, optimization and nanofiltration

Study of Polymeric Composites of Acid Polylactic Reinforced with Nanocellulose

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Abstract

This paper show the results of the evaluation of the wear of the polymer composites reinforced with nanocellulose (particle size ~ 100 nm) with potential biomedical applications. The addition of particles at a given matrix is a resource commonly used for more resistant materials. The reinforcements used are usually stronger and improve the mechanical properties of the original material, this arises from the need to obtain new materials with improved properties that would be impossible to bring together in a single type of material. Nanocellulose has excellent mechanical properties and come from natural sources like trees, cotton or agro-industrial waste. The areas evaluated in this research are composites of polylactic acid (PLA) reinforced with nanocellulose. The study includes analysis surface roughness, crystallinity, functional groups available features useful in the characterization of polymeric matrices, fibers, particles and other constituent materials of polymeric composites. Another feature that is expected to assess is the wear surfaces. Wear is the loss of mass of the surface of a solid material by mechanical interaction with another body in contact, is an important characteristic to assess the potential of a composite as biomaterial for applications such as prostheses, than could constantly be subject to wear in the presence of a fluid such as blood or saliva.

Keywords: wear, polylactic acid, nanocellulose, composites, biomedical applications.

May Be Possible Generate a Docking Molecular Using Compounds of Gold by Attack the Kissing-Loop of HIV

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Abstract

It has been proposed that the kissing-loop complex of the Human Immunodeficiency Virus Type 1 (HIV-1), which initiates the dimerization of the genomic RNA, a key step to the virus replication, could be a target for neomycin-B and thymine-neomycin [1]. As additional hypothesis, because the supply of auranofin led to an increase in the count of the CD4+ cells [2], this drug could be another potential candidate to target the kissing-loop complex. In this work we used molecular dynamics to model the molecular docking of the drugs above mentioned to the kissing-loop complex, obtaining structural parameters such as the sites and interactions number in addition to electronic parameters such as the total energy and the Gibbs energy to characterize the molecular docking.

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Keywords: Dymanics Molecular, genomic RNA of HIV, docking molecular.

Optical Properties of Metallic and Semiconductor Nanoparticles in Zeolite A4 and their Antibacterial Applications

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Abstract

This study shows the optical properties and antibacterial activity of AgNPs y its chalcogenides of S and Se. The nanoparticles were synthesized and stabilized in the matrix of A4 zeolite AgNPs show an average size of 7.5 nm and the chalcogenides show a size around 9 nm nanoparticles have a quasi-spherical morphology. The calculated interplanar distances confirm the presence of metallic and semiconductors nanoparticles in hexagonal, monoclinic and orthorhombic phase for Ag, Ag_2S and Ag_2Se NPs respectively. SPR for AgNPs was obtained at 415 nm and absorption at 331 nm (for Ag2S) and 375 nm (for Ag2Se) were visualized for the semiconductors. The presence of surface-enhanced Raman spectroscopy (SERS) effect caused by AgNPs on the surface of the zeolite was observed. We suppose that the SERS effect in the material is caused by Electromagnetic enhancement mechanism (EEM). The antibacterial property of the nanoparticles stabilized in zeolite was analyzed against gram-negative Escherichia coli and Pseudomonas bacteria and gram-positive bacteria Staphylococcus aureus and agalactiae. In order to quantify the antibacterial effect of the nanoparticles, the inhibition zone was used as a parameter on the bacteria colonies grew the culture medium by conventional methods. AgNPs showed a better result against all bacteria. The bacteria better Inhibited with all material was S. aureus. The result also suggests the antibacterial activity is slightly mayor with (Ag_2S)NPs that (Ag_2Se)NPs.

Keywords: Nanoparticles, Antibacterial Activity, Optical Properties

Synthesis and Characterization of Nanoparticles of Silver Using Extracts of Aloe Vera, Applied to Bandages and Patches

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Abstract

With the help of the Nanomedicine, the aim is to search for systems of treatment of greater effectiveness of existing ones for the care of the affected area. A proposal for the care of the wound by burns is to implement bandages and patches with nanoparticles of silver and Aloe vera extract. Silver nanoparticles have great potential biomedical applications as an agent with bactericidal, fungicidal, antiviral or healing.

The work of research shows the way in which the bandages with nanoparticles of silver and Aloe vera eficientan The sanitation process and scarring of the skin; in the same way, are bacteriological tests for the verification of the effectiveness of silver nanoparticles with extract of Aloe vera.

Synthesis of a Shape Memory Composite Base on Polyvinylalcohol and Ag 0D Nanoparticles

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Abstract

Shape Memory Polymers (SMP) are those that can recover their original or permanent shape through the application of external stimuli, such as temperature, contact with water, among others. To do this, you must first "program" the polymer; Ie it must be deformed by the external stimulus to obtain a temporary form. This form is maintained even when the stimulus is withdrawn and can remain indefinitely. If the stimulus is applied again, the polymer will regain its original shape.

Obtaining SMP, which has nanoparticles, has been more recent and its usefulness lies in improving the already inherent properties of polymers and making multifunctional materials, and "intelligent" ones. In the case of their applications as sensors, the ability to react to stimuli such as temperature, to be used in food or medicines and to determine if they have been subjected to a temperature above the recommended temperature, or to present the effect of Memory of form in the presence of certain solvents or vapors of them, which would allow to detect the presence or absence of them.

In the present work, the polyvinyl alcohol (PVA) was used as polymer matrix because it presents thermal stability, chemical resistance, is biodegradable and biocompatible. Silver nanoparticles were used to incorporate them into the PVA, due to their high thermal conductivity, electrical conductivity and antimicrobial activity. The influence of the nanoparticles on the properties of the PVA was investigated and its shape memory was evaluated under the temperature stimulus

Synthesis and Characterization of Polymeric Nanoporous Microparticles as Potential Drug Carriers

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Abstract

Smart hydrogels can undergo significant changes in their physicochemical properties in response to a variety of environmental stimuli, such as temperature, pH, electrical fields and glucose. Hydrogels containing ionizable groups can take advantage of their ability to volume changes depending on the pH of the physiological médium1.

One of the ways to delay the therapeutic action of drugs are the functionalized polymer nano- and micro-particles (NP's or MP's)2. In this work, nanoporous MP's were synthesized with acrylic acid functionalized methyl methacrylate and crosslinked with ethylene glycol dimethylacrylate (PAA-PMA-EDGM) to achieve functionalization levels of 20 and 25% and several degrees of cross-linking 0, 0.1, 0.3 and 0.5. MP's were characterized by dynamic and static dispersion light, they have a spherical shape and an average size of 300-450 nm at a pH 3 depending on the functionalization and crosslinking degree. The hydrogels are pH-sensitive they show pH-dependent swelling behavior. After freeze-drying MP's showed BET area in 10-12 m2g-1 range and a porous size of 6-8 nm, in the range of mesoporous materials. The aim of this work is to develop a new form of drug delivery system for anticancer drugs.

Keywords: nanoporous microparticles, pH-sensitive, freeze-drying.

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Synthesis and Structural Characterization of Polylactic Acid Nanospheres Obtained by Microemulsion

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Abstract

The rapid advancement of nanotechnology in recent years has given way to a real perspective within the medical and biological area; Current researches are based on the synthesis of new materials with inherent properties that favor their passage, stay and exit of the human body. The potential use of polymer nanospheres in these areas had a great reachin the late 80's, due to the fine adjustment of their properties. In this work we report an efficient method to produce polylactic acid nanospheres (PLA) in CTAB-ammonium hydroxide-water-oil-TEOS microemulsion system and the effects of temperature on its structural properties observed with Scanning Electron Microscopy, UV-vis Spectroscopy and Thermogravimetric Analysis.

Keywords: Nanospheres, Polylactic acid, Drug delivery

Use of AFM to Detect Early Damage in Stored and Gamma Irradiated Red Blood Cells.

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Abstract

Blood gamma irradiation is the only available method to prevent transfusion associated graft versus host disease (TAGVHD), its important maintain the qualities of blood such as structural and functional for a successful treatment. However, it is widely known that Storage and ionizing radiation are stressing agents of human red blood cells (RBCs) and produce morphological and biochemical changes altering its function.

In this work, we systematically analyzed at nanoescale the topological changes in non-irradiated RBCs and stored gamma irradiated RBCs using atomic force microscopy (AFM). Also, we evaluated the functional properties of membrane by osmotic fragility and integrity of hemoglobin using Raman spectroscopy. The irradiation process alters the roughness on cell membrane in a dose dependence manner from the fifth day of radiation and the time of storage increases those effects. The changes on the roughness is visible at five days of storage true the fragility test, and fragility of the RBCs increase radically at thirteenth day of storage, related to time and radiation effects without dose dependence. The biochemical fingerprint of RBCs remained unaltered, indicate that hemoglobin structural remain unaltered. Our results showed that early markers as nanoscale roughness, allow us to evaluate blood quality since other perspective.

Keywords: Red Blood Cells (RBC’s), AFM, Roughness, Raman Spectroscopy.

Effect Changes in Osmotic Pressure of Red Blood Cells Stored and Gamma Irradiated

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Abstract

Blood transfusion is one of the most important therapies in various diseases, being vital to maintain the quality of the blood. In patients with compromised immune system the use of gamma irradiated blood is required to prevent graft versus host disease associated with transfusion (TA-GVHD). However, in the blood gamma irradiated oxidative damage in red blood cells occurs, including abnormalities in cell membranes causing hemolysis. In this work we study the changes in osmotic pressure of red blood cells stored and gamma irradiated. Different doses of gamma radiation were used the most recommended dose is 25 Gy and two higher dose 35 and 50 Gy. We calculated osmotic pressure, Dose lethal 50 (DL50) and force with data obtained of fragility osmotic and size. The obtained results show changes in structural integrity of the erythrocyte cell membrane components as a result of oxidative damage due to gamma radiation.

Keyworks: Red Blood cells ● Gamma irradiated ● Osmotic fragility ● Dose lethal 50.

Polypeptide-Based Nanoparticles Formulation for DNA Transport and Delivery

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Abstract

Nanotechnology has been extensively used for gene delivery and cancer therapy. Gene transfer principle relies on the use of DNA complexing agents, referred to as vectors or gene carriers, that can compact and protect the genetic material from degradation in biological fluids, and can deliver the genetic material inside the targeted cell. Few natural polycations possess the characteristics required for gene delivery, such as low immunogenicity, biocompatibility and minimal cytotoxicity. They also need to be able of binding to nucleic acids and provide good transfection efficiency. In this project we propose the development of original polypeptide-based nanovectors (elastin-like polypeptides, ELPs) able to compact and deliver nucleic acid chains into targeted cells. ELPs engineering allows controlling macromolecular dimensions, namely polypeptide sequence and length, the exact number of positively-charged groups and physico-chemical characteristics such as temperature responsiveness. A detailed study of the compaction process between the functionalized ELP-M-40 and nucleic acids (eGFP and pUC19 plasmids) was performed to find optimal conditions to develop stable nanoparticles with controlled size and surface potential at different charge ratios.

Membranes Electro Spun Poly Lactic Acid with Nanoparticles of Magnetite

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Abstract

The Tissue Engineering is a multidisciplinary area that involves combining scaffolding, cells, and molecules biologically to regenerate functional tissues. Presents the study of four types of cellular scaffolding on the basis of poly(lactic acid) and nanoparticles of magnetite. The scaffolding developed were: 1) PLA13%, 2) PLA13%-$Fe_3O_4$10%, 3) PLA13%-$Fe_3O_4$20% and 4) PLA13%-Fe3O430%, which were obtained by means of the technique of electrospun, using the following parameters: capillary distance to manifold 30 cm, volumetric flow 0.30 mL/h, 15 kV voltage and relative humidity of 30%. The morphological characterization was performed by scanning electron microscopy, where it was observed a reduction in the diameter of the fiber to increase the concentration of nanoparticles of magnetite. Thermal analysis was performed by thermogravimetric analysis to show the temperature difference of degradation between each one of the scaffolds. The mechanical characterization was performed by means of Traction tests carried out with a universal testing machine, the results show that the accession of nanoparticles decreases the modulus of elasticity of the scaffolds. In vitro cultures were performed on mesenchymal cells from the human during five days, by means of the indicator LIVE/DEAD, it was quantified the number of living cells and it was noted that a number of nanoparticles added to affect a number of living cells. From the experimental results, it is possible to show the utility of this new material in the biomedical area.

Keywords: electrospinning, nanoparticles, magnetite, scaffold, poly(lactic acid)

Evaluation of Antibacterial Activity of Different Nanocomposites of Calcium and Magnesium Oxides

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Abstract

Currently the research of nanomaterials with bactericidal activity has increased considerably since bacterial pathogens have become resistant to commercial antibiotics. Interesting reports have recently been reported using metal oxides where they have an antibacterial effect. The advantages of using oxides are that they are very environmentally friendly materials, can be used in small quantities and are generally considered to be safe for human beings. Under rigorous conditions they show a stability, which makes them more applicable. Therefore in this work we have sought the elaboration of nanoparticles consisting of oxides of magnesium, calcium and their nanocomposites.

The synthesis method consists of the precipitation of nanoparticles in the form of Mg(OH)2 and $Ca(OH)_2$ in dimethylsulfoxide using ammonium carbonate as precipitating agent. After calcining the samples, nanoparticles of MgO, CaO or their composites were obtained. The samples were analyzed with Infrared and Raman spectroscopy and X-ray diffraction. The results showed the formation of nanoparticles of MgO, CaO and their composites.

In addition, it is interest to apply the nanoparticles and nanocomposites to strains of Gram negative bacteria (Salmonella thypi) and Gram positive (Enterococcus faecalis) to observe their antimicrobial effect and measure their degree of inhibition.

Keywords: metal oxide nanoparticles, antibacterial activity.

Evaluation of Nanoestructures of Diatomite in Water Filtration

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Abstract

In recent decades, various water treatment technologies have been proposed and applied in the experimental and field levels. Thus, among the most used decontamination systems at present: centrifugation, filtration, separation, sedimentation, coagulation and flocculation, aerobic and anaerobic treatments, osmosis, nanofiltration, microfiltration, adsorption, etc. Also, chlorination, ultraviolet radiation, and the use of membranes. However, not all technologies achieve the same performance, meaning the percentage reduction of all pollutants, the same costs or have the same process of regeneration or cleaning. In this sense, the objective of this research is the study of nanostructured materials of diatomite for use in decontamination of water, the materials were modified by calcination and by mechanical action to increase the Surface area. The diatomite is a silicic sedimentary rock, a product of diatomaceous algae fossilization. The diatoms; microscopy unicellular algae cover by a silicic layer called frustule, this one is porous and has more of 10,000 shapes. The chemical composition of the fossilized skeleton fossilized (frustule) is opal, amorphous silicon $SiO_2.n.H_2O$.The use of this kind of material will complement the actual methods of treatment and filtration of water, and it will also reduce the costs of the processes.

Keyword: Nanofiltration, Diatomite, decontamination of water.

Magnetic Al_2O_3-Al_3Fe– $Al_3Fe_5O_{12}$ Nanoparticles Immersed in a Polycaprolactone Matrix: Preparation, Characterization and its Use in Biomedicine

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Abstract

Nowadays the nanomedicine necessity is searching for materials that produces innovative methods for drugs therapies and administration. Because of its multiple applications magnetic nanoparticles have been studied and employed in biomedical areas as hyperthermia, magnetic resonance imaging (MRI) agents, biosensors, magnetic carriers and targeted drug delivery. In this context, the aim of this study is to elaborate a nanostructured magnetic Al_2O_3-Al_3Fe- $Al_3Fe_5O_{12}$/ polycaprolactone composite in order to take advantage of the biocompatibility and biodegradable properties of the polycaprolactone (PCL) matrix, exploit the alumina (Al_2O_3) porosity and take advantage of the found iron aluminide-aluminum iron garnet (Al_3Fe- $Al_3Fe_5O_{12}$) magnetic “soft” properties. For the magnetic nanoparticles reaction synthesis was employed a $FeCl_3$ reduction with a lithium aluminum hydride in environmental conditions. The reaction was performed at 85°C during 72 hours in THF/Toluene 75/25 %V as solvent under continuous stirring. The resulting powder was then dried to 150°C during 4 hours. A thermal treatment was realized at 850 and 1100°C and posteriorly the Al_2O_3-Al3Fe- $Al_3Fe_5O_{12}$ nanoparticles were added in situ to the polycaprolactone matrix. Characterizations using Fourier Transform Infrared spectroscopy (FTIR), X-Ray Diffraction analysis (XRD), Scanning Electron Microscopy (SEM) and magnetic hysteresis parameters showed the formation of magnetic Al_2O_3-Al_3Fe- $Al_3Fe_5O_{12}$ nanoparticles immersed into a porous polycaprolactone matrix with excellent magnetic “soft” properties that makes it suitable for its use in biomedicine as a magnetic carrier and targeted drug delivery system (DDS).

Keywords: Polycaprolactone, iron aluminide, aluminum iron garnet, magnetic hysteresis, drug delivery system.

Noncovalent Interactions in Encapsulation of Molecules into Nanotubes

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Abstract

We investigate the absorption properties of some molecules on the inner surface of nanotubes (NTs) by first-principles density functional theory calculations. The nanotube that encapsulate the molecules is zigzag (12,0). Moreover, we study the behavior of the binding energie of this organic molecules with the inner walls of the NT, we also calculate the electronic Density of States (DOS) for each optimized structure, and we conclude that there is physical adsorption between the molecules and the nanotube, according to the chemically inert nature of NT. Results suggest that molecules can safetely pass through any cavity being protected by NTs, and can be useful in medical applications.

Chitosan Electrospun Nanofibers with Au/Ag Nanoparticles Synthesis and Characterisation

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Abstract

Chitosan solutions in acetic acid were studied for electrospinning process to stablish a method of synthesis to generate a biomaterial that could mimic the structure of an extracellular matrix for tissue engineering. Therefore, Chitosan based material are selected due to its biocompatibility, antimicrobial effect and biodegradability which makes it a good candidate for tissue engineering. We chose the electrospinning process due to the possibility to obtain a fibrous-like structure material with a high surface area and because it is a facile and easy method to get fibers under the nanoscale. Since Chitosan solutions are hard to electrospun because of its high viscosity and surface strength, a blend of Chitosan and Poly (Ethylene Oxide) were prepared in addition of Triton X-100 and Dimethyl sulfoxide to improve the electrospinning process and enable the fiber formation. Besides it was studied the incorporation of silver and gold nanoparticles into the polymeric matrix of the electrospun fibers to enhance the cellular proliferation and antimicrobial effect. The results indicated that it is possible to generate fibers without bead formation from Chitosan blend solutions with the nanoparticles inside the fiber structure but only when it is used a polymer concentration of 4 % w/v. We obtain fibers with diameters about 200 nm and the material generated was like a membrane with enough resistance to handled it and recovered easily from the aluminum foil collector. In this way, the purpose of this research was accomplish generating a biomaterial with a fibrous-like structure with properties that will be studied, applied and optimizing in a further researching.

Keywords: Chitosan, electrospinning, tissue engineering.

Transformation of CO_2 Into Value-Added Products in Reduced Graphene Oxide Supported TiO_2

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Abstract

The emission of pollutants is a problem to which we want to find a satisfactory solution. In the present case the research is focused on the elimination and / or reduction of CO_2 as a pollutant for the production of added value products such as methanol, ethanol, formic acid, formaldehyde and so on [1].

Titanium oxide is a n-type semiconductor with a high photoactivity absorbing in the UV region, so it is widely used as a photocatalyst. The performance of the catalyst depends of its physical properties such as pore size, specific surface area and active sites [2]. In this work, TiO_2 was prepared by the sol-gel method using two different precursors of titanium: titanium isopropoxide (A-serie) and titanium tetrabutoxide (B-serie). The supported sample were synthesized by the wet impregnation method: grapheme oxide onto titanium oxide (GO/TiO_2) at different percentages by weight and was evaluated in the CO_2 photocatalytic reduction reaction using water as a reducing agent. The synthesized materials were characterized by different techniques: DRX, nitrogen physisorption, UV-Vis spectroscopy in diffuse reflectance mode and Raman spectroscopy.

The X-ray diffraction patterns of the A-serie showed the presence of anatase phase of the TiO_2 used as a support, while in the B-serie, it was observed an anatase-brookite mixture. The results of the A-serie showed high yields towards ethanol, methanol and formic acid, while those in the B-series showed be selective towards the formation of ethanol. The graphene oxide supported onto TiO_2, increases the response of the TiO_2 towards the spectrum visible region and decrease its gap band, as well as retarding the recombination speed of the hollow -electron pair generated in the photonic activation of the semiconductor.

Keywords: Photocatalytic, TiO_2, graphene oxide.

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Based Quinoline Nano-Chemosensor for Detection of Metal Ions in Aqueous Medium

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Abstract

5,8-quinolinonebis(o-aminobenzimine) (QBI) were synthesized, then it converts into an Organic Nanoparticle (ONP) and applied for specific recognition of metal ions in an aqueous medium. The results show that fluorescence intensity decreases and increase with the increasing concentration of metal ion, in QBI solution metal ions (Ni^{2+}, Zn^{2+}, Hg^{2+}, Co^{2+}, Cu^{2+}, Al^{3+}, Fe^{2+}, and Pb^{2+}), proving that QBI-ONPs detect Cd^{2+} efficiently in the aqueous medium as chemo-sensor endorse that the metal ion that most increased was with Cd^{2+}. It appears that photo induced electron transfer (PET) occurs in the QBI-ONPs when the fluorophore is excited. For QBI/Cd^{2+} system, the PET is being inhibited considerably by lowering the receptor HOMO energy due to the formation of a bond between the metal ion and ligand, dismissing the fluorescence emission. This is consistent with the theoretical study that the energy of HOMO of the ligand is lower than that of $[Cd(QBI)]^{2+}$ complex.

Keywords: 8-hydroxyquinoline, Recognition of Cd^{2+}, Organic nanoparticles, heavy metals.

Surface Modification of Corncob Cellulose Nanocrystals by Acetylation

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Abstract

The corncob is the thresh residue of the corn from which the cellulose will be extracted. Cellulose is a molecular chain whose repeating unit is cellobiose, and is the most abundant polymer on earth that can be found in the cell walls of plant cells, is insoluble in water, has hydrophilic properties and has been used in many applications, the most representative is paper production. In order to obtain the cellulose, the corn pellet is crushed and sifted in a certain size of chips. Later, different samples are generated, which are then measured to measure the moisture content, to take into account the amount of water contained in the corncob. The percentage of ash is measured, to measure the amount of inorganic residues of the calcined organic material, then the extractives are measured in water and also in other solvents. Subsequently of all this happens to the chemical modification, which is the acetylation, which consists of covering the cellulose with the main reactants acetic anhydride and pyridine, where the acetic anhydride will participate in the acetylation and the pyridine will be the catalyst, the better temperature conditions and the time of the reaction process to obtain the highest degree of substitution. Subsequently, characterization tests of materials, including images in scanning electron microscopes, atomic force microscopy, X-ray diffraction and infrared spectroscopy with Fourier transform will be performed. Nanocrystals with chemical modification, are expected to be hydrophobic and then used as reinforcing material compatible with other materials.

Keywords: Agroforestry waste, cellulose, nanocrystals and acetylation.

Carbon Nanostructures Application for Oil Elimination Over Water Surface

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Abstract

The main purpose of this research is to find a solution to clean up crude oil when it enters in water. Were used low quantities to work in an environment with regular conditions of temperature and pressure. The results obtained from this research was removing crude oil from water used for testing and be able to reuse water without any risk. In order to make this happen was used to work a solution composed of CNT with alcohol and nanotori obtained by chemical treatment of MWCNT. Looking for a solution to be the most homogenized possible it was placed it on an ultrasonic machine. The CNT solution was tested by doping it in a mixture of crude oil and water, and nanotori solution was applied in the same way. Using an aluminum wire mesh solution was filtered through it making crude oil sticks to remain there and as an expected result water was without any contaminant. This processes was tested to clean fresh water and salt water. The results were confirmed comparing water during all the process with IR Spectrum to find out whether solution was getting back to original water or kept crude oil or CNT in its content. After getting water as a result of reaction it was monitored to make sure that this one will stay on the same way. The UV-Vis analysis is also presented.

Keywords: Oil Elimination, Carbon Nanotubes, Water Treatment.

Preparation, Structural Characterization and pH Stability of Sorghum Procyanidins/ Procyanidin B1-Gelatin Nanoparticles

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Abstract

Sorghum bran is an important source of procyanidins (PC), which have been recognized as antioxidants and anticancer agents. However, during passage through the gastrointestinal tract may undergo changes that alter the original structure, all of which limit their activity. A useful strategy to avoid such changes and facilitate their stable transport is encapsulating the PC in a biopolymer matrix, forming nanoparticles. For this instance the use of gelatin is contemplated as favorable because is a proline-rich protein, representing a natural crosslinking agent for PC, furthermore gelatin coating could increase the interaction of PC with metalloproteinases, which are endopeptidases related to the development of various pathologies, such as cancer and metastasis. The aim of this study was to characterize morphologically and structurally sorghum procyanidins (PCs) and procyanidin B1 (PB1) gelatin-based nanoparticles. Encapsulation was carried out by adding either dropwise PCs (0.5, 0.75 y 1, mg/mL) or PB1 (1 mg/mL) in an aqueous solution of A-type or B-type gelatins, with magnetic stirring. The results indicate no differences in nanoparticle size ($p> 0.05$) because of PCs concentration. PCs-gelatin nanoparticles showed an average size of 322.2 nm with A-type and 320.9 nm with B-type, and a zeta potential of +9.26 mV and -17.5 mV, respectively. Similarly PB1-gelatin nanoparticles had diameters of 321.5 nm with A-type and 338.2 nm with B-type, and a zeta potential of +3.97 mV and -14.3 mV, respectively. The nanoparticles were spherical with smooth surface as observed by electron microscopy SEM and TEM. The Fourier transform infrared spectroscopy (FTIR) suggests interactions due mainly to hydrogen bonds by changes in the region of 3000-3700 cm-1 and hydrophobic interactions. Antioxidant activity and SEM analysis revealed that the encapsulated PCs were not released during the gastrointestinal simulation against pepsins and pancreatin.

Keywords: Sorghum bran, Procyanidins, Gelatin.

Removal of Malachite Green from Aqueous Solution Using Maize Bagasse and Fe-Cu/Bagasse Composites

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Abstract

Water is a worldwide vital resource for sustaining life and due to the pollution of water by different classes of pollutants (inorganic, organic and pathogens) their quality has diminished. The application of nanomaterials for water treatment has gained impetus in recent years. Nanoadsorbents offer significant decontamination potential due to their unique characteristics. This study reports the synthesis of Fe -Cu nanoparticles loaded maize bagasse using reduction method and its use to remove malachite green dye. The properties of synthesized composite and maize bagasse were investigated by FTIR, XRD, SEM, EDS and N2 adsorption-desorption techniques and the presence of Fe-Cu nanoparticles was confirmed by TEM technique.

The adsorption properties of adsorbents for the removal of malachite green dye was examined using a batch method. The study of the sorption kinetics indicates that the adsorption on malachite green by Fe-Cu/bagasse and bagasse follows second-order model. The malachite green adsorption by Fe-Cu composite was faster than natural material and only showed two phases in the intraparticle diffusion model, probably due to the minor internal diffusion resistance. The adsorption isotherms experimental data were analyzed by the Langmuir, Freundlich and Langmuir–Freundlich models and the equilibrium data was well described by the Langmuir–Freundlich isotherm model. The adsorption was more favorable at basic pH. The OH-groups were proportional to dye adsorption capacities. Results showed that composite and bagasse possessed good adsorption abilities to malachite green.

Keywords: nanoparticles Fe-Cu, dyes, removal.

Treatment of Tequila Vinasse and Elimination of Phenol by Heterogeneous Photocatalysis Using TiO_2 NPs

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Abstract

In this work is presented the treatment of tequila vinasse and the elimination of phenol by heterogeneous photocatalysis (AOPs). In order to achieve these objectives were considered different factors: organic and inorganic coagulant, kind of NPs of TiO_2 (sintetized in the laboratory and buying by Aldrich), quantity of NPs, with and without H_2O_2, with and without black lamp with the effect of ultraviolet of 20 W/cm^2. In all this treatments was evaluated the ANOVA to determinate if the results were significantly different. It was found the elimination of phenol and the reduction of 70, 86.04 and 99.37% to organic chemical demand (DQO), color and total suspended solids respectively.

Keywords: tequila vinasse; heterogeneous photocatalysis; phenol; TiO_2 nanoparticles; sol-gel.

Green Synthesis of Bioflavonoid-Based Liposomes

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Abstract

In the present work, it was performed the nanoencapsulation of Quercetin and Capsaicin, which are substances present in different plants and foods such as chili, ginger and onion, which have properties to activate neurotransmitters in the nervous system. A novel green chemical method of liposome synthesis was carried out for the elaboration of a topical system to diminish the cellular stress. These liposomes are principal compound by Soy Lecithin, Shea butter and Aloe Vera. The results show an efficient and economic method that has a minimum polydispersion and suitable size of particle. The IR spectroscopy shows the presence of flavonoids. Simultaneously the topic delivery has shown biocompatibility on cells producing prolonged release.

Keywords: Liposomes, Green Chemistry, Flavonoid, Nanoencapsulation.

Synthesis of Silver Nanoparticles Using Hydro Alcoholic Propolis Extract

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Abstract

The development of silver nanoparticles using green methods, known as green synthesis, uses reducing agents and stabilizers to synthesize nanoparticles, which are friendly to the environment [1]. This method makes use of materials of natural origin, such as plant extracts and products made by some living beings such as honey bees, because these types of compounds have antioxidants, which can help in the reduction of nanoparticles. In this work we report a method of elaboration of nanoparticles, from the hydro alcoholic extract of propolis as a reducing agent [2]. Propolis is the resin produced by Apis mellifera honey bees, which collect from the buds of trees, to cover and desinfect the hive, has antioxidant, antibacterial, antiviral, and fungicidal properties, is chemically composed of phenols in the form of flavonoids and Amount of these depends on several factors, one of them is the plant species from where it was collected by the honey bees, plant health and season of the year [3,4] these properties are harvested by the bees within the hive. The obtained particles will be analyzed by the following characterization techniques: UV-vis spectroscopy; X-ray diffraction (DRX) and scanning electron microscopy (SEM). It is worth mentioning that the properties of silver nanoparticles are of interest for development in scientific research, because they have different properties in their characteristics that depending on their size, morphology and distribution, makes them have a good potential as agents antimicrobial [6] and highly effective in the presence of pathogenic microorganisms, since there are diseases caused by these, which over time have become more resistant to conventional biomedical treatments, developing resistance to drugs, and forcing to implement new technologies In microbial elimination products [7]. It is also proposed to elaborate a product of low cost and easy availability that, when potentializing the propolis antibacterial properties along with the antibacterial properties of the silver, must present a high and effective antimicrobial activity that will be evaluated with the use of antibiograms , In this way it will be possible to

provide information on the inhibition of microorganisms to avoid the bacterial resistance caused by the indiscriminate use of broad spectrum antibiotics, which have now promoted immunity and formation of new bacterial strains, becoming a serious problem for the world's population.

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Green Synthesis of Nanoparticles Through Honey (Apismellifera)

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Abstract

In recent years silver nanoparticles have become important because of the diversity of applications they have as drug-releasing agents, antimicrobial agents, catalysts as well as biomedical applications [1,2]. The synthesis of this type of structures is amused by the physical methods: evaporation-condensation and laser ablation, whose advantages are the absence of solvent contamination, uniform distribution of the nanoparticles, with the disadvantage of the difficulty in the size of the piece, as well as the high cost of equipment [3,4].

The chemical formulas control the size and shape of the piece, are usually more economic methods to perform the synthesis and sending the chemistry of homogeneity since the mixture is carried a molecular level; because the addition of more substances is unavoidable in most cases, the indispensable results are the need to purify the sample after synthesis [3] and in many cases substances like Dimethylsulfoxide (DMSO, C_2H_6OS) and N, N-dimethylformamide (DMF, C_3H_7NO) which may pose some health and environmental risks
[4,5,6,7].

Green Chemistry proposes the design of products or processes that reduce or eliminate the use or production of hazardous substances. [8] This current tries to prevent pollution by offering alternatives of synthesis with greater environmental compatibility, compared to the products or processes available in the which are more dangerous [9]. Bee honey Apis mellifera is a sweet natural compound with a wide variety of tones made from nectar of flowers and other extra floral secretions that bees liban, convert and store in the hive, its composition is related to the source of the nectar, soil and climate. has been shown to be an important reducing / stabilizing agent because of the carbohydrates it contains such as sucrose, fructose, glucose and maltose, the proportion of which depends on the place of

origin of the same. In addition enzymes, minerals and amino acids provide the encapsulation medium to avoid the agglomeration of metal nanoparticles [1,2,10] on the other hand has properties that have been shown to be anticancer because of the presence of antioxidants such as hydrogen peroxide, carotene, flavones and flavonoids [11,12,13], this makes honey a desirable option to be used as a precursor of silver synthesis with biomedical applications of low cost and green methodology avoiding the presence of solvents and hazardous or toxic waste.
The obtained particles will be analyzed by the following characterization techniques: UV-vis spectroscopy; X-ray diffraction (XRD) and scanning electron microscopy (SEM).

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Novel Treatment for Diabetic Foot Ulcers with Silver Nanoparticles

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Abstract

According to World Health Organization (WHO), the number of people with diabetes has risen from 108 million in 1980 to 422 million in 2014. One of the common consequences is the reduction of blood flow, which in combination with nerve damage in the feet increases the chance of diabetic foot ulcers (DFU), infection and eventual need for limb amputation (1). In addition, multi-drug resistant (MDR) microorganisms are a further complication for patients. This is why silver nanoparticles (AgNPs) that have shown excellent microbicidal activity against strains of MDR microorganisms (2) could be candidates for the treatment of DFU.

In this work, AgNPs fully characterized determining size distribution, morphology, hydrodynamic radius, zeta potential and plasmon resonance were present as a novel method to treat DFU. Three patients with DFU classified as Wagner ulcers II and III treated conventionally with an antibiotics schedule, and additionally AgNPs solution at 5% (1.8 mg/ml of metallic silver) was topically administered.

In the three cases lesion extent decrease was remarkable, as well as hyperkeratosis process and edema. Moreover, pigmentation confirms the imminent re-epithelialization process with active edges that favoring closure of the injury. After treatment, necrotic process was not observed and there was granulation tissue in the center of the ulcer

To the best of our knowledge, this work represents the first nanomedicine approach study performed in Baja California, Mexico in the world for the treatment of DFU of Wagner classification degrees II and III with silver nanoparticles (AgNPs) administered topically into the wound. Daily topical administration of AgNPs solution with metallic silver concentration of 1.8 mg/mL causes an improvement of the wound healing in average in less than 60 days of treatment. It is important to note that derived from this work, one technology reach the market and it is for sale as cosmetic product.

Keywords: Diabetic foot ulcers, silver nanoparticles, treatment

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Synthesis and Characterization of a Chitosan-Cholesterol Composite Projected to Tissue Engineering Applications

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Abstract

The Nanotechnology and Biomedical Engineering have been converted in crucial factors for tissue engineering, especially with the use of biocompatible materials, between them, biometals, bioceramics and biopolymers. This work presents the synthesis and characterization of a Cholesterol/Chitosan-g-GMA composite; the objective is to obtain a composite and to study its behavior as biomaterial. Inside this composite the function of Chitosan and Chitosan-GMA is to promote the tissue regeneration and avoid the bacterial growth, and de main function of cholesterol is providing the necessary conditions to growth quickly and orderly, due to the nature of cholesterol and its relation with epidermal tissue. The composite synthesis pathway is divided in three stages; the production of Cholesterol Succinate, the functionalization of Chitosan; the conjugation of both products. The cholesterol succinate was incorporated to hybrid Chitosan-GMA and raw chitosan, the composite was dispersed by vortex methods; after dispersion a film was obtained by casting and was used to subsequent for characterization by melting point, infrared spectroscopy, calorimetry and its application as a film in wounded tissue under controlled conditions is under evaluation. After the properties shown the film is proposed as a candidate which could allow accelerated epidermal regeneration and a film with chitosan used as reference.

Keywords. Chitosan functionalized, Cholesterol Succinate, tissue engineering.

Preparation and Characterization of Corncob Cellulose Nanocrystals

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Abstract

Corncob cellulose nanocrystals (CNC-corncob) were prepared by acid hydrolysis. In order to get the CNC, corncob was milled and screened and particles between 40 and 60 mesh were used. Chemical characterization was carried out according to TAPPI standards (Technical Association of the Pulp and Paper Industry) for lignocellulosic materials. Cellulose was isolated from corncob by several steps. First, delignification was made by pulping process with 50% ethanol solution (ratio 1:10) and 3% acetic acid at 175°C and 2.5 h. Corncob pulp was washed and air dried. Second, Pulp was bleached by WISE method using sodium chlorite and acetic acid at 70-80°C and 4 h. Holocellulose was washed and air dried. Third, 24% KOH solution was used to extract hemicelluloses and finally 17.5 % NaOH:4% H_3BO_3 solution was used to purified corncob cellulose, yield 40 to 45% dry basis. In order to prepare nanocrystals 64% sulfuric acid solution was used to hydrolyze cellulose. The CNC´s were characterized by analytical and spectroscopic techniques: infrared spectroscopy (FTIR), X-ray diffraction (XRD) and scanning electron microscopy (SEM). The importance of the characterization was to establish a correlation between the structure, shape and chemical composition of the CNC. The research indicates that the corncob could be an excellent raw material for the manufacture of CNC at low cost and respecting the environment.

Keywords: corncob, nanocrystals of cellulose (CNC) and characterization.

Nanoencapsulation of Lauric Acid with Chitosan for the Control Acne

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Abstract

In last decades, the implementation of new pharmaceutical forms of loaded and released drugs, have had great interest in representing a promising platform for the optimization of medical treatments. They are complex compound that provide better properties, such as stability, high ability to associate and reduction of adverse effects, improving the speed and place of drug release. This work presents he preparation of chitosan particles to nanoscale for loading and released drugs which were synthesized by ionic gelation method; using in chitosan particles crosslinked with sodium tripolyphosphate and lauric acid. The objective of this novel material is that chitosan nanostructured encapsulated lauric acid and apply this composite as an alternative to the treatment of acne vulgaris, with an expected efficiency upper 70 %, reducing significant the colonization of the propionabacterium acnes in 80 % in vitro system.

The synthesis of this Composite for release the active substance consist; of release consist; firts, in the formation of the chitosan nanoparticles and after nanoparticles loaded formed spontaneously in the incorporation of lauric acid in aqueous solution of chitosan (obtaining a stable solution) to subsequent for characterization by dynamic light scattering, infrared spectroscopy; Obtaining two populations in the particle size, the first with an average of 69 nm and the second 350 nm (formed by a particle agglomeration). With this solution was obtained a film which will be neutralized applied in vitro in an inoculum of P. acne, where the percentage of bacterial control is shown. This chitosan-lauric acid system will reduce the appearance of acne vulgaris as well as the reduction of scars caused by acne.

Keywords: Chitosan nanoparticles, Lauric acid, Acne vulgaris.

NANO TECH
Puerto Vallarta 2017

Transfer to Aqueous Medium of Rare Earth Magnetic Nanoparticles

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Abstract

At present, the use of nanotechnology for biomedical applications has had an important development, specifically the use of magnetite at nanoscale, where the main challenge is to obtain particles with high crystallinity and low polydispersity in aqueous medium for biomedical applications. Aim: Optimize the transfer of rare earth co-doped magnetic nanoparticles to aqueous media through ligand exchange. Methods and materials: We studied the synthesis of rare earth co-doped magnetic nanoparticles. The synthesis was performed by thermal decomposition. Subsequently, the size of the MNPs synthesized using TEM, as well as their crystallinity using their XRD spectrum, and their magnetic properties were determined with a vibrating sample magnetometer. Finally the nanoparticles were transferred to aqueous medium through the binder exchange reaction using thioglycolic acid. Results: Results showed that the maximum particle size obtained was 8 nm with superparamagnetic characteristics. Conclusions: The transfer to aqueous medium was suitably carried out, because the nanoparticles showed a high colloidal stability.

Keywords: Magnetic nanoparticles, functionalization, biomedical applications.

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Production of Silver Nanoparticles by a Filamentous Fungus

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Abstract

The potential applications of silver nanoparticles (AgNPs) has increased their demand in the market. The AgNPs synthesis can be done by physicochemical or biological methods and depending of the method and conditions, AgNPs present different characteristics. Biological synthesis of AgNPs include the use of plants, bacteria, yeast and fungi. The AgNPs biosynthesized present interesting characteristics, such as stability and solubility in aqueous solutions; moreover, AgNPs of fungi can be produced extracellularly. The aim of this study was to evaluate the effect of extracellular filtrate of fungus Penicillum sp grown in two different culture media and silver nitrate concentrations on AgNP production. Penicillum sp was grown in both Sucrose and Czapeck media then, biomass was used to obtain extracellular filtrates when it was exposure to water. Two extracellular filtrates were obtained, $AgNO_3$ at 1, 1.5 and 2 mM were evaluated to produce AgNPs. The AgNPs produced were monitored by UV-vis (200 to 800 nm), morphology was observed by TEM and size was determined by SPIP 6.0.2. Results showed that both extracellular filtrates have the capacity to produce AgNPs at all $AgNO_3$ concentrations. Microscopic analysis showed the formation of spherical AgNPs for all systems. The AgNPs synthesized using the extracellular filtrate coming from sucrose media at all $AgNO_3$ concentrations showed sizes within 2-12 nm at higher extent. When extracellular filtrate came from Czapeck media, AgNPs size were in the range of 2-12 nm, 12-22 nm and >22 nm. In summary, both extracellular filtrates had the capability to produce AgNPs at different extent, AgNO3 concentrations had effect on AgNPs size.

Keywords: AgNPs, biosynthesis, filamentous fungus.

Evaluación de la Citotoxicidad de la Doxorrubicina Sobre Andamios Poliméricos con FeNPs Utilizando Ondas de Choque Como Técnica de Transfección para el Tratamiento de Cáncer Hepático Metastásico

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Abstract

We present in this work the preliminary study by Raman spectra of the creation of a treatment alternative for metastatic liver cancer for future direct application in the lesion using a simple, easy to handle, biocompatible and biodegradable polymer matrix, in which embedded nanoparticles that provide radiopacity and an anthracyclic drug to provide localized cytotoxicity, coupled with the use of shock waves for the transfection of the drug into the tumor cell.

The matrix of the nanocomposite material is a hydrogel type polymer with degradation by thermal activation. The nanoparticles used in the work have specific characteristics such as radiopacity, biocompatibility and easy removal of these by the body through phagocytosis, also considering a low toxicity. Synthesized by the chemical coprecipitation method. The drug is well known for use as a chemotherapeutic agent in the treatment of malignant tumors, because it damages the genetic material of cancer cells as well as having antiproliferative properties.

The low frequency penetration power of the shock waves facilitates its application in internal tumors, so they were used to accelerate transfection to the tumor lesion without adding appreciable damage to the healthy tissue of the recipient organism. However, due to the modification in the molecular structure of doxorubicin caused by the use of shock waves we evaluated by Raman spectroscopy the nanocomposite material to establish a range of application where it is ensured that there is no change in functional groups which affects cytotoxicity.

Keywords: Liver Cancer - Nanocomposite Material - Shockwaves.

POSTER SESSION
WEDNESDAY

Computational Simulation of Molecular Interactions of Procyanidin B1 with Matrix Metalloproteinases -1, -2, and -7

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Abstract

Matrix metalloproteinases (MMPs) are a family of enzymes, capable of degrading the components of the extracellular matrix and are related to certain pathological processes, including cancer. For this reason, the MMPs are considered potential therapeutic agents against different types and stages of cancer, and have led to the development of synthetic inhibitors and the exploration of dietary bioactive compounds, which can act as specific inhibitors of MMPs. Among these compounds, are the procyanidins, that have been reported as efective inhibitors of certain MMPs. However, the specificity and molecular nature of the interactions between procyanidins and MMPs has not been described in detail. For studies in this regard the use of model systems at nanometric level and the use of methods of simulation and molecular modelling are relevant. The procyanidin B1 (PB1) dimer is an excelent model system because of their abundance in fruits and cereals, has the basic structure of the procyanidins and reaches dimensions of 1.2 y 1.22 nm of width and length, respectively. The goal of this study was to carry out a molecular docking study between PB1 in its compact conformation (more stable) and the catalytic domains of MMP-1, -2 and -7, obtained from the Protein Data Bank, employing the software AutoDock4. The results indicate that the interactions between PB1 and these MMPs ocurred in some exosites from the catalitic domain, as well as, subsites of the catalytic cleft of the enzymes. The bonding energies varied within a range of -6.46 to -4.89 kcal/mol and the complexes formed by the interactions were stabilized mostly for Hydrogen bonds established between the hydroxyl groups of PB1C and some polar aminoacid residues corresponding to each MMP.

Keyword: Matrix metalloproteinase, Molecular docking, Procyanidin B1.

Fabrication of Hollow TiO_2 Nanotubes Through Atomic Layer Deposition for Photocatalytic Applications

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Abstract

Carbon nanotubes (CNT) coated with TiO_2 have drawn attention for photocatalytic applications because this type of nanostructures can use the advantages that both components provide. Specifically, CNTs exhibit high surface to volume ratio, metal-like conductivity and have a large electron-storage capacity, which in combination with a semiconductor material (i.e. Titania), may accept photo-exited electrons and thus retarding the electron-hole pairs recombination. As for the Titania, it is one of the most investigated photocatalytic material mainly because of its strong oxidizing abilities for the decomposition of organic pollutants, but also because it is non-toxic, environmentally friendly, and chemically stable. The purpose of the present work is to combine the characteristics of CNT with TiO_2 to engineer enhanced materials for photocatalytic applications. Here we present a transmission electron microscopy (TEM) characterization together with a detailed high resolution elemental analysis by in-column energy dispersive X-ray spectroscopy (EDXS). XRD, TGA and XPS were also employed for the characterization of the resulting nanostructures. Finally, The CNT-TiO_2 were evaluated as photocatalytic material in the degradation of the alimentary azo dye amaranth.

We gratefully acknowledge financial support from the UNAM México funding through DGAPA IA103117, IT100314, PE101517 projects.

The authors would like to thank F. Ruiz, J. Diaz, I. Gradilla, E. Murillo. P. Piza and E. Aparicio for technical assistance.

Keywords: Carbon nanotubes, Photocatalytic applications, TiO_2.

Nanoparticles Photoluminiscent Synthesis to Obtain Concrete Additives

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Abstract

Nowadays, the construction industry has begun to implement the use of additives for concrete but most of this materials are common like the polymers one, it’s meaning that there is a high demand in the development of additives with new materials.

The Nanotechnology is an excellent option to obtain new materials, due to it has changed our vision, expectations, and abilities to control the materials world. The developments in nanoscience can also have a great impact on the field of construction materials.

The use of nanoparticles photoluminiscent improve the physical appearance of the concrete by using zinc oxide doped with cerium to get that the concrete produce an orange color.

The goal of this research is to obtain nanoparticles photoluminiscent by using the ultrasonic dot method to generate a new additive throw the use of nanotechnology. The results has been analyzed by UV-BIS, X ray diffraction (XRD) and Sweep Electronica Microscopy (SEM) techniques.

Keywords: nanoparticles photoluminiscent, ultrasonic dot method and concrete.

Oxidation Process of Tungsten Oxide Thin Films

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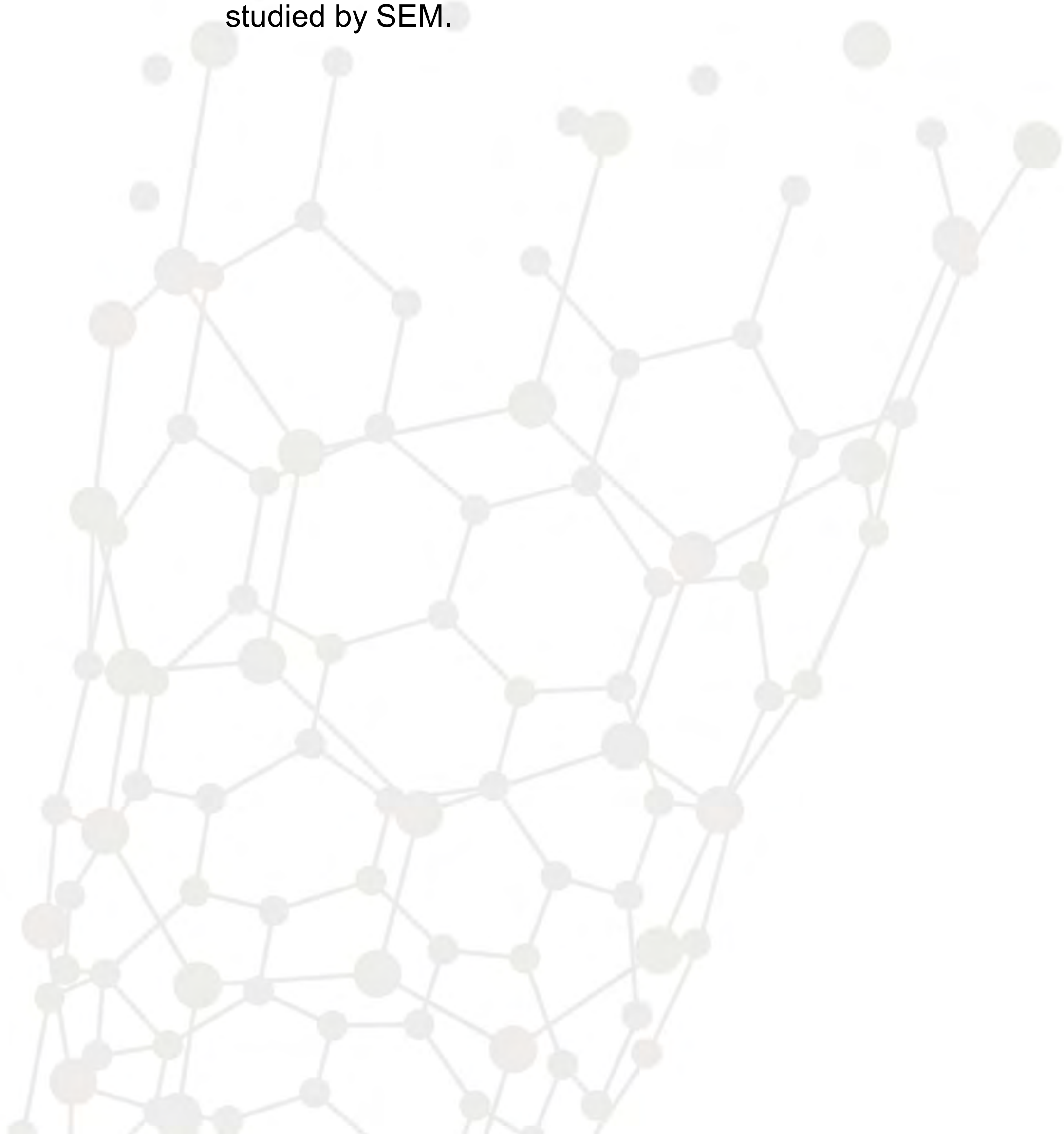
Abstract

Thin films were grown up over substrates of Si. We studied the change of the crystallography according to the temperature with XRD, the morphology was studied by SEM.



Incorporation of Additive Photoluminicent for Concrete

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Abstract

The photoluminiscent applied in construction of buildings has been an innovation in the world, the use of nanotechnology in this type of industry have beneficial properties, for example, decreases the use electrical energy for street lighting. Also its can be a decorative material by different color.

The different color are obtained by addition of several elements as well as europium or cerium, this materials are able to produce different game of colors.

In this study has been used nanoparticles of zinc oxide doped with europium to obtained blue nanoparticles photoluminiscent thrown co-precipitation method for zinc oxide and ultrasonic cube for europium doped.

All products obtained has been analyzed by UV-BIS, X ray diffraction (XRD) and Sweep Electronica Microscopy (SEM) techniques.

Keywoords: Concrete, Photoluminescence, Energy saving

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Synthesis and Characterization of Nanoparticles of Dioxide of Silica Applied in Cement

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Abstract

The work of investigation focuses in the analysis of the morphology of nanoparticles of dioxide of silica (SiO_2) with spherical geometry, synthesized by the process Sun - gel in a basic way. The above mentioned particles will be added to the cement to achieve a major hardness and resistance in the above mentioned material and to contribute (pay) to the industry of the construction. The investigation (research) shows the series of tests (essays) that have been done to the cement: analysis of resistance to flexotracción and compression, analysis of indexes of superficial ruggedness.

Keywords: Nanoparticles of dioxide of silica, compression, cement, method Sun - gel, spherical morphology.

Cu-Ag Nanoalloys Using Green Synthesis

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Abstract

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

Analyzing the Nitrogen Sites Activity from Doped Carbon Nanotubes for the Hydrogen Peroxide Generation (ORR)

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Abstract

Carbon nanotubes has generated commercial interest due to its electrical, mechanical, and thermal properties [1]. Recently, nitrogen doped carbon nanotubes (CN_x) has gained attention due to the change in catalytic activity of carbon near to the nitrogen sites and its ability to promote the Oxygen Reduction Reaction (ORR) [2]. Therefore, the doping of Carbon nanotubes gives them interesting activities as functional materials for fuel cell applications, photovoltaics, hydrogen production, and wastewater treatments due to its catalytic properties [3-4].

In this work the synthesis temperature of nitrogen doped carbon nanotubes was changed to try to modify the proportion among different nitrogen species (pyridinic, graphitic, pyrrolic, and molecular nitrogen) and the obtained samples were analyzed in detail by XPS to elucidate the proportion of such nitrogen species among the obtained samples. The nitrogen species proportion is correlated to the samples activity for the 2-electron process of the ORR. An electrochemical study is presented to show the ability of the nitrogen sites activity to promote the generation hydrogen peroxide by the ORR.

Once explored the nitrogen sites activity from the different CN_x, they were hydrothermally dispersed, decorated with iron oxide nanoparticles and assembled into a buckypaper, looking forward for a functional material which could enhance the electrochemical promotion of the Fenton reaction, a key reaction for wastewater treatment.

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Stabilized-Palladium Nanoparticles from Organometallic Precursors: Electrocatalysts for Methanol Electro-Oxidation

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Abstract

Stabilized Pd nanoparticles were synthesized from the organometallic precursor bis(dibenzylideneacetone) palladium(0), Pd(dba)2 under dihydrogen pressure and organic media in the presence of HDA as stabilizer. Well-defined stabilized Pd nanoparticles (<10 nm) were determined using transmission electron microscopy (TEM) and X-ray diffraction. The as-prepared materials were mixed in-situ with a carbon Vulcan matrix (10% wt. of the catalyst in turn) and used as electrocatalyst for the methanol oxidation in alkaline conditions. The i-E profiles obtained by cyclic voltammetry technique indicated redox process attributed to palladium, as expected. It was found that methanol oxidation-current performance is linked with the stabilizer, alcohol concentration and scan rate.

Keywords: Pd nanoparticles, methanol electro-oxidation

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Photocatalytic Performance of ZnO Hierarchical Nanostructures Decorated with Gold Nanoparticles: Effect of the Impregnation Method and Light Source

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Abstract

Because its physical and chemical properties, ZnO is a potential material in different technological fields. As a photocatalytic compound, it is considered an effective, inexpensive and non-toxic material for wastewater treatment. Here we report on the synthesis of hierarchical ZnO nanostructures decorated with gold nanoparticles (Au-NPs) using three different impregnation methods. The microstructure of the samples was fully characterized and their photocatalytic activity was evaluated in the degradation of Rhodamine B (RhB) pollutant. It is shown that the ZnO phase is constituted by aggregates of round-shaped nanoparticles, generating hierarchical structures. In any case, Au-NPs are uniformly distributed on the semiconductor support, however is the direct-Turkevich method which allows the highest metal loading. A strong visible-band (515 - 535 nm) dominates the absorption spectra of the nanocomposites. As expected, formation of Schottky barriers (Au/ZnO) leads to an increase of RhB degradation efficiency under UV-light (>90%). Nevertheless, contrarily to most reports, no photocatalytic activity associated with plasmon excitations was observed using pure visible-light, no matter the light-source has an intense green component. Therefore, it is proposed that meanwhile the emission spectrum of the light source is not shown, the photocatalytic activity of Au-NPs/ZnO composites under white-light can be attributed to a non-filtered UV component.

Keywords: ZnO, hierarchical nanostructures, photocatalysis.

Scanning Electron Microscopy Analysis at Low Voltage in Doped-Carbon Nanostructures

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Abstract

Carbon nanostructures have been developed as supporting material of active metals, and recently as doped carbonaceous materials using heteroatoms creating metal-free electrocatalysts for fuel cells, batteries and sensors. However, some features remaining as unknown need to be assessed regarding their effects in the electrochemical devices. On the other hand, recent development of new detectors for electron microscopes have allowed to better characterize the properties of new nanostructures, especially of graphene and doped carbon nanotubes. In this work, the high resolution scanning electron microscopy (HRSEM) study on carbon nanostructures doped with Si, S and N (CND-H) is investigated and correlated with other characterization techniques. The CND-H were synthesized using a modified chemical vapor deposition method using ferrocene, toluene and different organic reactants to dope them with sulfur, nitrogen and silicon, respectively. Pristine carbon nanotubes were also synthesized for comparison. CND-H were evaluated by high resolution scanning electron microscopy using not only the conventional secondary and backscattering electrons detectors but also a new electron energy loss spectroscopy (EELS) detector. Chemical microanalysis is performed using an X-ray energy dispersive spectroscopy (EDS) annular detector permitting to achieve high X-ray counts rates even at low primary energy. Transmission electron microscopy and X-ray photoelectron spectroscopy (XPS) were also used to correlate the results with HRSEM. Electron microscopy results show that morphologies were influenced by the dopants. CND-H with sulfur show a horn-like nanostructure with two different types of layers, the outer layer being more amorphous than the inner one. Meanwhile, CND-H with nitrogen show the typical bamboo-like structure. However, micrographs of CN-Ds with silicon show the same morphology that the pristine carbon nanotube. EDS elemental mapping results show the presence of the doping elements along the nanostructures which is in agreement with the chemical states detected by XPS.

Keywords: Nanohorns, carbon nanotubes, EELS.

Rhodium Nanostructures from an Organometallic Approach

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Abstract

The synthesis of Rh nanostructures has been investigated through different precursors under mild conditions. In addition, the influence of reaction parameters such as solvent polarity or stabilizer nature on size and shape of Rh nanoparticles was investigated. Various shaped assemblies of Rh nanoparticles were obtained depending on the chemical species formed in the reaction media. Transmission electron microscopy, X-ray diffraction and infrared spectroscopy were carried out as characterization techniques. Finally, this work shed light on how to control the formation of nanoparticle aggregates by modulating the nature of Rh precursor.

Keywords: Rh nanoparticles, organometallic precursor.

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DFT Study of the Interaction of Cisplatin Molecules with the Au_{18} $(SR)_{14}$ Cluster

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Abstract

Cisplatin molecule has an amply history about its use as a Cancer drug, and it is well known that cisplatin is able to help in the treatment of testicular Cancer with a 90% of success. [1] However, the presence of secundary effects is also known, being this an overcome to be solved in the meantime. It seems that the indiscriminated attack to ill and healthy cells can be reduced by improving the cisplatin delivery into the correct organ or tissue. We studied the interaction among one $Au_{18}(SR)_{14}$ cluster and cisplatin molecule(s) and our results indicate that it represents an option for cisplatin delivery given its bio--compatibility and their calculated adsorption energy. Our calculations based on DFT,[2] attests that $Au_{18}(SR)_{14}$ cluster is able to adsorb an important number of cisplatin units. Further analysis demonstrate that the interaction is strong enougth to avoid cisplatin loss during its transit toward the specific organ or tissue. However, cisplatin might be desorbed after approaching them. Moreover, our study involves the study of electronic and optical and chiroptical properties which provide us with fingerprints to characterize the proposed cisplatin/$Au_{18}(SR)_{14}$ system.

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Graphene Doped with Titanium Dioxide for the Improvement of Photoelectric Cells

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Abstract

The present work was carried out with the objective of realizing a photoelectric cell to take advantage of the heat energy transforming it to electrical energy, using the following materials graphene and TiO_2. Using the methods to obtain the precursor material to be used are, Graphene Synthesis from the modified method of Hummers (Y. Hao, M.S. Bharathi). The TiO_2 was used already elaborated from the supplier, for its doping of the graphene / TiO_2 was by semiquechimic means.

On the planet we find energies that we do not use to use for our daily needs. Electrical, solar, geothermal, thermoelectric, etc. (CIDETEQ 2010) We are not yet campás to have suitable knowledge for an apparatus to take advantage of these energies. As a clear example, the heat energy, which can be found in the sun, apparatus and humans, are capable of emanating this energy, different phenomena.

Wang D. et al. It attempts to modify the chemical properties of graphene by introducing titanium oxide crystals into the reticular structure of graphene in the hope of improving the voltage. Retention of material capacity under high stress conditions and discharge rates. His study tests rutile and anatase composed of TiO2-graphene products as cathode in electrochemical cells. These cells are compared with cells using the metal oxide as cathodic material.

Keywords: graphene hummer method, chemical exfoliation.

Synthesis of Graphene by Laser Ablation in Liquid

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Abstract

In this work we show the synthesis of graphene by laser ablation using a target graphite inside liquid nitrogen the laser used is Nd:YAG. The synthesis process is a single step does not need a high vacuum, chemical reagents or additional devices, this process can be controlled by changing the conditions of the laser, time and focus, the collection of the product obtained is easy. From the Raman analysis obtained, 3 bands are clearly visible in the 1000-3000 cm^{-1} range, corresponding to bands D, G and 2D. The band D located at 1328 cm^{-1} is associated with the defects in the graphene films, the band G located at 1577 cm^{-1} is designated to the C-C sp2 bond in the vibrations of the phonon in the plane: finally, the band 2D in 2658 cm^{-1} is the most characteristic of the graphene spectrum. The spectrum for bilayer graphene in the 2D band shows a wide and symmetrical peak, which was adjusted to four Lorentzian functions obtaining a FWHM of 58 cm^{-1}. Compared with monolayer graphene, the region of the 2D band for two-layer graphene is generally wider (50 cm^{-1}) and asymmetric with an I2D / IG of approximately 1.6, which is in line with that reported in the literature.

Keywords: Graphene, laser ablation, liquid nitrogen.

Visible-Light Driven Degradation of Ibuprofen Using Cu/CuO Nanocomposites Synthetized by Two-Step Approach

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Abstract

Semiconductor nanomaterials have attracted much attention in recent years because of their outstanding physical and chemical properties. The CuO is a p-type semiconducting material, exhibiting narrow band gaps (Eg=1.2 eV), has received considerable attention due to its wide applications in many important fields such as gas sensors, electrochemical, superconductors and photocatalysts.

In this work photodegradation of the non-steroidal anti-inflammatory drug ibuprofen (IBP) was carried out, for the photocatalysis test was used a solution of 200 ml of IBP diluted in distilled water in a concentration range of 20-50 mg L-1. The solution was irradiated with a white light UVP-XX-15S (8 Watts) lamp, stirred under constant air flow. To monitor the degradation process, aliquots were taken at certain time intervals to be measured in a Varian Cary 100 UV-Vis spectrophotometer. The composite material was fabricated by the two steps approach; the support copper oxide (CuO) was synthetized by the precipitation method, using copper acetate [$Cu(CH_3OO)_2$] as precursor of the metal, and sodium hydroxide (NaOH) as reducing agent. The CuO was decorated with copper nanoparticles; the CuO previously synthesized is added to an aqueous solution of copper chloride dihydrate ($CuCl_2$•$2H_2O$) and subsequently l-ascorbic acid ($C_6H_8O_6$) is added to form Cu nanoparticles in CuO surface.

The composite material was characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and diffuse reflectance spectroscopy to identify the crystalline phase, morphology, and determinate the band gap value.

Keywords: photodegradation, ibuprofen (IBP), Cu/CuO nanocomposite.

Raman Study of Eu^{3+}-W Codoped Nanosized TiO_2 and UV Light Induced Degradation of an Azo Dye, Quantum Size Effects on Relationships Betwwen Structure-Activity

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Abstract

Nanostructured photocatalysts have attracted growing interest because of their unique structures and properties. To obtain highly active TiO_2 particles are desired to provide a large specific surface area and enhanced catalytic activity due to quantum confinement effects in the semiconductor space charge [1]. By reducing the size of the synthesized nanoscaled anatase-brookite mixed-phase down to the nanometer order causes high efficiency in the effective parameters of photocatalytic activity of nanomaterials. The photoexcitation leads to the formation of electron–hole pair in TiO_2 and has received attention because of its excellent chemical stability, photoactivity, as it is easily available, stable to photocorrosion, cheap and present nontoxicity; controlling the incipient stages of crystal growth, is of vital importance because it is an important challenge in modern advanced catalytic oxidation process [2]. In order to enhance the catalytic activity, modification of TiO_2 by rare-earth element Eu^{3+} experienced significant changes during the recent years. Basically, the cationic doping of TiO_2 is performed by trivalent cations of suitable sizes can occupy Ti4+, modifications to the electronic structure of TiO_2 to shift the absorption into the visible range are under intense study in the photocatalysis field. In this work, we have prepared nanostructured Eu^{3+}-W codoped TiO_2 anatase-brookite mixed-phase. The present study is focused on the understanding of enhanced reactive property of Eu^{3+}-W codoped TiO_2 surfaces and relationships between structure-activity. Nanostructured photocatalysts have attracted growing interest because of their unique structures and properties. To obtain highly active TiO_2 particles are desired to provide a large specific surface areas and enhanced catalytic activity due to quantum confinement effects in the semiconductor space charge. Photocatalysis process has received much attention due to its potential applications in the fields of energy and environment. By reducing the size of the synthesized nanoscaled anatase-brookite mixed-phase down to the nanometer order causes high efficiency in the effective parameters of photocatalytic activity of nanomaterials [2,3].

High Methane Density Storage in Composite Materials

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Abstract

Use of the standard energy matrix, based in hydrocarbons, its direct related with an intensive damage to the environment in the extraction zone as in the final use destination. Other main limitation is related with the fact that the fossil fuels reserves are limited and its use is increasing in time, making harder (more expensive) its use. For that reason, one of the most important priorities today's, is the use of sustainable alternatives fuels that minimize the impact of its use in the environment and in its production cycle. Till now, attention has been focus to Hydrogen; but also its production as its storage for mobiles applications, are far away of the practical need. Natural gas has been used as alternative option, due to its availability and its low contaminant factor, this facts make it as a natural choice as a substitute of oil in cars and in other mobiles application. However, the lack of efficient storage methods has limited its use in the automotive industry.

The use of novel porous materials, as metal organic frameworks and carbonaceous structures, has been explored as matrix for methane storage (main constituent in natural gas), due to the exceptional high surface areas and its tunable chemical structures. Present work makes use of structural characteristics of both frameworks, for that reason a composite of these two structures was obtained. The structural versatility of these kind of compounds, bring us the possibility of control the chemical properties, like its pore geometry and dimensions and its channels structure, making it an alternative to explore the adsorption interaction of methane in porous materials.

Keywords: Methane, MOFs, carbonaceous structures and composites.

Structural and Optical Properties of PbS Nanocrystalline Thin Films Deposited by Microwave Technique

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Abstract

PbS thin films were obtained by microwave assisted chemical bath deposition on corning glass. Their structural and optical properties were studied by X-ray diffraction (XRD), scanning electron microscopy - energy dispersive X-ray spectroscopy (SEM-EDS) and transmittance and reflectance measurements in the wave length range 250–2500 nm. X-ray diffraction measurement revealed that all thin films have cubic rock salt (NaCl) type structure with crystal size up to 20 nm. The surface morphology was analyzed by atomic-force microscopy (AFM) showing that the films have uniform surface morphology and good quality over the entire sample. Optical measurements show that thin films have relatively high absorption coefficients between 104 and 105 cm^{-1} in the visible range. Additionally, the nanocrystalline films exhibit direct gap from 1.0 to 1.8 eV as particle size decreases.

Keywords: nanocrystalline thin films, PbS, microwave deposition.

A new 3D Framework Supported in Sipolar and Cuadrupolar Interactions. Intercalation of Thiazole in Layered Solids

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Abstract

Materials made from the assembling of inorganic and organic building units have receiving large attention in the last decades, mainly by the high diversity of construction blocks available and, in consequence, by the combination of them, which result in practically infinite number of 1D, 2D and 3D structures. Such hybrid porous solids have attractive properties for gas adsorption and separation, as molecular magnets and show many others functionalities. The tetracyanonickelate ion, $[Ni(CN)_4]^{2-}$, form 2D solids of formula unit $T(H_2O)_2[Ni(CN)_4]\cdot{}_xH_2O$ when react with divalent transition metals (T). These kind of inorganic layers have shown conformational flexibility which responds to steric and electronic requirements from the molecules bonded to the T metal. In this sense, tetracyanonickelate layers behave differently to the common inorganic layers, which maintain a rigid lamellar configuration. Neighboring layers remains together through a network of hydrogen bonding interactions between the water molecules coordinated to the axial positions for the metal T with the weakly bonded ones located in the interlayer region. These water molecules, both coordinated and weakly bonded, can be removed to intercalate organic molecules in the interlayers region. By these means it is possible to functionalize a whole gallery with specific organic functions. In this way, thiazole molecule is intercalated in layers of $T[Ni(CN)4_]$ (T = Mn, Fe, Co, Ni) in order to study the interaction between neighboring molecules and to characterize the 3D structure and related physical properties of the formed solids.

The intercalated molecules occupy the axial coordination positions for the metal T, which results with a distorted octahedral coordination. The Ni atom preserves its planar coordination to four C end of CN groups. In the interlayers region molecules coordinated to neighboring layers are found interacting between them through their dipolar and quadrupolar moments. In addition to the structural study, the distortion for the octahedral coordination environment for the metal T, is also detected as spin-orbit coupling, with a pronounced temperature dependence for Fe and Co. The pronounced decrease observed for the effective magnetic moment below 25K, reveals the contribution of zero field splitting to the magnetic properties of this series of hybrids materials. At low temperature dominates the antiferromagnetic interaction between T metal centers within the layers, and only for T = Ni, a weak

ferromagnetic effect was observed at 2K. This study shed light on the intermolecular interactions of thiazole molecules intercalated in 2D solids and contributes to understand the nature and properties of this type of hybrid inorganicorganic materials.

Keywords: X ray diffraction, crystal structure solutions, tetracyanonickelates, pillared solids.

Effect of Laser Repetition Rate in the Synthesis of Silver Nanoparticles in Distilled Water

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Abstract

Since 1993 year was used the laser ablation as a alternative method of metallic nanoparticles synthesis, which consist in the interaction of a high power laser on a target immersed in a liquid medium , being plasma the material generated from the target, that is confined by the medium high density. In this condition, electronic recombination occurs by rapid cooling causing the ions change to a neutral state favoring the formation of nanoparticles [1].

Laser parameters in combination with optical properties of the target, play a key role in the size and nanoparticles production. In this work is explored the effect of pulsed repetition rate in the synthesis of silver nanoparticles by laser ablation. For this purpose, the Nd:YAG laser at 1064 nm, with an energy of 0.1 J/pulse, a pulse duration of 7 ns and a repetition rate of 8, 9 and 10 Hz was employed on a silver coin immersed in distilled water. The obtained nanoparticles suspensions were characterized by UV-Vis absorbance and transmission electron microscopy. Resulting, the peak absorption, in UV-Vis measurements of each sample, increases as the repetition rate. According to the Beer-Lambert relation, we can conclude that nanoparticles yield increases with the repetition rate.

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Growth and Characterization of Tantalum Nitride Superconducting Thin Films

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Abstract

Since their discovery at 1911 by Kamerlingh Onnes, the superconductivity has been a promising property of specific materials that is important for scientist and engineers. Particularly, the superconducting materials have applications in lossless energy power supply, transport levitation and development of nanometric electronic devices. In this last, efficient fabrication of materials with a low superconductive energy gap and an intermediate transition temperature (Tc), results essential for the development and enhance of superconductive electronic devices in the GHz range. TaN thin films have previously showed superconductive transition temperatures up to 10.4 K with a superconductive energy gap lower than NbN, the most commonly used material for single photon detectors in the GHz range. The Tc of tantalum nitride depends strongly of the crystallinity and stoichiometry of the thin films. In the present work, the superconductive thin films of tantalum nitride grown by using laser ablation technique with a Nd-YAG laser on a Ta target (99.999%) varying the N2 (99.999%) partial pressure in the chamber as well as substrate temperature were obtained. X-Ray Diffraction Spectroscopy (Panalitycal X'pert Pro MRD system) and X-Ray Photoelectron Spectroscopy (XPS), with a X-ray monochromatic source and semispherical analyzer, from SPECS were obtained in order to study the crystallography and stoichiometry respectively. The R vs T curve of the films were obtained by using van der Pauw method. Finally, we report an ab initio study of a unit cells, fcc and hexagonal, of tantalum nitride using Quantum ESPRESSO software. We calculated the states density with the purpose of correlating with our experimental results obtained from XPS close to the Fermi energy.

Self-Assembly of Three-Dimensional In-Situ OGr Architectures Using a One-Step Hydrothermal Process

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Abstract

At present, there is a great deal of interest in the research and development of graphene-based carbon materials because of their properties attractive, making possible their use in multiple applications. This enormous potential of graphene only for the use and development of methodologies that allow its preparation and processing in large quantities, to give rise to useful macroscopic structures and controllable characteristics. Based on what is already known by other nano-structured materials (nanoparticles, nanotubes, etc.), the preparation and processing in liquid medium of graphene seems the optimal method to reach the objectives. To date, the technique in which the most are deposited is based on the exfoliation of graphite oxide and graphene oxide and its subsequent reduction, although alternative paths are also investigated, such as the exfoliation of the pristine graphite in medium Liquid by means of ultrasound.

The self-assembly has been recognized for a long time as one of the best strategies for bottom-up nanotechnology. Recent works have successfully demonstrated the self-assembly of graphene sheets in thin films of high performance through multi-stage processes, such as transparent and conductive membranes. In this work a high performance self-assembled graphene hydrogel prepared by an easy one step hydrothermal method is presented.

Keywords: carbon, graphene, self-assembly.

Synthesis and Characterization of Nanomaterials Based on Silica, Alumina and Titania Mesoporous Functionalized for Hydrogen Retention Applications

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Abstract

The need for technologies that can meet the energy requirements in an environmentally friendly way, since the production of hydrogen for energy purposes, gives a guideline to investigate appropriate systems for the storage, for this use. This paper describes activities taken to synthesize nanomaterials based on silica, alumina and mesoporous titania; with alkoxides of metals chosen from precursors and surfactants such as templates, established routes of synthesis, using ultrasonic radiation at one of the stages; for each of the structures were obtained samples of materials at one time considerably less employees in technique traditional sol-gel. The obtained materials were characterized by SEM, XRD, BET-AREA and the results give us consistent information to ensure that the established routes are suitable for obtaining the desired structures. The results obtained show a direct relationship between the structures of the materials obtained and the retention capacity of hydrogen.

Keywords: Nanomaterial, mesoporous, sol-gel, Silica, Alumina, Titania.

.Structures and Optical properties of Nanoforest-Like Carbon Nanotubes Decorated with Nanoparticles of Strontium Aluminate Doped with Rare-Earth Elements

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Abstract

Nowadays, carbon nanotubes have a lot of applications in daily life, being applied in the fabrication of cellphones, computers, nanotransistors, among many others. Currently, their new applications in biotechnology area are in search, particulary in order to find new biosensors with fluorescent properties applying on the basis of multi-wall carbon nanotubes (MWCNTs). In this work, the obtaining of carbon nanoparticles having fluorescent properties is presented. The synthesis was carried out by spray pyrolysis and heat treatment, with strontium aluminate SrAl12O19 doped with rare-earths ions. MWCNTs were synthesized from distinct organic precursors and the corresponding metal oxides. The metal oxides used was samarium (Sm), europium (Eu), neodymium (Nd), lanthanum (La), cerium (Ce) and some their combinations.

The synthesis via spray pyrolysis was realized on the surface of optical fibers to obtain a uniform growth of forest-like MWCNTs, adding to metal oxide nanoparticles to their surface, in dry nitrogen atmosphere in the temperature range from 780 to 850ºC. The process by heat treatment was made using MWCNT´s doped with COOH, dissolved on Isopropyl Alcohol at different concentrations con strontium aluminate. The formed products were characterized by Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), FTIR spectroscopy and UV/visible spectroscopies. The best results were observed with lanthanum oxide as a dopant. Possible applications as persistently luminescent phosphors for the formed MWCNTs-supported luminescent materials are proposed.

Keywords: Fluorescent Carbon Nanotubes, Spray Pyrolysis, Biosensors.

First Order Plasmonic Resonances in Hybrid Systems of Few Layer Graphene on Aluminum Nanocavities Arrays

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Abstract

The 2-dimensional materials such as graphene [1] and the plasmonics are used in multiple applications. Many of them require of efficient materials operating in the UV range of electromagnetic spectrum. In this region, aluminum is a good candidate due to its optical and electronic properties, natural abundance and low cost compared to other noble metals[2]. Combining these two materials, systems with novel properties can be obtained.

The present work presents results of fabrication of nanocavities in aluminum surfaces by electrochemical anodization using phosphoric acid and mixture of phosphoric-citric acids [3] as electrolytes in the 160-600 V range at ambient temperature and multilayer graphene synthesized by CVD [4,5]. The morphology and topography of these structures were evaluated by SEM.

Plasmonic properties of Al cavities arrays and hybrid sistems were analyzed based on specular reflectivity. Al cavities arrays fabricated with different acids dramatically reduced their optical reflectivity as compared with unstructured Al. At the same time pronounced reflectivity dips were detectable in the 200nm-400nm and 300 nm-600 nm ranges, which were ascribed to (1,1) and (0,1) corresponding to second and first plasmonic modes [6,7] respectively. In the hybrid systems an overall decrease in the reflectivity is observed which is related to an increase in absorbance; additionally a dip in the reflectance around 274nm characteristic of graphene is also observed. It has recently been theoretically demonstrated that graphene on metal gratings [8] can significantly improve the absorbance of graphene because of the excitation surface plasmon polaritons (SPPs).

All samples present a colored notable appearance depending on the observation angle. Our hypothesis is that the surface plasmons decay radiatively emitting photons in the visible range; this process because the strong coupling of plasmons and photons through the irregularities on the aluminum surface [6].

Keywords: Graphene, Plasmonics Sistems, Aluminum Nanocavities Arrays,

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Characterization and Cathodoluminescent Properties of Carbon Nanotubes Coated with ZnO by Atomic Layer Deposition

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Abstract

Surface engineering nanostructures through the incorporation of few atomic layers of metallic, inorganic or organic molecules on oxide surfaces, can substantially modify their properties opening to new ranges of possible applications. Furthermore, the formation of heterostructures is believed to be of importance in tailoring the physical properties of 1D nanostructures. The heterostructures with various compositions and interfaces have already demonstrated the distinctive performance in nanodevice applications. Being a wide band-gap semiconductor (3.34 eV), zinc oxide (ZnO) has been extensively investigated for electronic and optoelectronic devices, such as field emitters, photodetectors, gas sensors, and so on. Therefore, the formation of the heterojunction of ZnO and CNTs should extend the application scopes and reinforce the pristine properties of simplex ZnO and CNT materials. As a specific one-dimensional morphology, ZnO nanotubes attract extensive attention due to their high surface area, low density, biocompatibility, photocatalytic activity, turning into a promising candidate for lots of potential applications. MWCNTs were coated by atomic layer deposition (ALD) method, at 120 °C on a hotwalls ALD reactor, using Diethyl Zinc (DEZ) as precursor and deionized water as oxidant. XPS and FTIR were used to corroborate ZnO deposition. Through TEM was confirmed the homogeneous and conformal coating of CNTs. The luminescent properties were evaluated by Cathodoluminescence and HR-XPS was used to study defects involved on emission process.

Keywords: ALD, ZnO coating, Carbon nanotubes.

Design and Construction of a Chemical Vapor Deposition Reactor to Obtain High Quality Graphene at Low Cost

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Abstract

Graphene has attracted a lot of attention because of its peculiar mechanical, electrical and potential applications in industry and technology. It has several synthesis methods and depending on each method will be the properties obtained. The Chemical Vapor Deposition (CVD) is a large-scale method to obtain a two-dimensional material, this method is being used to obtain graphene in applications of electronic devices. In this work, a CVD reactor was designed and built to obtain graphene, the most promising synthesis route for the production of graphene on a large scale. The different variables to be controlled, such as temperature, pressure and gas flow, were studied to optimize the reactor design. As well as the lower consumption of energy and reagents. The synthesis of graphene is carried out by the method of chemical deposition in vapor phase, the methane gas (CH4) is the desirable precursor to obtain the graphene in an inert atmosphere.

Keywords: Graphene, Chemical Vapor Deposition, Electronic devices.

Understanding the Open-Circuit Voltage of Organic Photovoltaics: A Theoretical Perspective

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Abstract

A detailed analysis of the parameters affecting the open-circuit voltage, VOC, in a P3HT/PCBM dimer is provided in this poster. Electron transfer parameters are evaluated via CAM-B3LYP/6-31G* under the time-dependent and unrestricted density functional theory formalisms. The charge recombination driving force is found to mainly affect the recombination rate and, in turn, VOC. The analysis reported in this poster encourages further quantum-chemical investigations in organic photovoltaics with the aim of estimating and improving VOC so that more efficient organic solar cells may be predicted.

Keywords: organic photovoltaics; density functional theory; open circuit voltage.

Facile Encapsulating of Magnetite Nanoparticles in Silica

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Abstract

We report the successful encapsulation of magnetite nanoparticles in particles of silica formed by modification of Stöber method in presence of ultrasound stirring. The irradiation power (130W, 120 KHz) allows to obtain adequate encapsulation in 180 minutes of process. In order to control the silica thickness we modify the tetraethylorthosilicate (TEOS) concentration. This results allow control the coat of silica, reducing the agglomeration and preserve the properties in time.

Keywords: magnetite nanoparticles, Stöber method, TEOS.

Physicochemical Properties of Composite Material Graphene-Polymer

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Abstract

The study and development of materials is of the utmost importance for creation of new technology. One of the interesting areas of study is graphene, due to its special properties that can be used in many potential applications. Nonetheless, there are still problems to solve related with the mass production of graphene. The chemical methods represent a feasible option for industry production because of the higher and cheaper amount of material obtained in comparison with other methods. Hummers' method is a viable option to obtain reduced graphene oxide (rGo). This method consisted in two phases, oxidation and reduction, obtaining graphene oxide (GO). The synthesis of graphene oxide via Hummers' method and a modified Hummers' method [1] was done. To synthesize a composite nanomaterial, rGo was combined with polypyrrole nanoparticles. The results were analyzed and compared to establish the most appropriate option for the composite nanomaterial. To further improve the properties of the rGo, polypyrrole polymer nanoparticles prepared by chemical oxidation were added. The characterization of this composite nanomaterial to determine its physicochemical characteristics was performed by scanning electron microscopy (SEM), Raman spectroscopy and X-ray diffraction techniques. To determine properties such as hardness and elastic constant was performed by atomic force microscopy. The application of this material is for aerospace environments and could be used in the future for space exploration missions.

Keywords: Graphene, composite nanomaterial, polymer nanoparticles.

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Synthesis of g-C_3N_4/CeO_2 Nanocomposite for Photo Catalytic Applications

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Abstract

In the field of photocatalysis, graphitic carbon nitride (g-C_3N_4) is considered as promising material due to its 2.7 eV band gap. However, photocatalytic efficiency of g-C_3N_4 is limited, because of high recombination rate of electron-hole pair. To overcome the issue, development of hetrojunction with other semiconductors has been studied by researchers and successful in increasing photocatalytic efficiency to some extent. Among such materials CeO_2/ g-C_3N_4 nanocomposite is considered vital as it comes with Ce^{3+}, Ce^{4+} and oxygen vacancies.

Here, we will report the effect of g-C_3N_4/CeO_2 mass ratio on photocatalytic degradation of organic contaminant. About10 nm sized CeO_2 nanoparticles were synthesized in green chemistry methods using α-amino acid at low temperatures. Graphitic carbon nitride was obtained by pyrolyzing urea around 550 °C. In the later stage, various samples with different mass ratios were prepared using ultrasonicator. Variations in bandgap value (from 2.7 eV) with increase in the mass ratios were observed with UV-Vis analysis. Specific surface area and pore size were obtained using BET analysis. Changes in photocatalytic efficiencies will be correlated in detail with structural, optical and morphological changes and finally a proper degradation mechanism will be discussed.

Keywords: graphitic carbon nitride, photocatalysis, ceria nanoparticles.

Synthesis and Characterization of CeO_2 Doped with Sm_2O_3 and Eu_2O_3 for Potential Use in SOFCs

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Abstract

To free ourselves from the use of fossil fuels that are highly polluting, life-threatening and not easily regenerated, new technologies are being developed to obtain alternative energy sources more efficiently. Among these technologies, there is the option to improve the performance of solid oxide fuel cells (SOFCs) to make them highly energy efficient. Solid oxide fuel cells (SOFCs) have attracted much attention because they are environmentally benign, sustainable, generate low emissions and have relative low cost. However, conventional SOFCs with yttria-stabilized zirconia (YSZ) electrolyte require high operating temperatures (800-1000°C), which often lead to material degradation problems. Given that the greatest disadvantage of SOFCs is their high operating temperature, samples of CeO_2 were synthesized by spray pyrolysis method and doped with Sm_2O_3 and Eu_2O_3 to improve the ionic conductivity of the electrolyte so that it can operate at lower temperatures without losing its efficiency. The samples were analyzed using SEM, EIS and DRX and tested in a SOFC prototype.

Bulb Based on Silver-Functionalized Carbon Nanotubes

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Abstract

Since the invention of the focus has been tried to improve the light source over the years, all studies and experiments sought to obtain the longest emission time, best white light and saving electricity consumption in addition to reaching the reach Of all our homes and as we well know the essential part of the light source are the filaments, which are the ones that emit light, but also the energy consumption is essential. We present a method of light emission with the substitution of nanotubes decorated with silver instead of tungsten, with a small energy consumption and long life of useful life.

The production of our nanotubes made in the laboratory of the UTFV with the help of consultants the same institution, is by the CVD method, is a production already known, in the state of the art, is to produce a steam from the solution. The preparation of the solution, is a mixture of 2 chemicals, Toluene $C_6H_5CH_3$ and Ferroceno $C_{10}H_{10}Fe$, with percentage of 96.5% and 3.5% respectively. The positioning of the above solution is in a steam generator, which may be of the atomizing nozzle type or of an ultrasonic generator. Its connection of the steam generator with a ceramic tube or the connection to a quartz tube, a high purity inert gas selected from the group comprising Argon, Helium, Nitrogen, etc. Once the system is sealed, at a rate of less than 0.5 l / min. The heating of the tubular furnaces is left at a temperature within the range of about 650°C to about 1000°C.

Keywords: white light, nanotubes, energy saving.

Study of Electronic Properties, Spectral and Temporal Optical Behaviour of CdSe/ZnS Quantum Dots

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Abstract

Among different QDs those based on CdSe are the most extensively studied systems. However, from an application point of view these bare CdSe QDs are not at all suitable because of their sensitivity toward photo-oxidation of the surface which affects the photoluminescence quantum yield (PLQY) badly. Thus, CdSe/ CdS or CdSe/ZnS QDs are observed to be more stable at the ensemble level with respect to chemical degradation or photo-oxidation in comparison to bare CdSe QDs. In this work study blue, green, and red emission, abosortion, quantum yield, charge carrier dinamics and lifetime of these quaternary CdSe/ZnS QDs have been reported and analyzed in detail. Steady-state emission and nanosecond time-resolved PL decay for CdSe/ZnS QDs. Examination of the PL decay dynamics would be very much useful in elucidating the nature of the exciton state and characterizing the competitive radiative and nonradiative recombination processes. For the CdSe/ZnS QDs time-resolved PL decay traces have been observed to be multiexponential in nature and could be successfully fitted with a three exponential function. In general with the growth of the shells the overall decay gets faster. Three different time constants have been observed, one faster component of 3-4ns, a moderate component of 16-30ns, and a slowest component >30ns.

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Keywords: Lifetime, Quantum Dots (QDs), Photoluminescence (PL)

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Synthesis and Characterization of Chitosan Nanoparticles and their Antifungal Application in Plant Protection

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Abstract

Plant pathogenic fungi is one of the most important sources of seed and plant diseases, causing important losses in agriculture. In order to fight these organisms, chemical fungicides are used to protect economically important crops, however, the extensive and uncontrolled use of these biocides can also cause environmental toxicity to other living organisms, including human. An alternative is to produce nanoscale systems derived from natural materials, e.g. chitosan. Chitosan is a cationic biopolymer composed of β-(1-4)-linked d-glucosamine and residues of N-acetyl-d-glucosamine, obtained by deacetylation of chitin, an abundant polysaccharide isolated from the exoskeleton of crustaceans. Chitosan Nanoparticles (CS NPs) have been widely studied due to their high biocompatibility, biodegradability, non-toxicity, cost effectiveness and antimicrobial properties. Nowadays they are extensively used in biomedical applications, such as drug and gene delivery. The purpose of this work is to study the in vitro antifungal properties of chitosan nanoparticles against phytopathogenic fungi. The CS NPs will be prepared using ionic gelation method (a non-toxic, controllable organic solvent free process) using Tripolyphosphate-pentasodium (TPP) as a cross-linking agent. Different chitosan/TPP ratios (3:1, 6:1 and 9:1) will be tested against three strains of plant pathogenic fungi using poisoned food technique. Fungi were previously isolated from local regions. Particle size, morphology and chemical structure of CS NPs will be evaluated using SEM and FT-IR. This study pretends to evaluate the applicability of chitosan nanoparticles as a novel antifungal agent.

Keywords: Chitosan Nanoparticles, antifungal, biocide.

Dielectrophoresis As a Nanofabrication Technique for Transmon Quantum Bits

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Abstract

During the past years, Quantum Computing has become in one of the most studied fields among the emerging technologies. The capability of high processing computing makes this technology the best tool for solving complex processes in super-fast time frames, such as 3D molecular modeling, astronomical data analysis or statistical models. The reason for such an impressive behavior lies in the way of how data is saved and read in such machines: qubits. As a quantum system, qubits can be represented as atoms or another atomic particle (electrons, protons, ions) which allow the superposition of two different states at a time.

During the last years, different types of qubits have been tested in order to find the most functional way of making them. There are many parameters that should be considered. Among them are the quantum coherence of the system and the facility of physical manipulation outside the system. Following this line, transmons seem to be one of the favorites to achieve these.

In this poster, it is presented the analysis of the parameters to use in the qubit nanofabrication technique called Dielectrophoresis in order to achieve the optimum alignment of AlAg Nanowires in microelectrodes for nanochips. The desire transmons were easily formed at a very wide range of tuning parameters, which could easily be improved manually and could be implemented in a faster form of fabrication.

Biopolymer from Organic Banana Peel Debris Capable of Retaining the Carbon Dioxide from the Internal Combustion of a Gasoline Engine to Oxygen

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Abstract

Nowadays, it has been witnessed a growth in using petroleum derivatives polymeric materials, such as Polystyrene (PS), Polyethylene terephthalate (PET), Polyhexamethylene diamide (Nylon 66), Polyvinyl chloride (PVC), Polypropylene (PP) and annexes. The medium life of this polymeric materials, on average, is from 100 to 1000 years. Conventional plastics are causing environmental and health problems, such as climate change, depletion of abiotic resources, depletion of the ozone layer, and annexes. The solution use polymeric materials from natural and renewable fibers. Biopolymers have become increasingly important in everyday life for the development of new materials degradable to the environment and with characteristics similar to synthetic ones. Another very common problem is the combustion of automobiles to the environment, the emissions of carbon dioxide and suspended particles, counting also free radicals resulting from the combustion of fossil fuels. The proposal is the development of a biopolymer from organic banana peel debris capable of retaining the carbon dioxide from the internal combustion of a gasoline engine to oxygen. To increase its properties, it will be doped with graphene oxide to acquire the characteristics of the functional groups thereof, such as epoxy, hydroxy and carboxylic, as well as mechanical properties such as hardness, high resistance to deformation, highly hygroscopic, among other characteristics. The carboxylic groups will allow anchoring of the lithium, which will fulfill the function of forming a lithium arc, and attract the carbon, dissociating it from the oxygen when the emission is emitted by the muffle of a gasoline engine.

The equipment and techniques for characterization are the following: Scanning Electron Microscope (SEM), Transmission Electron Microscopy (TEM), Infrared spectroscopy (IR), Ostwald's Viscometer.

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