GENERAL PROGRAM

2nd International Symposium on Nanoscience and Nanomaterials

Ensenada, Baja California, Mexico, March 4-8, 2012

“Welcome to the Bionanotechnology Group”

Universidad Nacional Autónoma de México

Centro de Nanociencias y Nanotecnología

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LDG. Marina Curiel
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PRESENTATION

One of the main goals of the Symposium on Nanoscience and Nanomaterials formerly kown as Symposium on Material Sciences, traditionally held at our Center of Nanosciences and Nanotechnology now for 17 years, is the academic exchange that takes place between our researchers and the students of our three graduate programs. The growth of our research programs is reflected in these meetings, which initially lasted 2 days and, since 2012, updated to 5 days of academic activities, as will be experienced in the 2nd International Symposium on Nanoscience and Nanomaterials

During the 2nd International Symposium on Nanoscience and Nanomaterials to be held from March 4 to 8, we will offer 14 plenary conferences by outstanding international and national researchers who have been invited to this meeting. We will also be able to attend 27 oral presentations, and 88 posters will be exposed. I invite you to appreciate the variety of subjects presented and the high level of research that is being practiced in this, our research center. In particular, we welcome the always important participation of our students. The participation of a new research group recently incorporated to our Institution contributing a new line of research on Bionanotechnology will highlight our meeting. There will be more than a few plenary and contributed talks as well as poster presentations on that topic.

This event was made possible by the time and dedication of the members of the Organizing Committee, which on this occasion is integrated by Drs. Gustavo Hirata Flores, Noboru Takeuchi Tan, Alejandro Huerta Saquero, Mario A. Curiel Álvarez, Felipe F. Castillón Barraza, Jesús A. Maytorena Córdova, Trino A. Zepeda Paricda as well as José Juan Gervacio and Margot Sainz, under the coordination of Jesús M. Siqueiros Beltrones (Chairman). We wish to express our gratitude to our administrative and academic staff and to the students who will participate in this annually held event, thus ensuring its success. Last but not least, we are especially grateful to the Coordinator of Scientific Research of UNAM for his unconditional moral and financial support.

Sincerely,

"POR MI RAZA HABLARÁ EL ESPÍRITU"

Ensenada, B.C., March, 2013

THE DIRECTOR

DR. SERGIO FUENTES MOYADO

Centro de Nanociencias y Nanotecnología Universidad Nacional Autónoma de México

CONFERENCE TOPICS

Bionanotechnology

Structural properties of nanomaterials

Electronic, optical and transport properties of nanostructures

Nanomagnetism and spintronics

Micro and nanoelectromechanical systems (MEMS/NEMS)

Carbon and related systems

Quantum computing

Surfaces and interfaces

Thin films

Synthesis of nanomaterials

Nanocatalysis

SPEAKERS

Rafael Vázquez Duhalt
IBT-UNAM

Maxim Sukharev
ARIZONA STATE UNIVERSITY

Francisco Javier Espinoza Beltrán
CINVESTAV-QUERÉTARO

Kevin O'Donnell
APPLIED PHYSICS-CICESE

Olivia A. Graeve
UC SAN DIEGO

John Schliemann
UNIVERSITÄT REGENSBURG

Jorge O. Sofo
PENN STATE UNIVERSITY

Mark Tsodikov
RUSSIAN ACADEMY OF SCIENCES

Irina Simakova
ÅBO AKADEMI UNIVERSITY

Alexei Licea
CICESE

Milan Makale
UC SAN DIEGO

Laura Palomares
IBT_UNAM

Talat Shahnaz Rahman
UNIVERSITY OF CENTRAL FLORIDA

Gian Carlo Delgado Ramos
CIICH-UNAM

WORKSHOPS

Nanoscience and Nanotechnology for Beginners

Dr. Leonel Cota

Dr. Noboru Takeuchi

Spectroscopic Techniques for Materials Analysis

Dr. Wencel de la Cruz

Principles and Applications of Electron Microscopy

Dr. Oscar Edel Contreras

From Molecular Biology to Bionanotechnology

Dr. Alejandro Huerta Saquero

Dra. Karla Oyuky Juárez Moreno

EXHIBITS

Instrumentación y Servicios Analíticos
S.A. de C.V.
http://www.isasa.com.mx/

JEOL de México
S.A. de C.V.
http://www.jeol.com.mx/

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Carl Zeiss de México S.A. de C.V.
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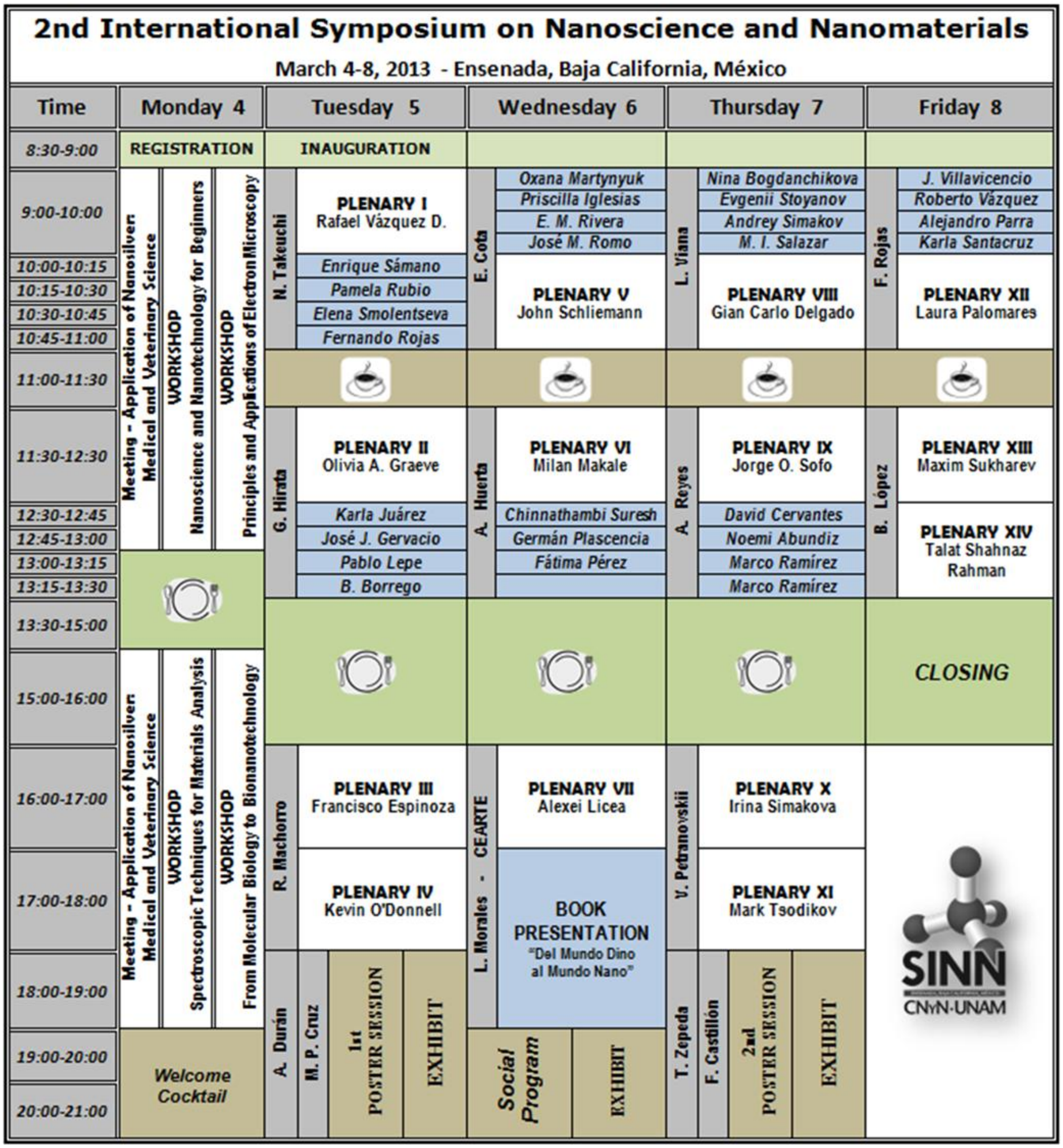
WEEK SHEDULE



2nd International Symposium on Nanoscience and Nanomaterials

March 4-8, 2013 - Ensenada, Baja California, México

Time	Monday 4	Tuesday 5	Wednesday 6	Thursday 7	Friday 8
8:30-9:00	REGISTRATION	INAUGURATION			
9:00-10:00	Meeting - Application of Nanosilver: Medical and Veterinary Science WORKSHOP Nanoscience and Nanotechnology for Beginners WORKSHOP Principles and Applications of Electron Microscopy	N. Takeuchi **PLENARY I** Rafael Vázquez D.	E. Cota Oxana Martynyuk Priscilla Iglesias E. M. Rivera José M. Romo	L. Viana Nina Bogdanchikova Evgenii Stoyanov Andrey Simakov M. I. Salazar	F. Rojas J. Villavicencio Roberto Vázquez Alejandro Parra Karla Santacruz
10:00-10:15		Enrique Sámano	**PLENARY V** John Schliemann	**PLENARY VIII** Gian Carlo Delgado	**PLENARY XII** Laura Palomares
10:15-10:30		Pamela Rubio			
10:30-10:45		Elena Smolentseva			
10:45-11:00		Fernando Rojas			
11:00-11:30		☕	☕	☕	☕
11:30-12:30		G. Hirata **PLENARY II** Olivia A. Graeve	A. Huerta **PLENARY VI** Milan Makale	A. Reyes **PLENARY IX** Jorge O. Sofo	B. López **PLENARY XIII** Maxim Sukharev
12:30-12:45		Karla Juárez	Chinnathambi Suresh	David Cervantes	**PLENARY XIV** Talat Shahnaz Rahman
12:45-13:00		José J. Gervacio	Germán Plascencia	Noemi Abundiz	
13:00-13:15	🍽	Pablo Lepe	Fátima Pérez	Marco Ramírez	
13:15-13:30		B. Borrego		Marco Ramírez	
13:30-15:00		🍽	🍽	🍽	*CLOSING*
15:00-16:00	Meeting - Application of Nanosilver: Medical and Veterinary Science WORKSHOP Spectroscopic Techniques for Materials Analysis WORKSHOP From Molecular Biology to Bionanotechnology				
16:00-17:00		R. Machorro **PLENARY III** Francisco Espinoza	L. Morales - CEARTE **PLENARY VII** Alexei Licea	V. Petranovskii **PLENARY X** Irina Simakova	
17:00-18:00		**PLENARY IV** Kevin O'Donnell	BOOK PRESENTATION “Del Mundo Dino al Mundo Nano”	**PLENARY XI** Mark Tsodikov	
18:00-19:00		A. Durán M. P. Cruz 1st POSTER SESSION EXHIBIT		T. Zepeda F. Castillón 2nd POSTER SESSION EXHIBIT	
19:00-20:00	*Welcome Cocktail*		*Social Program* EXHIBIT		
20:00-21:00					

***Workshops will be imparted at CNyN-UNAM facilities on Monday 4.**

****2nd General and 1st Satellite Meeting of “Application of Nanosilver in Medical and Veterinary Science” will be held at the Centro Social, Cívico y Cultural Riviera de Ensenada on Monday 4.**

FORMAT RESTRICTIONS OF ABSTRACTS

The proceedings of the 2nd International Symposium on Nanoscience and Nanomaterials are a compilation of the accepted abstracts of the plenary, contributed oral and poster presentations. Due to format restrictions figures and cited references, although mentioned in the abstarct, were not included in the printed version. If you require additional information please write to the authors.

PLENARY SESSION

PLENARY I

CYTOCHROME P450, VIRUS-LIKE NANOPARTICLES AND CHEMOTHERAPY

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Keywords: Bionanotechnology, Cytochrome P450, Prodrug, Virus-like nanoparticles.

The encapsulation of enzymes inside virus-like particles (VLPs) or other protein cages is a fast growing topic because of its implications in biocatalysis as well of their potential as enzymatic delivery systems. We report, for the first time, the encapsulation of a CYP450, which belong to a family of enzymes with relevant importance in medicine. First, combined quantum mechanical and molecular mechanical (QM/MM) calculations were used to explore the electron pathway involved in the suicide inactivation of cytochrome CYPBM3 from *Bacillus megaterium*. This method allowed a rational identification of key oxidizable amino acid residues in order to replace them for less oxidizable residues by site-directed mutagenesis. Double mutants of CYPBM3 21B3 (W96A/F405L) resulted in a more stable variant in the presence of hydrogen peroxide than native enzyme. The CYPBM3 21B3, with improved peroxigenase activity, has been encapsulated inside two different VLPs through a charge complementarity strategy. The VLPs used were CCMV and VP1 from murine poliomavirus. The encapsulation of CYP inside CCMV was favored by the fact that the enzyme and the interior of the capsid have opposite charge at pH 7.2. The VLPs formed showed an average diameter of 19.9 nm. On the other hand, to promote the interaction of the CYP with the negatively charged interior of the VP1 capsid, we chemically modified the surface of the enzyme with ethylenediamine to increase the number of positively charged groups at pH 8. The VLPs formed have an average diameter of 23.6 nm. We have demonstrated that it is possible to encapsulate the CYPBM3 inside CCMV and VP1 VLPs using a charge complementarity approach. The encapsulation of this CYP450 in viral structures will provide a model for the design of biocatalytic nanoparticles with potential medical applications, especially in chemotherapy.

PLENARY II

LIMITS OF PRECIPITATION AND COMBUSTION PROCESSES FOR THE SYNTHESIS OF NANOPOWDERS OF UNIQUE MORPHOLOGIES

Olivia A. Graeve
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This talk will present an overview of fundamental responses and limits of precipitation processes for the synthesis of nanostructured ceramic nanopowders, with special emphasis on combustion synthesis for the preparation of borides and reverse micelle synthesis for the preparation of oxides. Advanced sintering techniques for nanostructured materials will also be described. Boride compounds have proven essential for myriad applications such as reinforcing phases in metal-matrix composites and armor materials. One particular sub-group in this large class of materials includes the hexaborides. We will demonstrate the first instance of the preparation of boride materials by the efficient combustion synthesis technique at a temperature of 320°C. Combustion synthesis has been utilized since the 1990's for preparing many types of nanocrystalline oxides, as has been shown in countless studies. However, boride materials were thought to be unfeasible by this technique. We have selected two compounds, the hexaborides LaB_6 and $Sm_{0.8}B_6$, as model materials for representing the effectiveness of the process for the preparation of borides. The technique results in high-purity powders with unique cubic morphologies (as shown below), where the surfaces correspond to the {001} faces of the crystals. We will also present an analysis and systematic investigation of the structure and stability of reverse micelle systems with the addition of NH_4OH, $ZrOCl_2$, and $Al(NO_3)_3$ salts. The concept of an electrical double layer, as it applies to reverse micelles, will be considered for explaining features of destabilization, including the initial decrease in reverse micelle size, the destabilization concentration, and the effect of cation valence. We propose that the reduction in size prior to instability is caused by compression of the reverse micelle electrical double layers, as higher concentrations of salts are present. All these effects have important implications for the preparation of nanopowders by reverse micelle synthesis. If the reverse micelles are unstable before the precipitates are formed then the advantage of reverse micelle synthesis is immediately lost.

PLENARY III

QUANTITATIVE MECHANICAL AND PIEZOELECTRIC PROPERTIES OF MATERIALS AT NANOSCALE BY SPM

Francisco Javier Espinoza-Beltrán[1]*, Christian Ivan Enriquez-Flores[2], Francisco Javier Flores-Rodríguez[2], Eleazar León-Zarabia[2]
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Quantitative measurements at micro- and nano-scale of mechanical and piezo-electric properties using SPM techniques are gaining increasing importance in the development of new materials, characterization of MEMS devices and biological materials, etc. Dynamic atomic force microscope (AFM) working in the ultrasonic frequency range modes, based on contact resonances of the AFM cantilevers such as atomic force acoustic microscopy (AFAM) and contact resonance piezoresponse force microscopy (CR-PFM), provides quantitative characterization of mechanical and piezoelectric properties at the nanoscale level. The resonance tracking (RT) methods [1] applied to AFAM and CR-PFM allow avoiding the topography cross talk, which is common and undesirable for the AFM modes working at contact resonance. Also, RT methods allow mapping the tip-sample contact resonance; from these maps the elastic modulus distribution of the sample surface can be determined. Resonance tracking AFM is particularly useful for polycrystalline materials where the crystals are in the nanoscale size and with a particular texture. In this case, by resonance tracking AFAM the differences in the elastic modulus for the different crystalline orientations can be achieved. If the polycrystalline material is ferroelectric, resonance tracking PFM shows the ferroelectric domains for each crystalline orientation. In addition, with CR-PFM mode, piezoresponse hysteresis loops can be also obtained even for ferroelectric materials with low piezoelectric coefficients. Combining piezoresponse and displacement measurements of the surface, a self calibration method was developed in order to have quantitative hysteresis loops from which the piezoelectric coefficient d33 is extrated. In the present talk, details of the dynamic AFM methods mentioned above will be described, including application on different materials (PZT, $BiFeO_3$, TiN, etc.).

PLENARY IV

RECOMBINATION OF QUANTUM-ENTANGLED PHOTON PAIRS

Kevin A. O'Donnell
Física Aplicada, CICESE, Ensenada, B.C., México

Much research has studied the quantum entanglement of photon pairs created by splitting the photons of a pump laser in a nonlinear crystal. Here, we describe recent experimental work done at CICESE in which the entangled photon pairs are recombined back to single photons in a second nonlinear crystal, but with a time delay of a few femtoseconds introduced between pair members [1]. Unlike the Mandel two-photon interferometer [2], these observations are sensitive to temporal dispersion (ie, stretching or compression) of ultrafast photon wavepackets, and so permit observation of previously unseen effects like Franson's quantum dispersion cancellation [3,4]. Quantum vacuum fluctuations allow the recombined pairs to reconstruct the phase structure of the original pump beam, even though the pairs are incoherent in the classical sense. Under certain experimental conditions, classical interference is observed in the recombination rate due to mixing of the signal and idler modes. Potential applications, particularly in biophotonics, are discussed.

PLENARY V

HARTREE-FOCK THEORY FOR GRAPHENE

John Schliemann
University of Regensburg

We study Coulomb repulsion among charge carriers in monolayer as well as multilayer graphene within Hartree-Fock approximation. Apart from in-plane solutions given by the single-particle states of the non-interacting system, we find further solutions with the sublatttice spin pointing out of the plane. At sufficienntly strong interactions, the latter configurations are lower in energy than the in-plane solutions. We point out physical (and measureable) consequences of such out-of-plane solutions in terms of symmetry breaking and optical as well as transport properties.

PLENARY VI

THERANOSTIC LIPOSOMAL NANOPARTICLES TO OPTIMIZE EXISTING THERAPEUTICS

Milan Makale
Translational Neuro-Oncology Laboratories
UC San Diego Moores Cancer Center

Multifunctional liposomal nanoparticles and related nanoscale structures hold promise for cancer therapy by making feasible the use of potent drug and prodrug compounds that have failed during translational development due to inadequate pharmacokinetics (PK) and/or unacceptable toxicity (TOX). Data will be presented on how PK and TOX obstacles may be circumvented by implementing recently emerging concepts related to liposomal assembly, functionality, payload loading, and payload release. Moreover nanoparticle translation to the *in vivo* setting is presently hindered by a lack of physiologically relevant models to facilitate direct visualization of nanoparticle targeting kinetics, efficacy, and the host tissue response. We are addressing this deficiency by developing and validating an intravital platform that is suitable for direct combined modality imaging, and which can potentially guide the optimization of nanoscale particles for testing in orthotopic preclinical cancer models and, ultimately, for clinical application.

PLENARY VII

SHARK ANTIBODIES AND CONUS TOXINS, NEW STRATEGY TO ISOLATE: MEDICINES FROM THE SEA

Alexei Fedórovish Licea Navarro
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Keywords: new drugs, antibodies, toxins.

We have been working in the isolation of new drugs for the last 20 years. Two types of proteins such as Shark antibodies and the Conus toxins are some of the most fascinating molecules for this purpose. Shark antibodies can be used for the neutralization of toxic molecules, such as drugs, scorpion toxins, snake toxins or even our own proteins that can induce diseases when they are overexpressed. On the other hand, the Conus toxins interact with different proteins from our cells. These toxins can regulate several cell activities, they can increase the insulin expression level in pancreas, they can kill the tuberculosis bacteria, they can block chronic pain in degenerative disease and they can stop the cancer cell division. These two kinds of proteins, Shark antibodies and Conus toxins represent a promising universe of molecules for the development of novel drugs.

PLENARY VIII

PERCEPCIÓN SOCIAL Y DIÁLOGO INTERDISCIPLINARIO, ELEMENTOS CLAVE EN LA REGULACIÓN DE LAS NANOTECNOLOGÍAS

Gian Carlo Delgado Ramos
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En el avance de la ciencia y la tecnología de vanguardia, la percepción social es de gran relevancia pues puede contribuir al avance o al rechazo de tales o cuales aplicaciones tecnocientíficas sin que ello necesariamente se relacione a una base sólida de información y valoración interdisciplinaria.

En ese último ejercicio, debe notarse que si bien ya desde hace varias décadas hay avances en el estudio y análisis sobre la lógica, estímulos, incertidumbre e implicaciones del avance científico y tecnológico, la exclusión de ciertas visiones y valores en la toma de decisiones, en distintos ámbitos, no sólo el político, sigue aún arraigado. Es por ello que se considera necesario reinventar e incentivar el diálogo como instrumento clave para, por un lado, enfrentar la incertidumbre y la complejidad tecnocientífica propia de principios del presente siglo, y por el otro lado, para abrir canales interdisciplinarios más robustos útiles para ampliar el ejercicio de repensar los objetivos mismos de la actividad tecnocientífica. Para el caso de las nanociencias y la nanotecnología, lo anterior responde a la intensión de que éstas sirvan socialmente, esto es, en el sentido de que contribuyan a resolver problemas o necesidades sociales de modo genuinamente responsable (lo cual requiere de cierta regulación consensuada) y, sobre la base de un amplio y diálogo social que ayude a la construcción de percepciones sociales informadas pero al mismo tiempo no-modeladas.

El trabajo presenta resultados de análisis de percepción social en múltiples entidades universitarias del centro de México, analiza sus implicaciones y de cara al planteo de implementación de lineamientos de regulación de las nanociencias y las nanotecnologías acordados en Noviembre de 2012 por diversas entidades del gobierno federal, se reflexiona sobre la utilidad de promover en dicho contexto el diálogo interdisciplinario a la nanoescala así como la creación de espacios informativos y de divulgación de manera relativamente coordinada. Para esto último se presenta brevemente el proyecto LABnano – Laboratorio SocioEconómico en Nanociencia y Nanotecnología, su estado de situación y futuras actividades.

PLENARY IX

ELECTRONIC CORRELATIONS, MAGNETISM, AND TRANSPORT IN FUNCTIONALIZED GRAPHENE

Jorge O. Sofo
Department of Physics, Department of Materials Science and Engineering, and
Materials Research Institute.
The Pennsylvania State University

Graphene, a single layer of carbon atoms in the honeycomb structure, exhibits electronic states at the Fermi level with unique symmetry properties. These are responsible for graphene’s large electronic mobilities at room temperature that are almost independent of doping level. To harness this uniqueness into devices we need to modify the material. We need to find a way to inset carriers and open a band gap. Chemical functionalization has been the method of choice for these modifications; but it resulted in a box of surprises. It opens the way to magnetism, localization, and other interesting phenomena that are unexpected in materials made of carbon. We will review the fascinating magnetic states produced with hydrogenation and fluorination of graphene as well as their influence on its transport properties.

PLENARY X

NANOCATALYSIS IN VALORIZATION OF BIO-DERIVED CARBOXYLIC ACIDS

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Keywords: nanocatalysis, bio-mass.

The conversion of biomass into chemicals and fuels is one of the most relevant research areas at the present time being important for both academia and industry. For the latter it is a challenge to find alternative syntheses for substances that are currently obtained starting from petroleum. The challenge, that might also be a chance, is due to the differences in the feedstock that possesses opposite polarity characteristics. Contrary to petroleum, biomass consists of highly oxy-functionalized molecules that have to be dehydrated and hydrogenated, especially if fuels are the desired products. In the case of chemicals, alternative syntheses might be possible that might even be more economical when advantage can be taken from the structure of the molecules. Currently arising needs encourage a search for novel catalysts with unique properties that are necessary for new processes. Carboxylic acids are important intermediates in transformation of biomass which could serve as platform molecules in future biorefinery. Several promising reactions of carboxylic acids processing will be considered in this lecture; some of them such as hydrogenation are similar to processes widely known in chemical industry. At the same time, reactions less common for oil refining, for example ketonization, and decarboxylation are required in valorization of biomass components into fuels and chemicals. One of the most ambitious targets in catalyst preparation is to design and produce tailor made catalysts with well defined catalytic properties. The way of doing this is to develop multi-site catalysts involving single isolated sites for the different desired catalytic activities. The feasibility of this concept will be demonstrated for biomass conversion using, as examples, transformation of fatty acids and valeric acid into motor fuel components as well as valuable chemicals.

PLENARY XI

CATALYSIS BY HETEROMETALLIC CLUSTERS FORMED ON SUPPORT SURFACE. SYNERGISM AND STRUCTURAL ORGANIZATION OF ACTIVE COMPONENTS

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Keywords: heterogeneous catalysis, mono- and hetero metallic precursors and active components, structure, catalytic activity, selectivity, non additive effect.

In this communication analytical review of world-wide achievements, including the results of author's group, related to heterogeneous catalytic- and electro-catalytic reactions on Pt, Au, Ni, Pd, Zn mono- and hetero-metallic nanosized active components distributed on surface of Al_2O_3, ZSM-5 and TiO_2 supports

will be presented. Special attention will be done on the evolution of catalytically active components during preparation and preliminary activation stages of catalysts, as well as on correlations between structure of metal-containing sites and their catalytic properties in reactions of natural gas and row of biomass products, such as methane, alcohols and rapeseed oil conversion into hydrocarbon fuel components, olefins, as well as the process of methane steam reforming for hydrogen producing. Using X-Ray, XAS, TEM and Mössbauer spectroscopy it was shown, that non-additive increasing of activity and selectivity of materials can be provided by the forming of the clusters of metal-containing active components consisting of intermetallic, or core-shell configuration, or independent metal-oxide systems, undergoing with each other. Mechanistic aspects of reactions carried out will be considered. This work was supported by Russian Foundation for Basic Researches (Grants N 11-03-12014-офи-м-2011;12-03-00489-a; 12-03-00489-a); TOTAL DS 2715; the Grants of Russian Academy of Science (Programs 3 and 18); and Grant of President of Russia MK-2151.2012.3.

PLENARY XII

BIOTECHNOLOGY

Laura Palomares
Instituto de Biotecnología UNAM, Mexico

PLENARY XIII

MOLECULAR NANO-PLASMONICS IN LINEAR AND NONLINEAR REGIMES

Maxim Sukharev

School of Letters and Sciences Arizona State

Modern optics fueled with both tremendous advances in nano-fabrication and laser physics is currently experiencing significant growth. Researchers are now experimentally capable of producing structures with an outstanding precision of 1 nm. We are presently witnessing a unique situation – the research centered at interaction of matter with electromagnetic radiation is fully diving into nanoscale, where one considers purely quantum systems optically driven by nano-materials. The possibilities are indeed vast ranging from fundamental ideas on single atom/molecule optical manipulation, through control of light far below the diffraction limit, to optical engineering and photonic circuitry. Despite progress, the research in optics of quantum media coupled to nanomaterials is not complete. Many recent works consider just several quantum emitters driven by near-fields altered by plasmonic materials with a few very promising attempts to include collective effects, which as I will show in this talk play a pivotal role in quantum optics of nano-materials. It is hence important to merge well-established computational procedures in nano-optics and atomic and molecular physics at the nanoscale taking into account both significant spatial dependence of evanescent fields and strong electromagnetic field enhancement. The basis of the approach is to blend computational techniques in optics together with fundamentals of quantum atomic and molecular physics. A self-consistent model of Maxwell-Liouville-von Neumann equations is at the center of this presentation. This model is used to scrutinize both linear and nonlinear optical properties of ensembles of molecules strongly coupled to plasmonic nano-structures. The ideas of coherent control and STIRAP with collective effects taken into account are also discussed.

PLENARY XIV

SINGLE LAYER MOS$_2$ – A PROMISING MATERIAL FOR NANOSCIENCE AND NANOTECHNOLOGY: INSIGHTS FROM THEORY

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Single layer Molybdenum disulfide (MoS$_2$) appears to be a promising material for next generation applications owing to its low-dimensionality and intrinsic direct band-gap of about 1.9 eV. Several experimental groups have reported novel electronic and transport properties. Efforts are underway to also grow the material on support (copper, silica, boron nitride, etc.). We have carried out density functional theory (DFT) based calculations, to provide a fundamental understanding of some of the characteristics of this material. In this talk I will show how our calculations have helped identify the geometric and electronic structure of a reactive phase (Mo$_2$S$_3$) of MoSx when grown on Cu(111) [1], while also providing qualitative and quantitative agreement to the Moiré pattern of MoS$_2$ on Cu(111) observed in STM measurements [2]. To examine the effect of defect, I will present results for a single-layer MoS$_2$ with a sulfur vacancy row which shows the emergence of a defect state in the band-gap. This state is unoccupied and localized at the vacancy row. I will consider possible vacancy configurations which may provide a route for alcohol synthesis from syngas (CO, H$_2$, CO$_2$) from single layer MoS$_2$. In the same vain, we find that mirror joined-edge defects formed between two MoS$_2$ domains exhibit metallic behavior. More interestingly, we find signatures of magnetism at specific joined-edge defects formed between two sulfur edges with 0% sulfur coverage. From the analysis of the geometric structure, we show that some joined-edge defects undergo (2 x 1) reconstructions. I will present the implications of the above findings on electronic, transport and catalytic properties of the material and their relevance to ongoing experiments in several labs. I will also summarize our findings on the role of the support (several metal surface and BN(0001)) on the characteristics of MoS$_2$. Finally, I will present our results for the binding energies of exciton and trion of a single layer of MoS$_2$ obtained from our version of time-dependent DFT formalism. *Work done in collaboration with D. Le, V. Turkowski, T. Rawal and A. Ramirez (UCF), and L. Bartels (UC Riverside) and supported in part by DOE under grant DE-FG02-07ER15842.

ORAL SESSION

O-001

AN APPLICATION OF ELECTRON BEAM LITHOGRAPHY: LOCATION OF NANOSTRUCTURES BASED ON DNA

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Keywords: DNA Nanotechnology, Electron Beam Lithography.

Electron beam lithography (EBL) is a prime top-down technique used to write a pattern on a substrate, usually a dielectric material. Among many other applications, it is employed to localize and isolate specific nanostructures for future experiments. This is done by creating an array of apertures, or “windows”, with a size slightly larger than the nanostructures to be positioned. A series of patterns on SiO_x substrates to place DNA origami nanostructures, before and after metallization, with a rectangular shape (70 × 90 nm) are presented. The main goal of this work is the isolation and alignment of metallic nanostructures.

O-002

DENSITY FUNCTIONAL THEORY STUDY OF THE ORGANIC FUNCTIONALIZATION OF HYDROGENATED SILICENE

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Keywords: acetylene, ethylene, graphene, molecule, reaction, silicon, styrene.

Silicene, the silicon analogous of graphene, is a newly synthesized two dimensional nanomaterial, with unique features and promising potential applications. In this letter we present density functional theory calculations of the organic functionalization of hydrogenated silicene with acetylene, ethylene, and styrene. The results are compared with previous works of the adsorption on H-Si(111). For styrene, binding energies for the intermediate and final states, as well as the energy barrier for hydrogen abstraction are similar for the two systems, indicating that the functionalization of hydrogenated silicene by styrene molecules is also possible. The results for acetylene an ethylene are surprisingly different in H-silicene. The intermediate state in both cases is much more stable in H-silicene, and also the abstraction barrier is much smaller than in Si(111). Therefore, we believe that the reactions are also possible for acetylene and ethylene on H-silicene.

O-003

CO OXIDATION AT ROOM TEMPERATURE OVER GOLD CATALYSTS SUPPORTED ON NANOSTRUCTURED Ce-Zr-Al MIXED OXIDES

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Keywords: Ce-Zr-Al mixed oxides, sol-gel, gold nanoparticles, CO oxidation.

Gold nanoparticles supported on various metal oxides have been found to be active in many reactions: low-temperature CO oxidation, water gas shift reaction (WGS) (CO+H_2O), NO reduction etc. It is well known that the catalytic activity of gold catalysts strongly depends on the gold particle size, method of gold deposition, pretreatment conditions and nature of the supports. The reducible support plays a decisive role in the formation and distribution of oxygen vacancies as well as in gold particle dispersion and shape, which are directly reflected on catalytic activity. In the present work the catalytic activity in CO oxidation of gold catalysts supported on nanostructured Ce-Zr-Al mixed oxides was studied. The Al_2O_3 and Ce-Zr-Al oxides synthesized by sol-gel method via organometallic precursors were used as supports for gold (3 wt. %) catalysts preparation applying deposition-precipitation (DP) technique using $HAuCl_4 \times 3H_2O$ as a gold precursor and urea ($CO(NH_2)_2$) as a precipitation agent. Commercial CeO_2 and ZrO_2 (Alfa-Aesar) were used as supports as well. The prepared samples were characterized with XRD, BET, TEM, XPS and UV-Visible spectroscopy. Catalytic activity of gold catalysts in CO oxidation was studied at 30 ºC in a flow reactor with a gas mixture 1%CO + 0.5%O_2 and total flow 80 ml/min during 20 h of reaction. Before catalytic test gold samples were activated in oxygen or hydrogen flow at 350 ºC with a ramp rate of 20 ºC/min. The tested catalysts revealed high catalytic performance at the first minutes of reaction and the level of their activity was higher than that for comparable systems published in the literature. It was observed that gold supported on Ce-Zr-Al mixed oxides showed the enhanced activity than that supported on individual oxides (Al_2O_3, CeO_2 and ZrO_2). The activity of catalysts decreased with time: during 2-3 min for alumina based catalysts and 20-30 min for ceria including catalysts. The type of the samples pretreatment (reductive or oxidative) influenced drastically the activity of the gold catalysts. As a rule, oxidized ceria based samples were characterized with higher initial catalytic activity than reduced ones. The initial significant difference in the catalytic activity for studied catalysts became less noticeable after prolong catalytic test during 20 h. This effect could be explained by the transformation both gold species and catalyst support during catalytic reaction. The authors thank to E. Flores, F. Ruiz, E. Aparicio, P. Casillas, V. García, J. Peralta and M. Sainz for their kind technical support in this work. This project was supported by CONACyT (Mexico) and DGAPA–PAPIIT (UNAM, Mexico) through the grants 179619 and 203813, respectively.

O-004

QUANTUM DISCORD AND SPIN ENTANGLEMENT BETWEEN A MAGNETIC IMPURITY AND THE SPIN OF AN ELECTRON IN A GRAPHENE LAYER: THERMAL EFFECTS

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Keywords: quantum discord, entanglement, graphene , spin.

Quantum correlation such as entanglement (E) and quantum discord(QD) are valuable resources in quantum information and computation. They represent quantum non local correlations among two or more subsystem with no classical counterpart and are an active subject of study. The graphene has been extensively studied due to its unique physical properties in the electronic and transport properties. However, less is known of what are the effects on the induced quantum spin correlations of interacting particles embedded in a graphene layer. In this work we study the spin entanglement and quantum discords between a magnetic impurity and the spin of an electron in a graphene layer. We consider the model of an electron in a graphene layer that interacts with the spin of a localized magnetic impurity through the Heisenberg exchange coupling (HEC). We characterize the entanglement with the concurrence and quantum discord using mutual information technique. We computed these properties as a function of the temperature and HEC amplitude. We observe, in addition to the known lineal behavior of the critical temperature (CT, null entanglement) with HEC, certain HEC points where the CT decreases or increases non-linearly. This is associated with the existence of thermal spin mixtures of singlet S and triplet T_0 with a distinctive non zero QD, correlation different from entanglement that extends to temperatures beyond the CT. Thanks to DGAPA, project PAPPIT IN112012 for financial support and sabbatical scholarship for F. Rojas .

O-005

GENE UPREGULATION IN BREAST AND OVARIAN CANCER CELLS BY USING ARTIFICIAL TRANSCRIPTION FACTORS BY VIRAL AND NANOPARTICLES DELIVERY

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Keywords: Artificial Transcription Factors, breast cancer, serous epithelial ovarian cancer, Zinc Finger Proteins, Nanoparticles, Epigenetics, DNA methylation, Oct4.

Breast and ovarian cancer are the major cause of death among gynecological malignances, the later, most of the time is detected at latest stages when the disease is spread trough the peritoneal cavity. Therefore, is necessary to develop novel therapeutic tools to detect and target advanced stages of ovarian cancer. Herein we described a novel designer zinc finger protein (ZFP) able to upregulate the endogenous *Oct4* promoter in a panel of breast and ovarian cancer cell lines carrying a silenced gene. *Oct4* is considered as a key transcription factor and is involved in the maintenance of self-renewal and pluripotency in embryonic stem cells. We have found that in some ovarian tumor cell lines, the ZFP triggered a strong reactivation of *Oct4*, with levels

comparable with exogenous *Oct4* cDNA delivery. The upregulation of *Oct4* also modifies the capability of some ovarian cancer cells to form compact-self renewal spheroids or tumorspheres, this represents an *in vitro* assay to monitor the capability of single cells to proliferate in low adherent plates to assess stemness and tumorigenic potential. Surprisingly, the reactivation of *Oct4* required a KRAB domain; while KRAB-containing ZFPs are traditionally described as transcriptional repressors, our results suggest that these proteins could, in certain genomic contexts, function as potent activators and thus, outline an emerging novel function of KRAB-ZFPs. Additionally; we document a novel ZFP that could be used for epigenetic reprograming of cancer cells. In other complementary study we have shown that tumor growth and cell invasion can be diminished in a mouse model of ovarian cancer when treated with a systemic delivery of nanoparticles encapsulating a chemically modified ATF mRNA, thus outlined the first attempts and importance to use nanoparticles as a non-viral delivery system of ATFs into tumor cells with the potential of clinical applications for metastatic ovarian cancers.

O-006

PIEZORESPOSE FORCE MICROSCOPY CHARACTERIZATION OF MULTIFERROIC YCRO3 THIN FILMS

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Keywords: multiferroic, YCrO3, piezoresponse, ferroelectric, piezoelectric.

The research in materials that are both, ferroelectric and ferromagnetic, called multiferroics, has been increased dramatically in recent years due to the impact in the spintronics, a new generation of memory devices, and high frequency magnetic devices. $YCrO_3$ is one of the few known multiferroics. Its ferromagnetic response, highly reproducible, is quite well understood, but not the origin of the ferroelectric properties. Moreover, the *weak* ferroelectricity observed in ceramics has not been clearly characterized in films, this is the aim of this work. The ferroelectric domain distribution of $YCrO_3$ films, deposited by r.f sputtering, was studied as a function of thickness by piezoresponse force microscopy (PFM) in the resonant mode. Additionally, for the first time, amplitude and phase hysteresis loops, the coercive voltage and the d_{33} coefficient were obtained for this material. A resonance tracking piezoresponse technique was also used to obtain images of domains without topography effects. The results shown in this work widen the knowledge about the ferroelectric properties of $YCrO_3$ thin films. Thanks are due to E. Aparicio, P. Casillas, and I. Gradilla for their technical assistance. This work has been supported in part by PAPIIT-UNAM Proj. IN107708, IN103213 and CoNaCyT Proj. 174391, 166286.

O-007

ON THE ELECTROSPINABILITY OF SACCHARIDES

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Keywords:-------.

The electrospinning of natural and modified glucose based carbohydrates with linear (sucrose, maltose, etc.) and cyclic structures (cyclodextrins) into sub-micron and nano fibres is observed for the first time. The possibility of electrospinning short carbohydrate molecules expands the possible mechanistic theories regarding conventional electrospinning of polymeric nanofibres [1, 2]. Electrospinning of long chain molecules into nanofibres is thought to be depend on extensive chain entanglement. On the other hand supramolecular polymers, which are linear chains of low molar mass monomers held together by reversible non-covalent interactions, such as hydrogen bonding; do not present the typical chain entanglement associated with conventional polymer thermodynamics theory. Thus the discovery that short carbohydrate molecules can be electrospun, expands the range of applications for electrospinning of bio-based materials [3 - 5]. Furthermore, these results suggests that conventional polymer thermodynamics and electro hydrodynamics descriptions of the process are limited when describing charge transfer mechanisms in electrospinning; usually by ionic convection, surface charge migration and/or electronic diffusion by means of chemical potential flow. Since there is no single physical force that can be ascribed to hydrogen bonding; which arises naturally in supramolecular structures from the dynamic molecular interactions in the solution. These findings suggest a revaluation of the mechanisms underlying the electrospinning process.

O-008

ANALYSIS OF THE ANTIVIRAL ACTIVITY OF NANOSILVER PARTICLES AGAINST VIRUSES RELEVANT FOR ANIMAL HEALTH

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Keywords: silver nanoparticles, antivirals, veterinary and zoonotic viruses.

Silver nanoparticles have been described to exert some inhibitory effect against some enveloped viruses, such as human immunodeficiency virus, hepatitis B virus, herpes simplex virus, and monkey pox virus, among others (reviewed in Galdiero et al., 2011). For these and many other pathogenic viruses the development of new approaches to inhibit viral replication and transmission is a must since conventional treatments do not allow an efficient control of the diseases caused. Our work is dedicated to analyzing the potential antiviral effect of ARGOVIT silver nanoparticles against viruses which are causative agents of the so-called emerging and transboundary diseases. These are diseases which are very relevant for animal health, due to the economic losses associated to outbreaks, and in some cases also for human health, since the virus can infect not only animals but also humans (zoonotic diseases). Selected viruses require the experimental work in the certified laboratories with bio security level 3, which are available at the Center of Investigation of Animal Sanity CISA- INIA. As a first step of the study, the antiviral activity of nanosilver particles against two selected viruses we have analyzed the toxicity of silver nanoparticles over the cultured cell lines susceptible to be infected by the viruses. The next step includes determination of the optimal silver nanoparticle dose to be used on each particular cell line.

O-009

PHENOMENON OF SELF-ASSEMBLING SiO_2 NANORINGS

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Keywords: Gold complex, nanomateriales, morphology visualization, HRTEM.

The nanomaterials possess unique, beneficial chemical, physical, and mechanical properties; they can be used for a wide variety of applications in catalysis, medicine and biology.

Unexpected unique property of mesoporous silica with $[Au(en)_2]Cl_3$ complex such as the formation of self-assembling biomorphic nanostructures was observed by HRTEM. The self-assembly tendencies is manifested by different hierarchy structures of SiO_2 nanorings. Effect self-assembling of SiO_2 nanorings revealed in our work demonstrates that the silicon can form self-organized structures similar to biological systems (DNA). These unique properties of mesoporous silica can be compared with self-assembled SiO_2-carbonate biomorphs. Results showed, that time and temperatures are important factors for formation five-level hierarchy structures. There is the hypothesis, based on theoretical calculations, of the template role of water for biological system formation. Our results can be considered as experimental confirmation of these theoretical calculations. Water molecules and clusters can be templates determining the complex five-level hierarchy organization of “light” nanorings. In this case the nanorings only repeat complex water structure, which could permit to call observed effect “water-assembling” phenomenon.

O-010

ABSENCE OF THERMO-SPIN HALL EFFECT IN RASHBA AND DRESSELHAUS SPIN-ORBIT COUPLED SYSTEMS

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Keywords: Two-dimensional electron gas, spin-orbit interaction, spin caloritronics.

The central theme of spintronics is the generation and control of nonequilibrium electron spin in solids. So far, the spin generation has been done by optical, magnetic and electric means. Until recently, the possibility of generating spin currents by thermal means, has been neglected. The generation of spin currents by thermal gradients is now one of the central points of spin caloritronics. In addition to the recently observed spin Seebeck effect in ferromagnetic conductors, a transverse thermoelectric effect has been proposed, called the thermo-spin Hall current, which refers to the generation of a spin Hall current by a longitudinal temperature gradient in a two-dimensional electron gas (2DEG) with Rashba spin-orbit interaction (SOI)[1]. Here, we consider the thermo-spin Hall conductivity tensor of the spin current response induced by a frequency dependent temperature gradient in a 2DEG with Rashba and Dresselhaus SOI; the cases of quantum wells grown in the main crystallographic directions are considered. Relations between the thermally driven spin conductivity and the thermoelectric conductivity are derived. We found from these relations that the thermo-spin Hall conductivity tensor vanishes at arbitrary frequency and temperature. This is in contrast to the non-vanishing thermo-spin Hall effect predicted for the pure Rashba case[1]. This work was supported by DGAPA UNAM IN114210 and CONACyT-México.

O-011

MICROSTRUCTURAL STUDIES OF WO_3 MONOCLINIC NANOSTRUCTURES OBTAINED BY HYDROTHERMAL SYNTHESIS

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Key words: Tungsten oxide, WO_3, monoclinic structure, hydrothermal synthesis.

Nanostructured materials play an important role in different science areas. From the large variety of nanostructured compounds, the transition metal oxides have interesting properties as sensors, semiconductors and field emitters. Also are currently being exploring new applications for these materials as precursors for catalysts and lubricants. Several methods have been reported for the synthesis of WO_3 nanostructures which include physical deposition, chemical vapor deposition, arc discharge method, solid-vapor in air at atmospheric pressure, sol-gel, thermal evaporation and hydrothermal synthesis. Compared with other synthesis routes, the hydrothermal method is a good alternative because of its simplicity and reproducibility, besides that it is possible to control the particle size obtained. So, this paper presents the synthesis of nanostructures of monoclinic tungsten oxide (WO_3) using a hydrothermal method. The samples were analyzed by Raman spectroscopy, High Resolution Transmission Electron Microscopy (HRTEM) and X-ray

Diffraction (XRD). It was observed that hexagonal phase of WO_3 is obtained at a pH = 5, but the most favorable condition for obtaining the monoclinic phase occurs at a pH = 1. Authors acknowledge the support of Dr. Beatríz Millán Malo for XRD analysis as well as the financial support of DGAPA-UNAM PAPIIT IN107311-3 project.

O-012

TEM ANALYSIS OF CONCENTRIC Bi-LAYER CABLE GROWN BY ALD ON CNTs

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Keywords: transmission electron microscopy, atomic layer deposition, concentric, nanotubes.

Atomic layer deposition (ALD) can be used to deposit thin and conformal films with great uniformity on different types of substrates. When the substrate is a nanotube, it can be obtained coaxial tubes at the nanoscale. Different ceramic materials can be synthesized by ALD such as ZrO_2, HfO_2, Al_2O_3 or TiO_2 with applications going from electronics and bioengineering to catalysis. Here, alternating reactive gas sources one can obtain a concentric bi-layer cable with an Al2O3 layer and a TiO2 layer with controllable thickness according to the amount of ALD cycles used, a result that can be extrapolated to obtain multilayer coaxial cables. In this work it is presented a full detailed characterization at the nanoscale level using High Resolution Transmission Electron Microscopy (HRTEM) and the in-column Energy Disperssive X-rays Spectroscopy (EDXS) to show how the coating on the carbon nanotube (CNT) template looks, its thickness, the composition of the two layer forming the concentric bi-layer cable and the approximate thickness of each of its layers. We thanks F. Ruiz for technical assistance and projects CONACyT 83275, CONACyT 82984, CONACyT 155388, DGAPA-PAPIIT IN114209 and DGAPA-PAPIIT IN109612-3.

O-013

HDS OF DIBENZOTHIOPHENE OVER NANOPOROUS SBA-15 SUPPORTED COBALT-MOLYBDENUM CATALYST

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Keywords: Nanoporous, SBA-15, Co-Mo, acetate salts, Dibenzothiophene.

Transportation fuels are receiving the highest scrutiny because of the pollution from exhaust gas. Environmental restrictions regarding the quality of transportation fuels and the emissions from the refinery itself are currently the most important and most costly issues. Pollutants of major concern include SOx and NOx. The main aim of hydrotreating is to diminish air pollution emissions, to avoid poisoning of noble metals and acid catalysts used in catalytic reforming and cracking and finally to improve the fuel quality[1]. Among the various hydrotreating processes, hydrodesulfurization is the most important one, which is used to remove the most refractory sulfur compounds from the crude oil. Ni(Co)Mo(W) supported on alumina is used as conventional hydrotreating catalyst. The alumina support base of hydrodesulfurization catalyst leads an excellent activity, however, this support have lower surface area than mesoporous materials based on alumina-silicates. In order to improve the catalytic performance, many attempts have been made by making modifications on the support, method of preparation, etc. After the invention of mesoporous materials like MCM-41, SBA-15 and KIT-6, these materials have been employed as supports for Co(Ni)-Mo(W) catalysts and tested for hydrotreating reations[2-3]. Among these materials SBA-15 type support possess wide attention due to its unique thermal stability, high surface area and tunable pore size. The present investigation deals with the methods to improve the efficiency of Co-Mo catalyst for hydrodesulfurization of dibenzothiophene. In this view, series of supports viz., mesoporous SBA-15 and SBA-15 modified with Aluminium and Titanium will be synthesized and used them as support for Co-Mo catalyst preparation. To identify the role of metal precursor and formation of active molybdenum sulfide sites, in this study, molybdenum acetate and cobalt acetate were used as metal precursors. The structural and textural properties of the supports and catalysts were studied by different techniques. Finally, the catalytic activity will be correlated with the physico-chemical properties of the catalysts. The authors acknowledge CONACyT for financial support (Project 155388) and the valuable technical assistance to J. Peralta, M. Sainz, F. Ruíz, E. Flores, I. Gradilla, and E. Aparicio.

O-014

IMAGING ADSORPTION-UPTAKE OF METAL OXIDE NANOPARTICLES ON MACROPHAGES BY ULTRA-HIGH RESOLUTION SEM

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Keywords: nanotoxicology, metal oxide nanoparticles, electron microscopy.

Use of engineered metal oxide nanoparticles in a plethora of biological applications and custom products has warned about some possible dose-dependent cytotoxic effects. Macrophages are key components of the innate immune system used to study possible toxic effects and internalization of different nanoparticulate materials. In this work, ultra-high resolution field emission scanning electron microscopy (FE-SEM) was used to offer new insights into the dynamical processes of interaction of nanomaterials with macrophage cells dosed with different concentrations of metal oxide nanoparticles (CeO(2), TiO(2) and ZnO). The versatility of FE-SEM has allowed obtaining a detailed characterization of processes of adsorption and endocytosis of nanoparticles, by using advanced analytical and imaging techniques on complete unstained uncoated cells, including secondary electron imaging, high-sensitive backscattered electron imaging, X-ray microanalysis and stereoimaging. Low voltage BF/DF-STEM confirmed nanoparticle adsorption and internalization into endosomes of CeO(2) and TiO(2), whereas ZnO develop apoptosis after 24 h of interaction caused by dissolution and invasion of cell nucleus. Ultra-high resolution scanning electron microscopy techniques provided new insights into interactions of inorganic nanoparticles with macrophage cells with high spatial resolution.

O-015

MAGNETOELECTRIC EFFECTS IN MULTIFERROIC $TbMnO_3$ THIN FILMS DOPED WITH AL AND GA

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Keywords: Multiferroics, ferroelectrics, ferromagnetics, magnetoelectric coupling.

Magnetism and ferroelectricity coexist in materials called multiferroics. Search for these materials is driven by the prospect of controlling electrical dipoles with magnetic fields and magnetic moments with voltage, and using this to construct new forms of multifunctional devices. Early work was directed towards bringing ferroelectricity and magnetism together in one material. The simultaneous presence of electric and magnetic dipoles does not guarantee coupling between them, as microscopic mechanisms of ferroelectricity and magnetism are different and do not interfere with each other. The long-sought control of electric properties by magnetic fields was found (2003) in crystalline $TbMnO_3$ (TMO). The reason for the sensitivity of the dielectric properties to magnetic fields lies in the magnetic origin of their ferroelectricity, induced by complex spin structures. We present the dielectric properties and magnetoelectric measurements of TMO thin films doped with Al and Ga. Evidence that the magnetic field causes changes in the dielectric properties of the films is given. Doping highlights the ferroelectric transition temperature not observed in pure films. We acknowledge support from NSF-MRSEC, Grant No DMR 0520471, PAPIIT Proy. IN112610 and IN107708, CoNaCyT 166286 and 101020. We thank B. Noheda and the Zernike Institute for Advanced Materials at the University of Groningen for the use of their facilities. F. Pérez acknowledges the Beca-Mixta CONACyT scholarship. Thanks to J. Baas, E. Aparicio, I. Gradilla, D. Dominguez, W. de la Cruz, H. Tiznado and V. García for their technical assistance.

O-016

CREATION AND ADVANCEMENT OF INTERDISCIPLINARY, INTER-INSTITUTIONAL AND INTERNATIONAL GROUP “APPLICATION OF ARGOVIT IN BIOMEDICINE AND VETERINARY”

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Keywords: creation and advancement, interdisciplinary, inter-institutional and international group, application of Argovit, biomedicine and veterinary.

In 2012, under the leadership of the UNAM, a new “spin-off” Group “Application of Nanosilver in the Areas of Biomedical and Veterinary medicine” working in the area of nanobiotechnology has been created. The Group is interdisciplinary, inter-institutional and international. It includes 26 groups, 115 participants from 27 government institutions and 11 private companies of Mexico, Russia, Spain, Puerto Rico and United States. The results obtained by the group are of great impact for public health, especially in the treatment of diabetic foot syndrome, which is a direct consequence of diabetes; the number one cause of death in Mexico. More than 70 amputations have been avoided in patients with legs exhibiting diabetic ulcers which were recommended for amputation. Amputations were prevented during clinical studies of the treatment of diabetic foot with an innovative product of Argovit silver nanoparticles. Currently, clinical trials in hospitals of ISSTECALI are beginning. Progress in the comprehensive studies of toxicity (geno-toxicity, histological, dose, etc.) of Argovit silver nanoparticles in Russia and Mexico shows, that this drug is not toxic. The development of the new type of footwear with nanosilver for diabetic foot is one of the main achievements of the group. Currently the group is at the stage of transferring this technology to a spin-off company named Nanofit. The innovative nanosilver product represents an alternative to antibiotics; whose use and development is currently in crisis. Argovit application in the prevention and treatment of epidemics and pandemics of livestock and poultry is expected to make a great contribution in the economy of Mexico. Four emerging spin-off companies are diving forward towards the creation of high level skilled jobs. It is important to mention that all technology transfer high impact projects grows rapidly, incorporating new universities, institutions and companies.

O-017

CARBON MONOXIDE ABSORPTION ON THE SUFACE OF THE STRONGEST SOLID SUPERACIDS

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Keywords: Carbon monoxide, absorption, strongest superacids.

Carbon monoxide is widely used as test molecules in studying the acidity strength of Lewis and Brønsted acid sites on the surfaces of acidic catalysts. Attaching of CO molecules to the metal atoms of the Lewis centers result in increasing the stretch νCO vibration (ΔνCO) up to 107 cm^{-1} that can be used as a measure of acidic strength of the Lewis centers. At the same time attaching of CO molecules to the Brønsted centers, which are usually acidic OH groups, results to minimal νCO increasing (ΔνCO ~ 10 cm^{-1}). Possibly, there is some difference in the nature of the acid-base interaction of CO with Lewis and Brønsted acid sites that not allowed to use the values of ΔνCO as unified scale in measuring the strength acidity of both Lewis and Brønsted acids. In the present work we study the CO adsorption on the strongest known Brønsted superacids, carborane acids, in the absence of any Lewis centers. At that conditions the proton transfer on the CO molecules take place with formation of formyl cation, HCO^+. It had been shown that even one-component solid acids contain non-equivalent Brønsted centers. The IR spectra of HCO^+ cations indicate on the principal distinctions between the nature of CO bonding with Lewis and Brønsted acidic centers.

O-018

NANOREACTORS IN CATALYSIS

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Keywords: nanocatalysis, nanoreactors.

One of the most ambitious targets in catalyst preparation is to design and produce catalysts with well defined catalytic properties through the development of multi-site catalysts involving single isolated sites for the different desired catalytic activities. Considerable efforts have been devoted to the fabrication of nanomaterials with well-defined morphologies for specific applications. This is the case of nanocapsules that simultaneously provide the advantages of hollow and porous systems. Particular interest in the performance of chemical reactions in these confined environments has led to catalyst-containing hollow nanocapsules, so that a diffusional product/substrate exchange between the inner cavity and the bulk solution takes place in an efficient way. Thus, the design and synthesis of hollow/yolk-shell mesoporous structures with catalytically active ordered mesoporous shells can infuse new vitality into the applications of these attractive structures. Thus, the nanoreactor is the "space of nano level" (1-100 nm) where catalytic process including transport of

reactants, reaction and transport of products could be performed. The nanoreactors are characterized with some nanoscale advantages common for nanoscale materials such as elevated surface/volume ratio, unique electronic properties, huge amount of low-coordinated sites and high homogeneity. The current presentation is dedicated to the classification of the nanoreactors, methods of their fabrication and catalytic applications. The authors thank to E. Flores, F. Ruiz, E. Aparicio, P. Casillas, V. García, J. Peralta and M. Sainz for their kind technical support in this work. This project was supported by CONACyT (Mexico) and DGAPA–PAPIIT (UNAM, Mexico) through the grants 179619 and 203813, respectively.

O-019

Pt-Pd BIMETALLIC NANOPARTICLES ON MWCNT: CATALYST FOR HYDROGEN PEROXIDE ELECTROSYNTHESIS

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Keywords: Nanoparticles, bimetallic electrocatalyst, MWCNT, O_2 electro-reduction, H_2O_2 generation, electro-Fenton.

Electrosynthesis of H_2O_2 is powerful oxidizing agent, which finds applications in a wide variety of organic and inorganic synthesis reactions; also, H_2O_2 is considered a green chemical in the treatment of waste water as a replacement for chlorine. H_2O_2 is commercially produced by the Riedl–Pfleiderer process. However, the transport, handling and storage H_2O_2 are potentially hazardous. Alternatively H_2O_2 can be directly synthesized by Oxygen Reduction Reaction (ORR) in either alkaline or acidic media. There are many publications where is reported different electrode material for ORR, like carbon-based electrodes[1,2]; furthermore, addition of several metals and metal oxides to bias the activity of the oxygen reduction reaction toward the two electron transfer in ORR[3,4] is already known. Bimetallic nanoparticles of Pt-Pd were deposited by the microemulsion method on a multiwall carbon nanotube (MWCNT) to obtain a Pt-Pd/MWCNT for electrocatalytic reduction of O_2 to H_2O_2. The activity and selectivity of the catalyst was determined qualitatively by the rotating disk electrode method in acidic medium. The catalyst was spray-coated onto a reticulated vitreous carbon substrate and quantitatively was tested in bulk electrolysis for 20 minutes under potentiostatic conditions (0.5 V vs SHE) in a 0.5 M H_2SO_4 electrolyte using dissolved O_2. The bulk electrolysis experiments show that the Pt-Pd/MWCNT catalyst is more efficient for H_2O_2 electrogeneration than a MWCNT catalyst. Nitrobenzene degradation by electrogenerated H_2O_2 alone and electro-Fenton process were also tested. Our results show that both processes decompose nitrobenzene, but the Electro-Fenton process does it more efficiently. The prepared nanoparticulated catalyst shows a great potential in environmental applications.

O-020

WHITE-LIGHT EMITTING PHOSPHOR BASED IN THE COMBINATION OF RARE EARTH ACTIVATED Y_2SiO_5:Ce,Tb AND $Sr_2Si_5O_7$:Eu POWDERS

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Keywords: colloidal silica, yttrium silicate, white light and strontium silicon nitride.

Synthesis and characterization of a white-light emitting phosphor based in the combination of rare earth activated Y_2SiO_5:Ce,Tb (YSO) and $Sr_2Si_5O_7:Eu^{2+}$ (SSN) powders. The YSO was prepared by pressure-assisted combustion synthesis while SSN was prepared by solid-state reaction in N_2/H_2 atmosphere. In order to induce the formation of both X1-Y_2SiO_5 and X2-Y_2SiO_5 crystalline phases the YSO samples were post-annealed at 1100°C in 1350°C, respectively. On the other hand, the SSN powder which was prepared at different temperatures during the processing, presented the $Sr_2Si_5O_7$ crystalline phase which was verified by X-ray diffraction analysis. Photoluminescence measurements showed the contribution of a broad-band emission of Ce^{3+} ions located in the blue region of the electromagnetic spectrum, a well-defined green emission of Tb^{3+} ions with the main peak located at □$_{Em}$= 545 nm, in the YSO phosphor, and a broad-band emission in the red region due to Eu^{2+} ions in the SSN phosphor. It is noteworthy that the excitation wavelength used was in long UV radiation at 357 nm. An improvement in the luminescence properties of the YSO powders was achieved by coating the phosphor surface with colloidal silica. The absolute fluorescence quantum efficiency measurements showed an increase of around of 12% in efficiency for the silica-coted YSO in comparison to the YSO bare powders. The colloidal silica distribution and the thickness of the coating over the YSO nanocrystallites surface determine the increase in the quantum efficiency. Finally, a blend of the two luminescent powders Y_2SiO_5:Ce,Tb and $Sr_2Si_5N_8:Eu^{2+}$ were properly combined in order to obtain a white-light emitting phosphor with high color rendering index. Technical work performed by E. Aparicio, F. Ruíz, I. Gradilla and D. Domínguez is gratefully acknowledged. Financial support from CONACyT (Project No. 10555) and PAPIIT DGAPA-UNAM (Project No. 109913).

O-021

GAUSSIAN INDEX PROFILE THIN FILM LAYER CONTROLLED BY OPTICAL SPECTROSCOPY

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Keywords: Inhomogeneous thin films, optical spectroscopy of plasmas.

Inhomogeneous thin films have an important role in the new trend of thin films. Many practical limitations restricted a massive manufacturing, but even laboratory applications have been possible until recent years. A relationship between the optical properties of the film at any particular stage of process is essential. Several monitors are available, but none of them provides a real time indication of the film, which may allow us to verify, or correct, parameters during deposition. In this work we propose the use of optical spectra analysis of the light emitted by the plasma during sputtering deposition. The same idea may extend to any other plasma assisted deposition technique, e.g. pulsed laser deposition, plasma enhanced chemical vapor deposition, etc. Our goal is to get Gaussian index profile of oxynitride inhomogeneous thin films, monitoring the emission spectra of the plasma. To create changes in refractive index, we varied the flux of two gases, oxygen and nitrogen, to change film stoichiometry. The plasma was monitored with a spectrometer in the entire visible spectrum. We analyzed the spectral lines of the elements Ar, N and O, to observe their temporal evolution during the growth of the layers. Partial support from the Conacyt-Mexico project 60351 and DGAPA-UNAM projects IN100910 is acknowledged, Miss Abundiz thanks Conacyt for her scholarship.

O-022

CORRELATIVE MICROSCOPY APPLIED TO MATERIALS AND BIOLOGICAL SAMPLES

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Keywords: photon microscopy, electron microscopy, biological samples.

Historically, how photon and electron microscopy samples are processed have been different, and the simultaneous observation and analysis on the same particles or cells by these two methodologies is almost impossible in conventional microscopes. However, for the last 10 years a new type of microscopy has been created, which nowadays allows the fusion of both technologies and gives additional information, EDX elemental analysis imaging, cathodoluminiscence, for the solution of difficult problems. Currently it allows the interaction between microscope images and stereoscopes with SEM and TEM. This new technology called correlative microscopy can be applied to materials like nanoparticles, cells, tissues, rocks, bullets or bacteria, with applications in many fields, including forensic sciences.

O-023

LIGHTSHEET EXPERIMENTS IN REAL TIME

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Keywords: photon microscopy, electron microscopy, biological samples.

The needs of scientists change and grow in parallel with technological developments, sometimes towards unexpected directions. Since 2012 it is possible to perform experiments capable of maintain live cellular cultures or complex organisms in observation for long periods of time; and to monitor with high detail, growth processes, degeneration or regeneration of damaged tissues, drug expositions or nanoparticles in bacteria cultures, fungi, or virus in tissues, recording real time high definition 3D images for the study the sample evolution from the beginning and over the time. This is the science of the future, known today as Lightsheet.

O-024

SPIN ORBIT EFFECTS IN A TRIPLE QUANTUM DOT SHUTTLE

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Keywords: quantum dots, spin-orbit interaction.

Electron transport in triple quantum dot (TQD) arrays has become the subject of intense investigation recently, due to their importance as components for future quantum information systems e.g. coupled quantum bits (*qubits*). In TQD systems, charge stability diagrams have been obtained, entanglement, and interference effects in a triangular setup have also been studied; spin and electronic properties in a magnetic field have been analyzed as well. When one of the dots in the TQD system is set in motion by means of an external interaction, the system becomes a nanoelectromechanical system. Oscillating TQD's in linear array configurations have been proposed as shuttle systems, *i.e.*, the oscillating element acts as a shuttle carrying one electron from one contact to the other. In this work, we explore spin current features through a triple quantum dot shuttle (TQDS), with different Zeeman splitting in each quantum dot (QD), by using the Reduced Density Matrix master equation approach. We find that new resonances in the spin current appear due to the presence of spin-orbit interaction (SOI), and the asymmetry in Zeeman splitting. We also show that these resonances correspond to anticrossings in the energy spectrum, due to the level coupling induced by the SOI. Also, spin current polarization is analyzed as a function of tunnel coupling and detuning. For the case of an asymmetric TQDS, we show that in the weak coupling regime the device can act as a spin filter.

O-025

EFFECT OF SILVER NANOPARTICLES IN *Candida albicans*

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Keywords: Silver nanoparticles, *Candida*, antifungal effect.

Infectious diseases represent a public health challenge worldwide. Conventional antimicrobial agents are one of the factors for the development of multiple drug resistance and adverse side effects; therefore the development of new antibiotics and treatments is a global need. Candidiasis is the most common fungal disease, having a rapid increment of its prevalence. This disease is caused by the dimorphic yeast *Candida* spp., with *Candida albicans* as the main agent causing the infection. Several species of *Candida* are reported to present resistance to antifungal agents, representing a health problem that affects mainly immunocompromised patients. Silver has long been recognized for its antimicrobial effects and recently, silver nanoparticles have been reported to have antifungal properties. Therefore, in this study, we used silver nanoparticles (AgNPs) of 3-10 nm to assess their effect against *Candida albicans*. Preliminary results show high antifungal activity at very low concentrations (3.15 µg/mL), lower than those of common antifungal agents. However, the mechanism of action of AgNPs has not been truly elucidated, so more research is needed to understand the way AgNPs interact with the living cell and how to improve their use in the clinic. For that, the next step will be to determine the ultrastructural distribution of AgNPs in the fungal cell, and the effect of AgNPs in *Candida*´s clinical isolates.

O-026

A STUDY OF THE SELF-ASSEMBLY OF SUPPORTED LIPID BILAYERS ON SILICON WAFFERS BY MEANS OF ELLIPSOMETRY

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Keywords: Self-Assembly, Ellipsometry, Vesicle fusion.

The kinetics of the formation of Supported Lipid Bilayers (SLBs) from vesicle solutions was investigated using ellipsometry. The self-assembly process of the bilayer took place on silicon dioxide surfaces from 100 nm diameter 1,2-dimiristoyl-*sn*-glycero-3-phosphocholine (DMPC) and 1,2-dilauroyl-*sn*-glycero-3-phosphocholine vesicles. For DMPC, the range of concentrations studied was 0.025 to 0.380 mg/mL and the rate of the process was found to be concentration dependent and adsorption limited. Further experiments, particularly at concentrations above 0.380 mg/mL, presented evidence of net mass desorption as an intermediate step to supported SLB formation. For DLPC SLBs the apparatus used was a different one from the one used in the DMPC studies, with the new apparatus allowing for temperature control of the self-assembly process. A first study of the temperature-dependence of SLB formation is presented.

O-027

OPTICAL TRAPPING HEATING EFFECT IN LYMPHOCYTES

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Keywords: Optical trapping, cellular heating, quantum dots, CdSe.

Optical trapping is a powerful tool for manipulation and analysis of individual cells by controlling their dynamic. In this technique the particles are immobilized on gradient forces generated by a highly focused laser beam. The magnitude of these forces is too small to cause cell damage. However, heat generation can be induced by light absorption of the surrounding medium, which must be considered. In this work, we investigated the photothermal effect in optical trapped lymphocytes by using two laser wavelengths, λ_1= 820 nm and λ_2= 980 nm. The temperature was obtained indirectly from the displacement of the emission spectrum of the CdSe quantum dots. Our experiments indicate that the lymphocytes morphology keeps unchanged when using the λ_1= 820 nm laser however, it is found to be altered when we apply the λ_2= 980 nm laser at the same power of 259.5 mW. Those changes were associated with local temperature increases of approximately 7˚C. With these results we recommend to use the λ_1= 820 nm laser for cellular trapping in biological applications, but suggest that optical trapping with λ_2= 980 nm laser at a power of 250 mW or higher can be used as heater devices.

1st POSTER SESSION

P-001

EFFECT OF SILVER NANOPARTICLES IN MICROALGAE DUAL BIOREACTOR

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Keywords: bionanotechnology, microalgae, photobioreactor.

Microalgae are eukaryotic, photosynthetic microorganisms, mainly found in water ecosystems. Most of them are unicellular and they have a very important ecological role, because they can fix carbon and are in the first step in the trophic networks. Some species of microalgae are known for their great capacity to produce metabolites of research and economical interest. Microalgae are both important for their potential relevance in green energy production, such as biodiesel and, on the other hand, because they are a potential problem and source of ecological disruption when they bloom. In biodiesel production, microalgae have many advantages over other organisms, such as fast growth, lower requirements and facilities, genetic manipulation techniques, and so on. For this reason, it is very important to study and develop new procedures and techniques to improve their capacity to produce biomass, lipids or any other substance of economic interest. This work presents an approximation of the silver nanoparticles effect in the microalgae biomass production, in a hybrid photobioreactor. Overgrowth of microalgae or their presence when they are non-desired (such as in hydroponic systems) can disturb the water systems and deplete the available nutrients. Also, microalgae can produce toxic metabolites that worsen the problem and which can be toxic for human health. For these reasons, in the present work the interaction and inhibitory effect of silver nanoparticles, in microalgae cultures, is also studied.

P-002

TWO NANOSCALE SELF-ASSEMBLING BIOMORPHIC SYSTEMS: SIO_2 NANORINGS AND SIO_2-CARBONATE CRYSTALS

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Keywords: Gold complex, nanomateriales, morphology visualization, HRTEM.

In the present work SiO_2 nanorings self-assembling phenomenon consisted in the formation of biomorphic structures with size ~ 20-80 nm was discovered. This phenomenon showed different hierarchy of structure formation (separated nanorings, toroids, chains, spheres, sphere chains, spirals, loops, etc.). These nano-structures were revealed self-assembled SiO_2 nanorings (with size ~ 10 nm) impregnated with $[Au(en)_2]Cl_3$ complex. Biomorphic nanostructures observed in this work are compared with the closest analogous biomorphic systems of self-assembled SiO_2-carbonate biophorms (silico carbonates of alkaline earth compounds), for which it was found that adding proteins in the biomineralization process brings to formation of such biophorms as twisting rods, sunflowers, mitotic cells, leafs, worms, screws with size 70,000-700,000 nm were obtained in the presence of proteins. Finally, the plausible mechanisms of formation of both systems (SiO_2 nanorings and SiO_2 -carbonate crystals) are discussed.

P-003

ANALOGY OF SELF-ASSEMBLING PHENOMENON OF SiO_2 NANORINGS AND BIOLOGICAL SYSTEMS

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Keywords: Gold complex, mesoporous silica, self-assembling, biological system analog.

In recent years, the design and fabrication of hierarchically structured nanomaterials have been focused because they provide a large number of improved or new properties. While in biological systems hierarchical organization levels are well defined (e.g. nucleotides-DNA-nucleosomes-chromosomes-chromatin), in inorganic systems are currently not. In this work, we described self-assembling nano-structures of hexagonal mesoporous silica. This nanomaterial represents SiO_2 nanorings with external and internal diameters of 9 and 5 nm, respectively, and 8.5 nm in length. Structural evolution of nanorings was studied by HRTEM technique. Ethylenediamine gold complex was used for the nanoring contrast increase. The self-assembly tendencies is manifested by five-level hierarchy structure of nanorings. Revealed similarity of self-assembling of SiO_2 nanorings and biological systems is discussed.

P-004

APPLICATION OF GOLD COMPLEX AS VISUALIZATION AGENT FOR SILICA NANORINGS IN HRTEM

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Keywords: Gold complex, nanomateriales, morphology visualization, HRTEM.

The nanomateriales are attracting a great attention due to their fundamental significance and potential applications in catalysis, medicine and biology. Silica nanorings prepared with surfactant-templated synthesis have unique properties such as good thermal and chemical stability, high surface area and nanosize (< 10 nm). In the present work the following samples containing SiO_2 rings were studied by HRTEM: SiO_2, $[Au(en)_2]Cl_3/SiO_2$ (supported ethilendiamine gold complex) and Au/SiO2. Our results showed that in the cases of SiO_2 and Au/SiO2 samples, in the vast majority of images of SiO_2 were observed “shapeless clouds”, so the morphology of nanorings was not easy detectable. Unexpectedly, in the microphotographs of $[Au(en)_2]Cl_3/SiO_2$ the nanoring morphology was clearly observed. Further investigation of $[Au(en)_2]Cl_3/SiO_2$ samples revealed self-assembling phenomenon consisted in formation of complex structures with different hierarchy (separated nanorings, toroids, chains, spheres, sphere chains, loops, etc.). The obtained results showed that $[Au(en)_2]Cl_3$ complex can be used as contrasting agent for the “visualization” of nano-rings morphology and probably other nanomaterials in HRTEM studies. Application of $[Au(en)_2]Cl_3/SiO_2$ is more preferably than Au/SiO_2 and SiO_2 probably due to its bulky volume (compared with Au/SiO_2 with the same Au loading) and high contrast (compared with SiO_2).

P-005

BIOSYNTHESIS OF GOLD NANOPARTICLES BY *NEUROSPORA CRASSA* EXTRACT AND THEIR SERS PROPERTIESS

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Keywords: Biosynthesis, nanoparticles, *Neurospora crassa*, SERS.

The development of ecofriendly methods for the synthesis of metallic nanostructures has become an interest of research in several countries. The so-called "green chemistry" employs biological material to fabricate nanostructures and has the benefit of improving the biocompatibility of nanomaterial. However, to successfully compete with existing chemical and physical methods, strict control over average particle size and uniform morphology is required but still a challenge. In this work, we present the use of *Neurospora crassa* extract for the biosynthesis of gold nanoparticles of controlled size and shape. Fungal extract was

incubated with the gold precursor solution under different conditions of temperature, pH value and reaction time. Best results were obtained from incubations at 60˚C; at pH 3 we observed the formation of different shaped nanoparticles (e.g. spheres, triangles, hexagons etc.) while at pH 5.5 mostly quasi-spherical nanoparticles of 6 to 21 nm were formed. At pH 10 only small, quasi-spherical nanoparticles of 3 to 12 nm were obtained. High resolution transmission electron microscopy (HRTEM) confirmed the crystalline and elemental character of the gold nanoparticles. Furthermore, obtained nanoparticles are shown to possess excellent surface-enhanced Raman scattering (SERS) properties. Using methylene blue as target molecule it is shown that small, quasi spherical NPs of 3 to 12 nm enhance the Raman signals about 2 times, quasi-spherical NPs of 6-21 nm enhance Raman signals about 25 times and different shaped NPs in a broad size range enhance Raman signals about 40 times. Results are promising and show that these gold nanoparticles might have potential applications for biological sensing and labeling systems.

P-006

PERSPECTIVES FOR SILICON BASED LIFE

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Keywords: silicon-based life, water structure, humanity long term perspectives.

Life on Earth as well known is built upon carbon and carbon-based compounds. The possibility of different chemical foundation of life elsewhere in the Universe has been discussed. Topic of life on the base of different elements attracts attention due to long term perspective programs of humanity, which sounds too fantastic nowadays. These programs include creation of humanoids with body on the basis of different elements and consequently possessing different physical, chemical and biological properties, which could survive under very different conditions, which are too severe for nowadays human bodies. Creation of these humanoids would permit to study and populate our universe. One of the most probable alternatives to life based on carbon can be "silicon life" because carbon and silicon are chemical analogs. Effect self-assembling of SiO_2 nanorings revealed in our work demonstrates that the silicon can form self-organized structures similar to biological systems (DNA). Results showed that time and the presence of water vapors are very important factors for formation five-level hierarchy structures. There is the hypothesis, based on theoretical calculations, of the template role of water for biological system formation. Our results can be considered as experimental confirmation of these theoretical calculations. Water molecules and clusters can be templates determining the complex five-level hierarchy organization of "light" nanorings. In this case the nanorings only repeat complex water structure, which could permit to call observed effect "water-assembling" phenomenon.

P-007

INFLUENCE OF PROMOTERS ON ACTIVE STATE OF GOLD SUPPORTED ON MESOPOROUS SILICA

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Keywords: Gold catalyst, promoter, mesoporous silica, CO adsorption, IR spectroscopy.

It is well known that the catalytic activity of supported gold nanoparticles are influenced strongly by a variety of factors, such as the gold particle size, the character of its interaction with the support, the nature of active sites, and the strength of metal-support interaction, etc. The nature of different Au sites is considered as one of the most important for their catalytic activity. The electronic state of different Au species supported on Ce, Fe, La and Mg-modified hexagonal mesoporous silica (HMS) has been studied by infrared spectroscopy of adsorbed CO. Modification with promoters was performed by direct synthesis (Me-HMS) and impregnation (Me/HMS) methods. The catalytic activity of gold supported on modified HMS investigated in liquid-phase aerobic oxidation of alcohol. Experiments revealed existence of the following states of supported gold: ions Au^+, neutral metal particles Au^o and a number of partly charged states $Au^{\delta+}$ with different effective charge. IR spectroscopic measurements showed influence of promoters on the electronic state of the supported gold. The influence of electronic state of gold species varied by addition of different promoters on catalytic properties and redox pretreatments is discussed.

P-008

NANOPARTICLES MODIFIED QCM BASED SENSOR FOR HYDROLASES ACTIVITY DETERMINATION

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Keywords: hydrolases activity, QCM sensor, nanoparticles, signal amplification.

Nanoparticles as an efficient signal amplifier were deposited onto the surface of a quartz crystal microbalance (QCM) together with the enzyme substrate to create a simple biosensing platform for the sensitive hydrolases activity determination. The large nanoparticles specific mass (more than 10 times than the specific mass of the substrate itself), results in about 10-fold response increase of the QCM during the enzymatic degradation of the nanoparticles loaded substrate. Enzyme activity U and QCM frequency change with time $\Delta f / \Delta t$, recorded applying the approach subject of the present work, were correlated using the following modified Sauerbrey equation, including the mass change due to the nanoparticles release: $\Delta f = -\mathrm{K}(\Delta m_{\mathrm{NP}} + \Delta m_{\mathrm{S}})$.Taking into consideration, that: $\Delta m_{\mathrm{NP}} + \Delta m_{\mathrm{S}} = A\Delta n_{\mathrm{NP}} + M\Delta n_{\mathrm{S}}$ and $U = \Delta n_{\mathrm{S}} / \Delta t$, one can obtain: $U = -(\frac{1}{\mathrm{K}M}\frac{\Delta f}{\Delta t} + \frac{A}{M}\frac{\Delta n_{\mathrm{NP}}}{\Delta t})$, with: f – frequency, t – time, m_{NP} – mass of the nanoparticles, m_{S} – mass of the enzymatic substrate, A – atomic mass of the nanoparticles, M – molecular mass of the substrate, n_{NP} – number of micromoles of nanoparticles, n_{S} – number of micromoles of substrate, U – enzyme activity unit, and K – a constant, depending on the resonant frequency of the fundamental mode of the crystal f_{o}, the area B of the gold disk coated onto the crystal, the shear modulus μ of quartz, and the density of the crystal ρ ($\mathrm{K} = -2f_0^2 / B\sqrt{\mu\rho}$). The suggested approach was successfully applied for the determination of the activity of the enzymes lipase and trypsin, respectively.

P-009

LIPID PEROXIDATION AND PROTEIN PEROXIDATION INDUCED BY DIFFERENT NANOPARTICLES IN ZEBRAFISH ORGANS

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Keywords: Lipid peroxidation, protein oxidation, nanoparticles, oxidative stress, Zebrafish, Toxicity.

Nanomaterials have revolutionized technology. Nevertheless, they can pose a threat to the environment and the organisms because of the same nanoscale characteristics that make them useful. Nanomaterials that act as electron transfer agents have been shown to induce oxidative stress. The protein oxidation and the lipid peroxidation induced after 48 h of exposure to the different nanoparticles of europium-doped hydroxyapatite (HA:Eu), bismuth germanate (BGO), europium-doped yttrium oxide (Y_2O_3:Eu), silver nanoparticles (AgNP), and carboxylated multi-walled carbon nanotubes (MWCNT-COOH), were determined in different tissues of zebrafish (*Danio rerio*). Both oxidative stress markers showed to be dose-dependent, being higher at 1 ppm than the control experiments. Exposure to Y_2O_3:Eu and MWCNT-COOH nanoparticles produced protein oxidation values even higher than those obtained with H_2O_2 100 μM. In ovaries, testicles and brain, carbonyl content in proteins reached values up to 4-times higher than control. BGO and AgNP showed less oxidative effect; nevertheless, protein oxidation accounted for up to 3-times of the control fish values. HA:Eu had little effect, showing a maximum of two-fold in liver at 1 ppm. Lipid peroxidation values were usually less than 2-fold of those observed in control fish, except with MWCNT-COOH nanoparticles where exposure to 1ppm induced the highest lipid peroxidation in all analyzed tissues, reaching values up to four-times higher than control. In all cases, gills were the tissues less affected. On the other hand, no significant differences were found in gene expression of oxidative stress markers such as superoxide dismutase (Sod1), the transcription factor Forkhead box protein O1 (FoxO1), and the glutamate-l-cysteine ligase catalytic subunit (Gclc) after 48 h treatment. The results from this work clearly indicate that nanoparticles exposure induces oxidative stress in zebrafish organs. Nanotechnology now has the challenge of improving the nanomaterials design to prevent negative side effects.

P-010

MEMBRANES WITH $Ca(OH)_2$ NANOPARTICLES FOR THE REMOVAL OF H_2S AND CO_2 FROM BIOGAS

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Keywords: bionanotechnology, biogas, $Ca(OH)_2$ nanoparticles, membranes.

The developed of cellulose acetate membranes with $Ca(OH)_2$ nanoparticles had been improve in an anaerobic digester (AD), in order to obtain methane from biogas. It is known that cellulose acetate membrane[1], hold H_2S and CO_2 molecules, acting as a hydrophobic nanoporous membrane. Starting from organic food waste, obtained mainly from restaurant consortia, the AD produced biogas with CH_4 (70%-78%), CO_2 (28%-33%), H_2S (0.005%-2%) and others (1.995%-5%). A filter composed by a cellulose acetate hydrophobic membrane (approximated pore diameter 50 nm) with $Ca(OH)_2$ nanoparticles, was implemented for the reaction of CO_2 to H_2CO_3 and the neutralization of H_2S, to avoid environmental contamination. The AD yielded $11m^3$ of biogas daily per 100kg of organic food waste. After filtered, the biogas was acquired a lower concentration of CH_4 (92%), CO_2 (7%) and H_2S (0.0001%). The average purity of the biogas was 92%, which could be used directly as biofuel according to the regulations. By this bionanotechnological method is achieved the main purpose of biogas purification derived from food wastes.

P-011

ENHANCING OXIDATION ACTIVITY AND STABILITY OF ISO-1-CYTOCHROME C AND CHLOROPEROXIDASE BY IMMOBILIZATION IN NANOSTRUCTURED SUPPORTS

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Keywords: Chloroperoxidase, Cytochrome c, Immobilization, Kinetic stability, Nanostructured sopports.

The immobilization of enzymes in inorganic materials has been widely used because it can produce an enhancement of the catalytic stability and enzymatic activity. In this article, the effect of the immobilization of iso-1-cytochrome c (CYC-Sc) from Saccharomyces cerevisiae and chloroperoxidase (CPO) from Caldariomyces fumago on the enzyme stability and catalytic oxidation of styrene was studied. The immobilization was carried out in three silica nanostructured supports with different pore size MCM-41 (3.3 nm), SBA-15 (6.4 nm) and MCF (12.1 nm). The adsorption parameters and leaching degree of immobilized enzymes were determined. Catalytic parameters of immobilized and free enzymes were determined at different temperatures (20–60°C) and in different acetonitrile/water mixtures (15–85% of acetonitrile).The results show that there is low leaching of the enzymes in the three supports assayed and the adsorption capacity (qmax) was higher as the pore size of the support increased. The pore size also produces the enhancement of peroxidase activities on the styrene oxidation. Thus, CPO adsorption into SBA-15 and MCF showed remarkable thermal and solvent stabilities at 40 °C showing a total turnover numbers of 50 times higher than free CPO in both supports. The enhancement of activity and stability doubtless is interesting for the potential industrial use of peroxidases.

P-012

USE OF TYPE III SECRETION SYSTEM FROM ENTEROPATHOGENIC *ESCHERICHIA COLI* AS NATURAL NANO-MACHINE TO DELIVER THERAPEUTIC PROTEINS INTO EUKARYOTIC CELLS

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Keywords: Injectisome, T3SS, EPEC, bacterial vectors, vaccine carriers, drug delivery.

Enteropathogenic *Escherichia coli* possess a pathogenicity island called the locus of enterocyte effacement (LEE) which encodes structural components of a type III secretion system (T3SS) among other genes. T3SS or injectisome is employed by the bacteria as a molecular syringe to translocate effectors into the host cell to subvert normal host cell functions to benefit of bacteria. The use of live attenuated bacteria as carriers for recombinant vaccination strategies has been partially successful. Taking advantage of heterologous expression of EPEC LEE genes in commensal *E. coli* strains offers the opportunity to express and deliver therapeutic proteins into host cells avoiding effector translocation. Accordingly, we designed chimeric proteins recognized by T3SS as substrates that can be delivered into epithelial cells. Our aim is the employment of optimized delivery strategy of heterologous proteins for therapeutic purposes. Advantages and challenges of our dual heterologous expression system of both T3SS and chimeric therapeutic proteins are discussed.

P-013

NANOPOROUS MEMBRANES AND COATINGS

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Keywords: Bionanotechnology, biomedicine, nanoporous membranes, coatings.

This is an overview of nanoporous membranes for biotechnologycal applications. Nanoporous substrates and coatings distinguished by their large surface area have recently captured attention in different range of applications, including release and transport of drugs, gas purification, electronics and biotechnology. Nanoporous materials can be described as materials with pore sizes less than 100 nm. Recent advances in nanoscience have made it possible to fabricate by synthesis methods precisely control morphology, pore size, pore density and distribution. The acquired physical and chemical properties of the pores in nanoporous materials make them increasingly attractive for regulating and sensing transport at the molecular level. Technics such as track etching, lithography for organic polymeric membrane, anodization, sol-gel and microfabrication are some of the most used for nanomaterial synthesis. Nanoporous materials such as silicon grids (SiO_2), aluminum oxide (Al_2O_3), Nafión®, titanium oxide (TiO_2) and porous silicon are shown with illustrative examples. Despite the huge research about synthesis, characterization, and functionalization of nanoporous materials, there are still several issues that must be solved in order to create effective synthetic nanoporous systems.

P-014

ENCAPSIDATION OF DNA PLASMIDS BY THE CCMV CAPSID PROTEINS

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Keywords: CCMV, DNA.

The cowpea chlorotic mottle virus is an RNA icosahedral virus, which under certain conditions of pH and ionic strength have been disassembled and reassembled in vitro. In this work we analyze the self-assembly of CCMV protein around DNA molecules, which are stiffer than its RNA genome. We used two dsDNA plasmids, one of approximately 3000 bp and the other of 4700 bp, and a linear DNA plasmid with about 5500 bp. Gel electrophoresis was performed to determine optimal conditions for assembly and the assemblies were observed by TEM. For all experiments, the assemblies were done at pH 7.2. For circular DNA assemblies, we obtained spherical capsids with similar diameters to those found for the wild type virus, around 28 nm. In the case of the linear plasmid, we observed spherical capsids too with a diameter of 22 nm and some tubes.

P-015

ENTERAL ADMINISTRATION OF BILE SALT-PHOSPHATIDYLCHOLINE MIXED MICELLES LOADED WITH CLONAZEPAM IMPROVES THE ANTICONVULSANT RESPONSE IN PENTYLENETETRAZOLE-INDUCED SEIZURES IN MICE

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Keywords: Mixed micells, anticonvulsant effect, nanoparticulated pharmaceutical formulations, mixed micells, therapeutic activity, myoclonus generalized seizures, pentylentetrazole induced seizures.

In recent years nanotechnology has changed the functionality of various materials to offer new alternatives to current challenges. One of the exemplary cases is medicine, where it is desired to design new medicines more efficient and with lower side effects. In this work, the anticonvulsant effectiveness of clonazepam (CLZ) loaded in bile salt – phosphatidilcholine mixed micelles (MM, CLZ-MM) administered by enteral route (oral, p.o.) in mice (swiss webster) was investigated. Doses of CLZ and CLZ-MM at 0.01, 0.03, 0.1, 0.3 mg/Kg were administered by p.o. route to assess its anticonvulsant effect on pentylentetetrazole (PTZ) induced seizures (80 mg/kg, i.p.) The occurrence of myoclonus, generalized seizures and tonic convulsions or mortality induced by the convulsant agent PTZ was registered, statistical evaluation of latencies to seizures were evaluated as means by ANOVA and T Student tests (SigmaStat® SPSS). The size, zeta potential, shape and composition of mixed micelles were analyzed by transmisson electron microscopy, high-performance liquid chromatography and differential scanning calorimetry. CLZ-MM of 22± .59 nm diameter, a zeta potential value at -28.65 ± mV, a spherical shape without drug crystal formation, an entrapment efficiency of 48.7% (w/) and drug loading of 7.3% (w/w) were obtained for this pharmaceutical formulation. A higher anticonvulsant effect on generalized and tonic seizures was obtained with CLZ-MM at 0.1 mg/kg. This carrier system could reduce side effects and is a proposal to improve efficiency of the drug dosage. These experiments are evidence that nanoparticulated pharmaceutical formulations offer several advantages in the transport of drugs to enhance their therapeutic activity.

P-016

SYNTHESIS OF HEMATITE A–FE$_2$O$_3$ NANOPARTICLES USING THE CONTROLLED PRECIPITATION METHOD

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Keywords: nanoparticles, controlled precipitation method, hematite, MEB, FT-IR, Raman.

Magnetic nanoparticles show several interesting properties that can be used in applications such as catalysis and biomedicine. Among them, iron oxides are currently under investigation. Applications are known in the industry as an agent for paintings and polishing. Recently, medical applications have been found for this material in the treatment of brain tumors. It is also used in the treatment and recovery of catalysts. [1] This paper describes the synthesis of hematite nanoparticles by controlled precipitation method MPC. The synthesis was carried out in 3 stages: precipitation, washing and heat treatment. Aliquots were taken at different time intervals and thermal treatment in order to observe the formation of the crystalline structure [2].

Some samples were observed using metallographic microscope also observed by scanning electron microscope (SEM), surface morphology and samples were analyzed by FTIR and Raman spectroscopy with through which spectroscopic signals (peaks in the Raman spectrum) was evident formation α-Fe2O3 hematite. This material was analyzed and observed by FTIR, Raman spectroscopy and SEM respectively. This synthesis of nanostructured metal oxides is important not only for the results but also by the application that has this type of nanoparticles. It is also the first synthesis of this type developed in UTTT University, impacting positively on the motivation of TSU students in nanotechnology.

P-017

IN VITRO TOXICITY OF MULTIWALL CARBON NANOTUBES ON RESPIRATORY TISSUE

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Keywords: carbon nanotubes, bronchial epithelium, inflammation.

The constant development of new nanomaterials with different compositions has increased its use in science and technology, as in the case of carbon nanotubes, the need to assess the toxicological risk of these materials considering the different allotropes that can form and many of them new in the environment is crucial for the development of regulatory policy. In this study, the effect between exposure to carbon nanotubes obtained by microwave and amorphous carbon, in rat bronchial cells and alveolar macrophages was compared. For this purpose, individually cultured and co-cultured, bronchial cells obtained by primary culture and alveolar macrophages obtained by broquial lavage, were exposed to different nanomaterials. To determine the cytotoxicity, cell viability was measured by the MTT assay and for inflammation reaction levels of TNF-α and IL-6 was measured. The results show that during 24 hours of exposure there was no significant inflammatory response or cytotoxicity. Results demonstrate that these materials are of low biological reactivity, however not exclude the possibility that they are toxic, particularly in respiratory tissue, by impactation or deposition phenomena.

P-018

SYNTHESIS, CHARACTERIZATION AND ANALYSIS OF BIOCOMPATIBILITY OF STAR-SHAPED GOLD NANOPARTICLES

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Keywords: gold nanoparticles, nanotheranostics, electron microscopy.

Engineered nanoparticles have diverse applications in biomedicine, as diagnostics, image contrast agents, nanosensors and drug delivery systems. Anisotropic metallic nanoparticles possess potential applications in cell imaging and therapy+diagnostics (theranostics), but controlled synthesis and growth of

these anisotropic or branched nanostructures has been challenging. Star-shaped gold nanoparticles were obtained through a seed mediated route using 2-[4-(2-hydroxyethyl)-1-piperazinyl] ethane-sulfonic acid (HEPES) as a precise shape-directing agent. Morphology of gold nanoparticles was obtained by ultra-high resolution FE-SEM (HITACHI S5500) and aberration corrected atomic resolution TEM/STEM (JEOL ARM-200F) to obtain a detailed characterization of nanostructure and atomic arrangement. Nanoparticles showed absorbance centered into NIR region (700nm), dynamic light scattering and zeta potential showed a narrow size distribution (80 nm), monodispersity and high colloidal stability. Interaction of star-shaped gold nanoparticles (35-350 µg/ml) with *in vitro* cultured macrophages showed that after 24 h there are no signs of cytotoxicity, as viability remained at 94±1% even at highest concentration used. FE-SEM imaging techniques helped to analyze adsorption and uptake of gold nanoparticles. Gold nanostars showed to be biocompatible and efficiently adsorbed and internalized by cells, as revealed by advanced FE-SEM and backscattered electron imaging of complete unstained uncoated cells. Additionally, low voltage STEM and X-ray microanalysis revealed the ultra-structural location and stability of nanoparticles after endocytosis with high spatial resolution. Star-shaped gold nanoparticles have demonstrated their applications in biomedicine for SERS applications, thermal-ablation and nano-theranostics.

P-019

SYNTHESIS AND CHARACTERIZATION OF MAGNETIC NANOPARTICLES COATED WITH MESQUITE GUM AND GUM ARABIC

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Keywords: Mesquite gum, magnetic nanoparticles, colloidal stability, DSL, XPS, FTIR.

Mesquite gum (MG) (*Prosopis spp*) is a highly branched polysaccharide considered as a type II proteic arabinogalactan (AGP). This molecule has been studied to deepen the existent knowledge about the relationship between its structure and functional properties to be compared with gum Arabic (GA), which is another widely used AGP in pharmaceutical and food industry. Both molecules are quite similar regarding structure and chemical composition. The importance of magnetic nanoparticles (MNP) resides in the potential applications in biomedical sciences as contrast agents for nuclear magnetic resonance (RMN), and controlled drug delivery systems. Despite the great amount of advantages that MNP´s present, they need to be coupled with other molecules to improve their stability, functionality, and biocompatibility in a colloidal system. GA has recently attained this purpose with favorable results. The structural conformation and stabilizing properties of GM suggests that this molecule could be used to stabilize magnetic nanoparticles (MNP). In this work, we present Mesquite gum as an alternative MNP stabilizer as a substitute for gum Arabic. The synthesis of magnetic nanoparticles by chemical coprecipitation and surface modification, with both MG and GA, was successfully achieved. The resulting nanoparticles were characterized by dynamic light scattering (DLS), X-

ray photoelectron spectroscopy (XPS), and Fourier transform spectroscopy (FTIR). Dynamic light scattering showed an average radius of 103 nm for MG and GA coated magnetic nanoparticles. MG, GA, and MNP´s identities were observed by FTIR. XPS spectrum confirmed the presence of magnetite due to the clear appearance of Fe $Sp2_{1/3}$ and Fe $Sp2_{1/2}$ peaks. The N (E) values obtained for the C 1s region provided evidence of the presence of MG and GA gums in the MNP. The presented results let us conclude that both GA and MG has successfully adsorbed in the MNP surface.

P-020

RELEASE OF AMOXICILLIN FROM SUBMICRO/NANOSTRUCTURE OF POLYANILINE/L-GLUTAMIC ACID

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Keywords: Polyaniline, L-glutamic acid, Amino Acids, biomolecule, Amoxicillin.

Polyaniline (PANI) is an important conducting polymer, which has been the focus of much research in recent years because of its low cost, its good intrinsic properties such as conductivity, good environmental stability in its conductivity state, easiness of synthesis and its use in a wide range of applications. In the last five years PANI nanofibers have been considered suitable for applications in the field of nanoscience and nanotechnology based on the combination of the morphology and the chemical and physical properties of this polymer. A variety of methods have been reported for preparing PANI nanofibers through routes based on the chemical-oxidative polymerization and physical methods, for example the electrospining technique, polymerization *in situ* hard- and soft-templates, among others. Some applications of PANI nanofibers include its use in ion-exchange membranes, electromechanical prototypes, chemical sensors, biosensors and controlled drug release devices. The application of PANI in the biomedical field is supported by the possibility of preparation in nanodimensional structures with different geometries, which provides a versatile platform specifically for the detection of diseases and controlled drug release devices. Recent investigations have reported the incorporation of simple amino acids to polymeric nanostructures for promoting the functionalization and biocompatibility of the material which in turn enhances the interaction drug-nanostructures for subsequent controlled release. The present work reported the synthesis of PANI nanostructures in the presence of L-glutamic acid. The amino acid is used in order to increase the biocompatibility and the binding ability of PANI nanostructures to bioactive molecules as drugs, which favors their application in the area of investigation. The extent of amoxicillin release from PANI/glutamic acid hybrid was studied in various pH solutions.

P-021

SYNTHESIS OF CORE-SHELL PHOTONIC COLLOIDAL CRYSTALS MADE OF PMMA/PHA/PAA

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Keywords: Core-Shell, Photonics, Crystals, Polymers, Bottom-Up, Colloids, Microspheres, Photonic band gaps.

A photonic crystal is a material whose essential feature is the periodicity in its refraction index. As long as the behivour of the electrons obey the Schrödinger equation, the photons are a different story; they obey to the Maxwell equations. Hence, there is an analogy between the crystalline potential effect on electrons and the periodic variation in the refraction index on photons. In a classic crystal, the periodicity in the atomic potential impacts into the electron propagation itself, appearing permitted and prohibited bands. The last ones are energies whose electrons cannot spread in some crystal directions. In a photonic crystal something similar happens, the existence of periodicity on refraction index causes an interference of different diffracted waves by crystalline planes, either constructive or destructive to some directions and some energy. Resulting in a new band gaps but now they will be called photonic band gaps. It's quite interesting the possibilities to mold the wavelengths flow to give technological applications whose go since better laser efficiency to healthcare applications. Nevertheless it is quite interesting also the nature of the colloidal crystals to form photonic crystal films (bottom-up). In order to obtain polymeric colloidal crystal films, latex microspheres having 280~400 nm size range and narrow distribution were prepared by emulsion polymerization. Microspheres of methyl methacrylate (MMA) core and elastomeric hexyl acrylate (HA)/acrylic acid (AA) shell, were synthesized. A vertical and horizontal method was used for the self-assembled colloidal crystals films to reflect selective wavelength range of visible light. The 3D structures of colloidal crystals were characterized by Atomic Force Microscopy (AFM). For the reflectance measurement, a fiber optic UV-Vis spectrometer was used.

P-022

SYNTHESIS AND EVALUATION OF NANOSTRUCTURES ELECTROCATALYST FOR FUEL CELLS

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Keywords: Hydroxiapatite, Carbon Nanotubes, β-Cyclodextrin, Simulated Body Fluid.

In recent years, Direct methanol fuel cells (DMFCs) have received a lot of attention as the promising power sources for portable electric devices due to high energy density, simple and easily handled structure, easy transportation and storage of cheap liquid fuel as well as low temperature operation. The electrochemical reduction of oxygen, and methanol oxidation are very important reactions in electrochemistry due to central role in fuel cells. The activity improvement of the oxygen reduction reaction (ORR) represents one of the important issues in fuel cell development. Efforts to this fact have involved the utilization of bimetallic catalysts to increase the catalytic activity and to reduce cost. On other hand, the methanol oxidation reaction involves higher catalytic activity and selectivity for avoid side reactions. This work shows the synthesis of composites of metallic nanoparticles based on platinum on multiwall carbon nanotubes (MWCNTs) by the reverse microemulsion method for application as electrocatalysts in Direct methanol fuel cells. Figure 1 shows the linear voltammograms of the catalytic activity for ORR of the metal electrocatalyst Pt/MWCNT and bimetallic electrocatalysts Pt-Au, Pt-Pd, Pt-Ru and Pt-Ir on MWCNTs. The results in this figure show the current density for Pt-Pd/MWCNTs, Pt-Ru/MWCNTs and Pt-Ir/MWCNTs are much higher value than Pt/MWCNT and Pt-Au/MWCNTs, which suggests a high ORR activities, for hence these materials can be a good cathode electrocatalysts. The selection of the best electrocatalysts at anode and cathode leads to a better performance on methanol fuel cells.

P-023

CATIONIC NANOGELS WITH POLYETHYLENE GLYCOL (PEG) SHELL BY “SOAP LESS” EMULSION POLYMERIZATION

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Keywords: Nanogels, emulsion, cationic polymers, polyethylene glycol.

Nanogels are nanosized polymer networks swollen in a liquid, i.e. water. Nanogels that respond to certain pH changes as their volume have gain great importance do to the fact that tumor tissues are known to show slightly acid pH compared to healthy tissues. Therefore pH sensitive nanogels are good candidates for biomedical applications, for example, for pH triggered drug delivery. In this project a synthetic approach has been established for the preparation of nanogels formed by a pH responsive core of poly(*N,N*-diethylaminoethyl methacrylate) (PDEAEM) and a shell of the biocompatible polymer polyethylene glycol (PEG). Polymeric nanomaterials, in particular those containing PEG as coating, have gain great interest as biomaterials since the so called “PEGylated” biomaterials, are provided with a layer of “invisibility” against the immune system increasing the mean lifetime of nanocarriers in the bloodstream. The methodology used for the synthesis was the “soap-less” emulsion polymerization, i.e. an emulsion polymerization reaction without surfactant, where a methacrylate functionalized PEG (PEGMA) acts as stabilizer for the monomer droplets while it was incorporated by free radical reaction as shell over the PDEAEM nano-particle. For stabilizing the polymeric nanoparticles and giving them their network structure, three different crosslinkers were tested: ethylene glycol dimethacrylate (EGDMA), *N,N´*-bis-acrylamide (BIS), and a divinylacetal compound (DVA). Dynamic light scattering results show that the average diameter of the nanogels decreased from 274 nm down to 73 nm with increasing PEGMA content in the recipe, while maintaining a narrow size distribution. Under similar synthetic conditions the crosslinker type affects the average diameter and the size distribution of the nanogels. All prepared nanogels show a Zeta potential in deionized water of +4 mV evidencing that they are cationic. It was shown that adjusting the synthetic conditions, cationic nanogels with a PEG-shell can be prepared adjusting their diameter and ratio of PDEAEM-PEG.

P-024

REDUCTION OF Cu^{2+} IN THE PRESENCE OF Ag^{+} IN NATURAL CLINOPTILOLITE: STRUCTURAL CHARACTERIZATION

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Keywords: Natural clinoptilolite, Cu/Ag bimetallic system, EXAFS.

Modified zeolites with cations, clusters and metallic nanoparticles are of interest due to the possibility to develop materials with new properties. They can be used for different applications as catalytic materials, drugs and bactericides. Among other metals, Cu and Ag are of great interest due to both catalytic properties and olygodynamic activity [1]. The properties of the modified zeolites depend on the type of metallic species, their oxidation state, and their aggregation (or size), as well as their stability. We present a study concerning the thermal reduction under hydrogen flow of natural clinoptilolite from Tasajeras deposit, Cuba, exchanged with mixed Cu^{2+} and Ag^{+} bimetallic system. The study was conducted to analyze the influence of silver in the reduction of Cu^{2+}. Samples of Cu/Ag bimetallic system supported on natural clinoptilolite (CLI) were prepared by simultaneous ion exchange, and reduced in a H_2 flow at selected temperature. X-ray absorption spectroscopy experiments (XANES and EXAFS) were performed in beamline EXAFS2 LNLS, Campinas, Brazil in transmission mode. A double monochromator crystal Si (111) was used to vary the energy around the Cu K absorption edge (8979 eV). The energy calibration was made using metallic Cu. For the qualitative and quantitative analysis of XANES and EXAFS spectra CuO, Cu_2O and Cu standards were used. EXAFS spectra were reduced using the standard procedures by means of the Atenas software [2]. The results show that the presence of silver lowers the temperature and reduction of Cu^{2+} affects the aggregation of small metallic particles. EXAFS studies complement the results obtained by XRD and UV-Vis [3,4], and allow for new evidence on the formation of clusters and nanoparticles as a result of this reduction. The reduction of Cu^{2+} in the presence of silver can be an alternative for controlling the size of the resulting copper nanoparticles. This work was supported by the Brazilian Synchrotron Light Laboratory

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P-025

NATURAL IRON-EXCHANGED CLINOPTILOLITE AND MORDENITE: PREPARATION AND CATALYTIC ACTIVITY IN NO REDUCTION

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Keywords: Natural zeolite, Mordenite, Clinoptilolite, NO reduction, Iron.

In this work the preparation of different iron/zeolite samples through ion exchange of aqueous solutions of Fe^{2+}, Fe^{3+}, and Fe^{2+}/Fe^{3+} mixtures with natural clinoptilolite and mordenite from Cuban deposits Tasajeras and Palmarito de Cauto, respectively, as well as the test of their catalytic activity in NO reduction with CO/C_3H_6 mixture are presented. The obtained results showed that Fe^{3+} exchange is more favored than Fe^{2+} exchange for both zeolites. As a result of the ion exchange the surface area of both zeolites increases. All iron exchanged samples have higher catalytic activity in NO reduction than the starting natural zeolites. For both zeolites, the Fe^{2+}-only exchanged samples have higher catalytic activity than the Fe^{3+}-only or Fe^{2+}/Fe^{3+}-mixed exchanged samples. It was proposed that active centers of NO reduction are linked with divalent iron. We would like to thank E. Aparicio, E. Flores and J. Peralta for the technical support, and acknowledge granting by CONACYT (102907, 179619) and DGAPA (207511, 203813) Projects.

P-026

SYNTHESIS OF POLY (N-ISOPROPYLACRYLAMIDE) FOLIC ACID FUNCTIONALIZED

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Keywords: smart polymer, raft, poly NIPAAm, folate, bioconjugate.

The folate receptors are abundant form in cancer cells, since these have a very important requirement of folate for DNA synthesis [1]. A number of studies demonstrate that drug transporters nanosystems superficially decorated with folate ligand moieties show a very high affinity for tumor cells versus normal cells [2-4]. Development of chain transfer agents containing biomolecules is very important for obtaining smart polymers. One of the major branches of smart polymers is temperature sensitive polymers, or thermosensitive polymers. Poly *N*-isopropylacrylamide (PNIPAAm) is one of the most important thermosensitive polymer and of greatest interest, because its phase transition temperature its 32.8 ˚C, is close

to the physiologic temperature [5]. In this work, we prepared PNIPAAm containing folic acid using reversible addition-fragmentation chain transfer polymerization (RAFT). This polymerization method uses a chain transfer agent (CTA) to control molecular weight and polydispersity. Specifically, this synthesis involves a CTA containing a carboxylic end group and then makes the coupling of folic acid. Another important aspect of this work is the determination of the lower critical solution temperature (LCST) of folic acid-functionalized PNIPAAm, which is of fundamental importance in the potential biomedical application. Some polymer therapeutics can be functionalized using this strategy, and this approach is highly versatile for functionalizing RAFT polymers. To date, few transfer agents that incorporate biomolecules in structure and few polymers that can be vectorized.

P-027

SILICA- COATED MAGNETITE NANOPARTICLES FOR DNA MAGNETIC PURIFICATION

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Keywords: Silica, Magnetite, DNA, Magnetic purification.

Silica (SiO_2)/ magnetite (Fe_3O_4) core-shell nanoparticles were synthetized to allow rapid magnetic separation of DNA from biological samples. Fe_3O_4 magnetic cores were prepared by the aqueous co-precipitation of $FeCl_3 \cdot 6H_2O$ and $FeC1_2 \cdot 4H_2O$ with addition of ammonium hydroxide. The results reveal that the magnetic nanoparticles are crystalline with narrow size distribution. Also a sequential method has been used to prepare spherical silica nanoparticles using ultrasonication by sol–gel process. The silica particles were obtained by hydrolysis of tetraethyl-ortosilicate (TEOS) in ethanol medium. Particles in the range 100-300 nm were synthesized. Finally, a systematic investigation of the formation of silica- coated magnetite particles using ultrasonication via sol– gel approach. Silica, magnetite and silica coated magnetite nanoparticles were examined under scanning electron microscopy (SEM), atomic force microscopy (AFM), transmission electron microscopy (TEM), X- ray diffraction (XRD) and X- ray photoelectron spectroscopy (XPS). Silica/ magnetite surface area and mesoporosity were also analyzed using the Brunauer- Emmett-Teller (BET) isotherm. Core-shell solid phase adsorbent was tested for DNA extraction from E.Coli bacteria. The results show that the DNA templates displayed single bands and A260/ A280 ratios within 1.60– 1.72. These nanoparticles are reusable, non- toxic and have great effectiveness on DNA purification. The authors acknowledges to M.C. David Dominguez, Ing. Israel Gradilla Martínez, M.C. Martha Eloisa Aparicio Ceja, Sr. Francisco Ruiz Medina. Also acknowledges to Coordinación de la Investigación Científica- UNAM through a grant IN207511 for their economic support.

P-028

DEVELOPMENT AND CHARACTERIZATION OF POLYDIMETHYLSILOXANE NANOCOMPOSITE

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Keywords: nanocomposite, polidimethilsiloxane, silica nanoparticles, nanoindenter.

One unique application of polymer nanocomposite is the structural material for building nanoscale microfluidics, but when the material is required to perform in complex microfluidics systems which are commonly integrated in bioMEMS and lab-on-a-chip (LOC), the requirement for the stiff and other properties is higher. In this project, the focus is on the development of the capability of silicone nanocomposite materials to deliver the desired properties as specified by the researchers who use it as structural material for building the microfluidic devices. We used the traditional and simplest method for preparing polymer/silica nanocomposites that is the blending, what is direct mixing of the silica nanoparticles into the polymer. The main difficulty in this traditional method is always the effective dispersion of silica in the polymer matrix, because they usually tend to agglomerate. We implemented and compared two methods for dispersion, by surface chemical and physical modification of the nanoparticles to improve the dispersion in the polymer matrix. The chemical method used is modify with silane coupling agents, the functional group reacts with hydroxyl groups on the silica surface. The physical method used is treated silica nanoparticles with CTBA, this surfactant reduced interaction between the silica particles within agglomerates. The dispersion of particles in the polymer matrix has a significant impact on the properties of nanocomposites, sometimes the nanocomposite presents cluster of particles and exhibit properties even worse than conventional polymer systems, which we demonstrate using nanoindentaction test as approach to gather comparative elastic modulus and hardness data for the polymer composite systems. Also, we characterize the size and shape of the particles present in the nanocomposite system to confirm the manufacturer supplied data.

P-029

EVALUATION OF FINE PARTICULATE MATTER ($PM_{2.5}$) AND ULTRAFINE PARTICULATE MATTER ($PM_{0.1}$) IN THE AIRSHED OF TIJUANA, BC - SAN ISIDRO, CA. BORDER

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Keywords: Nanoparticles in air, Fine and Ultrafine particles in air, USA-Mx border pollutants.

The location of the Tijuana-Rosarito-San Diego within the same air basin has generated implications deteriorating air quality. Epidemiological studies on health concluded that high concentrations of particulate matter (aerodynamic diameter ≤ 2500 and ≤ 100 nm) is associated with increased mortality and morbidity (1, 2). Recent studies indicate that the levels of $PM_{2.5}$ and $PM_{0.1}$ in urban air show a high correlation with carbon monoxide (CO) and black carbon (BC) which are associated with vehicle emissions (3). This study presents the results of the evaluations performed in 3 simultaneous monitoring sites in Tijuana, México, and 3 monitoring sites in San Ysidro, USA, during the Calmex campaign in 2010. Preliminary results allow us to consider that the airshed of the Tijuana-San Diego region can be described as a funnel basin in which the prevailing winds during the day moving from northwest to southeast, causing a drag of air pollutants in the same direction and this is reversed at night. The average values of $PM_{2.5}$ and $PM_{0.1}$ in the reference site located in Playas de Tijuana are 4.14 $\mu g/m^3$ and 1648.91 pt/cm^3, respectively. Average $PM_{2.5}$ values show the same trend as BC, ie daytime highs and nighttime low levels. BC levels are up 10-20% compared to the levels of $PM_{2.5}$ and this relationship is consistent with other studies that evaluated air quality by mobile sources. Correlation between levels of BC and $PM_{2.5}$ indicate that probably generating emission sources are the same. Presented in UABC levels are approximately double those shown in Tijuana Technological University. Levels of $PM_{0.1}$ presented at both sites were higher in daytime, which indicates that probably the biggest contribution is from mobile sources. In UABC. High levels were observed at 13:00-14:00 and 02:30-03:30 hrs. due to plentiful arriving and departed aircrafts those times in the city's airport.

P-030

SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF HYDROXYAPATITE-WOLLASTONITE BIOCOMPOSITES, PRODUCED BY A SOL-GEL ROUTE

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Keywords: Hydroxyapatite, wollastonite, sol-gel, biocomposites.

Hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$, is a type of calcium phosphate-based material with great interest for biomedical applications, due to the chemical similarity between hidroxyapatite and the mineral part of human bone. This chemical similarity with appropriate porosity and crystallinity permits direct chemical bonding between bone and hydroxypatite. However, hydroxyapatite is brittle and relatively weak when compared with common implants such as metals, alloys and high strength ceramics. The best use of hydroxyapatite in load bearing implant applications is as a coating of one of those implant surfaces. In the present work, a composite of hydroxyapatite-wollastonite was synthesized by a sol-gel route, using calcium nitrate and ammonium phosphate as precursors immersed en aqueous medium and high purity natural wollastonite as reinforcement element. This composite was characterized by thermal analysis, X-ray diffraction, FT-IR and scanning and transmission electron microscopic techniques. Formation of hydroxyapatite occurs at a relatively low temperature of about 350°C. The characterization techniques demonstrated the synthesis of stoichiometric hydroxyapatite-wollastonita biocomposites as a final product.

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P-031

COMPARATIVE STUDY OF GOLD CATALYSTS IN CO OXIDATION AND NO REDUCTION UNDER LEAN BURN CONDITIONS

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Keywords: Gold catalysts, NO reduction, CO oxidation, Lean burn conditions.

The catalytic reduction of nitrogen oxides in the presence of oxygen has been one of the most important scientific challenges during the last few decades. Nowadays gold catalysts have attracted the interest of many researchers due to their high catalytic activity in reactions as NO reduction with CO and hydrocarbons under lean burn conditions. The aim of this work was a comparative analysis of several gold catalysts supported on metal oxides in order to reveal the role of the support nature in these reactions. Gold catalysts were prepared by gold deposition-precipitation on commercial oxides (CeO_2, ZrO_2, Al_2O_3, La_2O_3 and MgO) and mixed oxides synthesized by sol-gel technique (Al_2O_3, $Al_{1-x}Ce_x$ and $Al_{1-x}[CeZr]_x$). Pre-oxidized catalysts were tested in NO reduction and CO oxidation in a reaction mixture consisting of NO + CO + C_3H_6 in oxygen excess (λ=26), with a space velocity of 60,000 h^{-1}. Gold NPs supported on mixed oxides were characterized with higher activity, particularly in NO reduction. In contrast with catalysts supported on commercial oxides, gold over synthesized supports showed activity in NO reduction at low temperature (less than 100 ^{o}C). This effect could be attributed to the synergetic effect in mixed oxides used as supports. The authors thank to E. Flores, P. Casillas, V. García, F. Ruiz, E. Aparicio, M. Sainz and J. Peralta for their kind technical support in this work. This project was supported by DGAPA–PAPIIT (UNAM, Mexico) and CONACyT (Mexico) through grants IN207511, 203813 and 179619, respectively. E. Vargas is grateful for CNyN for grants IMPULSA UNAM and CONACyT (Project 50547).

P-032

VALERIC ACID KETONIZATION: GAS-CARRIER EFFECT ON THE CATALYTIC ACTIVITY AND REACTION MECHANISM

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Keywords: decarboxylation, carboxylic acids, mechanism, gas-carrier effect.

Organic acids are the largest group of the promising biomass derivatives, which are usually synthesized by fermentation and/or chemical transformation of glucose obtained by biomass hydrolysis.

Carboxylic acids can be converted into ketones by catalytic decarboxylation of two acid molecules with carbon dioxide and water as by-products over metal oxides [1, 2]. One-pot mode of carboxylic acid decarboxylation coupling followed by ketone hydrogenation into alkane over Pt(Pd)/M_xO_y bifunctional catalyst can be considered as a more attractive way to produce green diesel components (Fig.1). Although acid decarboxylation is typically carried out in inert atmosphere, consideration of ketonization as a part of one-pot technology requires studying catalytic behavior of metal oxides in an acid ketonization under hydrogen gas atmosphere. The aim of our work was to study catalytic activity of mono metal oxides ZrO_2, CeO_2, and bimetallic oxides CeO_2/ZrO_2 with varied CeO_2 loading in valeric acid ketonization carried out in hydrogen and nitrogen atmosphere. Using HRTEM, XRD, FTIR *in situ*, UV-Vis *in situ*, XPS *ex-situ*, and low temperature N_2 physisorption techniques structural and electronic changes in the state of the oxides being exposed to the corresponding gas-carrier were identified to interpret catalytic behavior. Additionally, FTIR *in situ* and UV-Vis *in situ* were applied to find a feasible mechanism of carboxylic acid ketonization. Thus, the process was occurred with high conversion and selectivity over ZrO_2 and (5-20%) CeO_2/ZrO_2 while neat CeO_2 showed very low valeric acid conversion regardless gas atmosphere (Table1). Insertion of inactive ceria into zirconia led to the notable increase of valeric acid conversion. Using XRD, HRTEM and XPS data for 10%CeO_2/ZrO_2 the reasons for increasing catalytic activity were proposed to be a solid solution formation with uniform cerium distribution, higher Lewis acid site content and the formation of a highly defective surface [3]. The research work was partly supported by Special Russian Federal program on scientific and educational staff for innovative Russia #8530, CONACyT (Mexico) grant 179619 and DGAPA–PAPIIT (UNAM, Mexico) grant 203813.

P-033

INFLUENCE OF THE OBTAINING PROCESS IN THE STRUCTURAL AND DIELECTRIC PROPERTIES OF THE DOPED KNN SYSTEM

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Keywords: Piezoelectricity, 77.65.-j, Piezoelectric Ceramics, 77.84.Dy, Permittivity, 77.22.Ch.

Doped KNN ceramics were obtained by two variants of the ceramic method: 1) mixing the starting powders by magnetic agitation and 2) using a mortar mill, during 24 and 12 hours, respectively, followed by calcination for twice those times. For (K0.5Na0.5)0.95La0.05(Nb0.9Ti0.05)O2.9 (KNNLaTi) and for $(K_{0.5}Na_{0.5})_{0.95}La_{0.0166}Nb_{0.9}Ta_{0.1}O_3$ (KNNTaLa) the reached density values were 94% and 97% of the theoretical value, respectively. The X-ray diffraction (XRD) patterns in both samples correspond very well with those of pure KNN. Additional reflections of secondary phases appear and were identified as $Na_2Ti_4O_9$ and a tungsten-bronze phase. The lattice parameters of all patterns were determined by least square fitting and the FullProf software. For KNNLaTa the majority phase was an orthorhombic and for KNNLaTi was monoclinic. The grain size and morphology are different for both cases: for KNNLaTa rectangular shaped grains and sizes between 0.7 to 0.9 μm (observed by SEM) were obtained as in KNN ceramics, while for KNNLaTi rounded grains are observed with sizes around 27-28 nm (observed by PFM). On the other hand, in KNNLaTa samples the ferro-paraelectric transition occurs around 315 °C which is a lower temperature than that reported for KNNTa, making evident the incorporation of the La ions into the structure. Also a widening of the permittivity vs. temperature transition curves with respect to those of the KNNTa compound is observed. However, for the KNNLaTi sample the ferro-paraelectric transition occurs at around 120^0C. Additionally, it is observed that this transition is diffuse, with a very marked widening of the permittivity vs. temperature curve. This work was supported by CONACYT Proj. No. 166286, 101020 and 127633 and DGAPA-UNAM IN113312, IN107312, and IN112610.

P-034

SYNTHESIS AND CHARACTERIZATION OF MWCNTs DECORATED WITH Pt AND Ni NANOPARTICLES

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Keywords: transmission electron microscopy, nanotubes, Pt nanoparticles, fuel cells.

The increasing development of nanotechnology has been the result of a continuous progress in the synthesis of nanostructured materials. The multiwall carbon nanotubes (MWCNT) have chemical, mechanical, electrical and high surface area properties that enables them to adsorb metal nanoparticles (NPs) over their surface. Some metal NPs such as Pt, Pd, Ru and Au are used as electrocatalysts applied in fuel cells. When metal NPs are supported on MWCNTs have shown improved catalytic activity, corrosion tolerance and durability due to the electronic properties, morphology and their size producing increments on the electrochemical active area. One of the main issue on the commercialization of polymer fuel cells is the cost reduction and long term performance which can be improved by nanostructured materials such as NPs on MWCNTs. The present work presents the in situ preparation of Ni NPs during MWCNTs synthesis by spray pyrolisis technique. The MWCNTs were grown on a TiO_2 thin film deposited on a Vycor tube (SiO_2) using as catalyst nickelocene dissolved in toluene as the carbon source. Then, about 3% of Pt was deposited by aqueous solution synthesis. The samples were characterized by transmission electron microscopy where it can be observed the presence and distribution of Pt-Ni NPs along the MWCNTs. We thank F. Ruiz for technical assistance and project CONACyT 155388, CONACyT 82984 and DGAPA-PAPIIT IN109612-3.

P-035

MAGNETITE-LOADED PLGA-CHITOSAN NANOPLATFORM WITH POTENTIAL MULTIFUNCTIONAL USES

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Keywords: Nanoplatform, magnetic nanoparticles, magnetite nanoparticle, PLGA and chitosan.

Nowadays, much attention has been paid to develop multifunctional nanosystems, able to be used in diagnosis and treatment of diseases such as cancer. In this way, magnetite (Fe_3O_4), poly(D,L-lactide-co-glycolide) (PLGA) and chitosan were used for the production of a multifunctional nanoplatform. Fe_3O_4 nanoparticles were synthesized by a coprecipitation method. Magnetic nanopartcicles hydrophobically modified were obtained coating the magnetite surface with stearic acid. Magnetite nanoparticles coated with stearic acid were encapsulated into PLGA nanoparticles using an oil-water emulsion technique. Finally, we used chitosan as stabilizing agent of the magnetite-loaded PLGA nanoparticles suspension. Different techniques, as dynamic light scattering (DLS), atomic force microscopy (AFM) and zeta potential, were used to determine the size and zeta potential of nanoparticles. FTIR and EDX corroborate the presence of magnetite into the nanosystem.

P-036

GALLIUM NITRIDE NANORODS GROWN OVER AU/SIO$_2$ BY MOCVD

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Keywords: semiconductor, nitrides, metal-organic vapor deposition.

Gallium nitride films were grown by metal-organic chemical vapor deposition (MOCVD) over silicon dioxide with a thin layer of gold (Au/SiO_2). The samples were grown at relative low temperature (600 °C) using trimethyl-gallium (TMGa) and UHP ammonia (NH_3). The grow process was between 60 and 30 minutes. The GaN grown in this work was characterized by scanning electron microscope (SEM), energy dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD) and photoluminescence (PL). The result of the surface morphology of two GaN films shows rods formations with a semi-spherical segregation on the top as shown by SEM. The length of the GaN nanorods are 2 micrometers approximately and the diameter of the segregation is near to the 500 nanometers. Oxygen contamination was observed by EDS however gallium oxide was not observed. This research was support by CONACYT, the Universidad de Sonora and the Centro

de Nanociencias y Nanotecnología (CNyN). The authors would like to thank Marta Eloisa Aparicio Ceja and Israel Gradilla Martínez for the help with the analysis.

P-037

ROUND ROBIN COMPARISON OF FULLERENE NANOFIBERS

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Keywords: Round Robin comparison, C_{60} nanowhiskers.

A recent study of fullerene-based supramolecular nanoarchitectures is opening new possibilities for technological applications of fullerene materials such as sensors, transistors, catalysts, and fuel cell electrodes [1]. Nanowhiskers possess high surface to volume ratios, which mean that they have a highly reactive and readily functionalizable surface [2]. The activities in the TWA34 working group of the VAMAS organization (Versailles Project on Advanced Materials and Standards) are focused on measuring the population of nanoparticles (NP's) such as metal nanowires, SWCNT, magnetic nanoparticles, nanopowders and quantum dots [3]. The main goal of the TWA working group is the standardization and comparison between different measurement techniques in order to understand the dimensional, electrical, chemical, optical or magnetic properties of nanoparticles. Recently, in the particular case of fullerenes nanofibers, the TWA34 "Project 4: Raman spectroscopy of fullerene nanofibers" has just been completed in the first step. The goal of the Round Robin study was to collect the basic Raman spectroscopy data of C_{60} nanofibers under various exposure conditions of laser beam that serve to prepare a protocol to obtain standard Raman profiles of C_{60} nanofibers.

P-038

DIAMETERS DISTRIBUTION OF CARBON NANOTUBES

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Keywords: Diameter, carbon nanotubes, dispersion, certified, AFM, SEM, Raman.

In this work we analyzed two types of carbon nanotubes, single-walled (SWCNT) and multi-walled (MWCNT). An aqueous dispersion of the nanotubes was prepared with sodium deoxycholate salts (SDO) and sodium cholate (SC) at 2% V/V, the samples were characterized by atomic force microscopy (AFM), scanning electron microscopy (SEM) and Raman spectroscopy. The AFM equipment was calibrated using reference material SRM 2483, the specification nominal diameter is in the range of 0692-0966 nm. Subsequently, diameters were measured with SWCNT and MWCNT nominal specification of 1.2 - 1.5 nm and 110 nm -170 by SEM and AFM, respectively. From the results, a statistical analysis was carried out using the general linear model, in order to determine the most appropriate technique for measuring nanotubes. The SWCNT diameter results measured by AFM and Raman signals were compared, due to the spectra representing the ratio of the diameter with the metallic or semiconducting nature of the SWCNT, while AFM images indicate the position of the nanotube. Finally, these techniques demonstrate the ability to study the diameters of nanotubes. The statistical model applied showed that the AFM technique is more appropriate than the SEM to measure the size of the diameter. Furthermore, it was observed that the samples prepared with ODS have a high dispersion, which facilitates the measurements. These are within the range of diameter certified reference material.

P-039

MULTIFUNCTIONAL $Gd_2O_3:Eu^{3+}@Fe_3O_4$ NANOCOMPOSITES SYNTHESIZED BY SPRAY PYROLYSIS

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Keywords: Luminescent nanoparticles, magnetic nanoparticles, multifunctional nanoparticles, gadolinium oxide, iron oxide, spherical nanoparticles, spray pyrolysis.

In this work we present the synthesis and characterization of $Gd_2O_3:Eu^{3+}@Fe_3O_4$ nanocomposites fabricated by spray pyrolysis. Firstly, $Gd_2O_3:Eu^{3+}$ nanoparticles were synthesized in order to study the effects of temperature, precursor solution concentration, Eu-doping concentration, and carrier gas flow rate on the material properties. After the optimum parameters were established for the maximum luminescence emission, luminescent and magnetic $Gd_2O_3:Eu^{3+}@Fe_3O_4$ nanocomposites were fabricated in a one-step spray pyrolysis process by using commercial Fe_3O_4 nanoparticles (SkySpring Nanomaterials, Inc.) as the magnetic component. The obtained nanomaterials possess both luminescent and magnetic properties, due to their composition, and spherical morphology, due to the nature of the spray pyrolysis method. Excellent luminescent properties and paramagnetic behavior were obtained in these $Gd_2O_3:Eu^{3+}@Fe_3O_4$ nanocomposites. The photoluminescence was measured under UV excitation (□$_{\text{Exc}}$= 258 nm) and showed the characteristic red emission of Eu^{3+} (□$_{\text{Em}}$= 612 nm). SQUID magnetometry was used for magnetic measurements and the powder morphology and crystallinity were observed by XRD, SEM and STEM. Maximum emission intensity was obtained at 10% Eu-doping concentration. Such properties assure applications of $Gd_2O_3:Eu^{3+}@Fe_3O_4$ nanocomposites in biomedical and biotechnological studies.

P-040

$(Lu_{1-\alpha-\beta}Y_{\alpha}Pr_{\beta})_2SiO_5$ SCINTILLATORS OBTAINED BY COMBUSTION SYNTHESIS AND SPRAY PYROLYSIS METHODS

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Keywords: Scintillators, decay time, luminescence, $(Lu,Y)_2SiO_5$, praseodymium.

In the present investigation we report on the synthesis of Pr-doped $(Lu_{1-x}Y_x)_2SiO_5$ (LYSO) powders by using two different methods: pressure assisted combustion synthesis (PACS) and spray pyrolysis. We examine the influence of the Y/Lu ratio and the rare earth (RE) activator concentration on the luminescence properties. LYSO single crystals activated with Ce^{3+} are proposed to be employed in the medical imaging field as detectors (scintillators) in positron emission tomography (PET) equipment [1]. The $(Lu_{1-\alpha-\beta}Y_\alpha Pr_\beta)_2SiO_5$ powders were prepared by using nitrates as the precursors in both methods, and hydrazine (N_2H_4) as the reductive fuel on the PACS. Subscripts α and β were varied between 0.2-0.49 and 0.005 or 0.05 respectively. All powders were thermally treated in air at 1200°C at different times. Regardless of the concentration of Pr^{3+} and post-synthesis annealing time, a $(Lu,Y)_2SiO_5$ (LYSO) solid solution as a majority phase is obtained in all phosphors. The diffraction peaks of the LYSO powders match perfectly to the reported for monoclinic Lu_2SiO_5 (JCPDS 41-0239). This is in good agreement to XRD data reported by other groups for this compound [2], confirming with this the formation of a LYSO solid solution. It is important to note that no Pr oxide phases were detected. Pr-activated samples emit in the UV region under short-UV excitation (250 nm). The emission spectra shows a principal peak at λ= 275 nm and a second one at λ= 313 nm which corresponds to the $^5D_2 \rightarrow 4f\ (^3P_2)$ and $^5D_1 \rightarrow 4f\ (^3H_4)$ "forbidden" transitions in Pr^{3+} [3]. The room temperature luminescence decay time profiles of the Pr^{3+} activated samples emission monitored at 270 nm upon excitation at 252 nm varies between 11 ns and 16 ns.

P-041

MECHANICAL PROPERTIES OF TANTALUM CARBONITRIDE (TaC_xN_y) THIN FILMS GROWN BY DC REACTIVE SPUTTERING

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Keywords: DC reactive sputtering, tantalum nitride (TaN_y), tantalum carbonitride (TaC_xN_y), microstructure, nanoindentation.

TaN_y and TaC_xN_y thin films were grown on Si (111) at various substrate temperatures using the DC reactive sputtering technique in an atmosphere of Ar/N_2 and $Ar/(N_2+CH_4)$, respectively. The nitrogen partial pressure (P_{N2}) was varied in order to synthesize TaN_y and TaC_xN_y films with different nitrogen content (y =

[N]/[Ta]). The methane partial pressure (P_{CH4}) was settled in ~0.07 and ~0.10 to grow the TaC_xN_y films with different content of carbon (x = [C]/[Ta]). The chemical analysis was performed using Auger electron (AES) and X-ray photoelectron (XPS) spectroscopies, while the structural and mechanical characterizations were done by means of X-ray diffraction (XRD) and nanoindentation tests, respectively. The structure of the TaN_y films changed from hexagonal γ-Ta_2N + cubic δ-TaN to cubic δ-TaN phase when increasing the P_{N2}. Likewise, the structural changes of the TaC_xN_y films were dominated by the P_{N2} rather than the P_{CH4}. The carbon content (x = ~10%) integrates within the TaN_y structure whether in replacing the nitrogen interstitial sites or in amorphous phase to form the TaC_xN_y solid solution. In the Ta-N system, the nanoindentation tests showed that the samples composed of mixed crystalline phases, hexagonal γ-Ta_2N + cubic δ-TaN, obtained the higher hardness values, from 26 to 29 GPa. On the other hand, the TaC_xN_y films with a hexagonal structure presented hardness values from 21 to 25 GPa, while the hardness for the TaC_xN_y formed by more than one crystalline structure is slightly higher than 30 GPa. The authors would like to thank for the technical support to D. Domínguez E. Aparicio, I. Gradilla, J.A. Díaz in UNAM-CNyN; and to F. Alonso in CICESE. This work was Partially support by Project DGAPA-PAPIIT No. 103711.

P-042

FLUORESCENCE PROPERTIES OF DYSPROSIUM-ACTIVATED HYDROXYAPATITE IN FLUIDS

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Keywords: Hydroxyapatite, fluorescence, biomarker, dysprosium.

Luminescence dysprosium-activated hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2:Dy^{3+}$, $HAp:Dy^{3+}$) nanopowders have been synthesized at different dysprosium concentrations (0.5, and 5 %) by L-tartaric acid-assisted sol-gel method and subsequently annealing at two different temperatures 800 and 1000°C. The nanopowders were analyzed by X-ray diffraction (XRD), the morphology by transmission electron microscopy (TEM), the chemical composition with energy disperse spectroscopy (EDS), and optical properties by photoluminescence (PL). The $HAp:Dy^{3+}$ nanopodwer presented a red emission when was excited with 350 nm. The PL analysis shows the contribution of four fundamental emissions peaks; the first centered at 484 nm ($^4F_{9/2} \rightarrow {}^6H_{15/2}$), the second at 575 nm ($^4F_{9/2} \rightarrow {}^6H_{13/2}$), the third at 767 nm ($^4F_9 \rightarrow {}^6H_{11/12}$) and the fourth at 775 nm ($^4F_9 \rightarrow {}^7H_{9/2}$), these emission peaks are attributed to the intraionic transitions of Dy^{3+} ions. The $HAp:Dy^{3+}$ nanopowders preserved their luminescence in human serum, urine and water. The luminescence properties of $HAp:Dy^{3+}$ may find important applications in medicine as biomarker.

P-043

STRUCTURAL AND FERROELECTRIC PROPERTIES OF THIN $BiFeO_3$ FILMS DEPOSITED BY RF MAGNETRON SPUTTERING

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Keywords: Ferroelectric thin films, RF Sputtering, XTEM, PFM, C-V.

Epitaxial thin $BiFeO_3$ films with good ferroelectric properties at room temperature are attractive for many micro- and optoelectronic applications. Ferroelectric thin films with well controllable structure and dielectric response are actively studied around the world for their potential usage in novel devices like non-volatile memories and new kind of solar cells. The aim of this work is to obtain epitaxial thin ferroelectric films ($\leq$ 100nm) in a conventional deposition system used in recent years by the microelectronics industry. The $BiFeO_3$ films studied here were deposited by RF magnetron sputtering using a target of the same material at 150 W and temperature of 700°C. The total pressure was 25 mTorr with a 4:1 $Ar:O_2$ gas ratio. The structure of the fabricated samples was studied by Cross-sectional Transmission Electron Microscopy (XTEM), X-Ray Diffraction (XRD) and Atomic Force Microscopy (AFM). Structural results showed films with single orientation determined by the substrate with an almost atomically flat surface. Ferroelectric response was analyzed by Piezo Force Microscopy (PFM) and Capacitance-Voltage (C-V) measurements. The ferroelectric behavior of the films is confirmed through electrical measurements after applying voltages in both directions. M. Curiel thanks DGAPA-UNAM for the postdoctoral fellowship. The author also thank to F. Ruiz, E. Aparicio, D. Dominguez, I. Gradilla and P. Casillas for their invaluable technical assistance. The support of CoNaCyT through grant 166286 is acknowledged.

P-044

STUDY OF FERROELECTRIC PROPERTIES OF HIGHLY TEXTURED $Pb(Fe_{1/2}Nb_{1/2})O_3$ THIN FILMS BY PIEZORESPONSE FORCE MICROSCOPY

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Keywords: PFN, Multiferroic Material, rf-Sputtering, Piezoresponse Force Microscopy.

In recent years, the interest in the study of multiferroic materials has increased due its degrees of freedom that makes them useful for the development of new nanoscale technologies and applications. A good candidate to be used in this new nanoscale applications is the multiferroic material $Pb(Fe_{1/2}Nb_{1/2})O_3$ (PFN); however the majority of studies have focused in ceramics of PFN at macroscale level and there are few papers about thin films of this material. For this reasons, the goal in this work is to study the local ferroelectric characteristics of highly textured PFN thin films deposited by rf-magnetron sputtering. To our knowledge, on PFN thin films, a switching ferroelectric image obtained from the application of dc bias to an area while scanning a larger area by piezoresponse force microscopy (PFM) in the resonance mode is shown for first time. Additionally, to obtain a clear distribution of ferroelectric domains in PFN thin films without cross talk topography, a resonance tracking PFM was used. Finally, the local hysteresis loops were measured by PFM. A piezoelectric constant d_{33} of 3.9 pm/V and a coercive voltage of approximately 9 volts were calculated from these measurements. This study shows, for the first time, the local ferroelectric characteristics of PFN thin films deposited by rf-magnetron sputtering. J. J. Gervacio-Arciniega thanks DGAPA-UNAM for the postdoctoral fellowship. Thanks are also due to E. Aparicio, F. Ruiz, and P. Casillas for their technical assistance. This work was supported by DGAPA-UNAM grant IN113312, and CONACYT grants 166286 and 127633.

P-045

SYNTHESIS NANODIAMOND GROWTH BY HF-CVD

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Keywords: Synthesis, Nanodiamond, HFCVD.

In recent years the nanodiamonds (ND) have gain a great importance in many areas of physics, chemistry and biology. Its wide range of applications have been derived from its unique characteristics such as high and thermal conductivity, extreme strength, chemically inert (anticorrosive) and biocompatibility. In the other hand it is know that many of these applications are based on the electrical and optical properties associated with defects in diamond crystals. In this paper, a novel method to synthetized nanoparticles of diamond on Si (111) and Au/SiO2 using an enhanced hot-filament chemical vapor deposition (HF-CVD) technique is presented. ND synthesis is carried out in a quartz tubular reactor using a HF-CVD method. The method consists in reacting methane gas (CH_4) and hydrogen (H_2) in suitable proportions into the quartz reactor at high temperatures (~ 2000 °C) to facilitate growth of the ND. The proccess parameters were, P_{S1} =

30 Torr, P_{S2} = 70 and P_{S3} Torr = 100 Torr / $T_{SUSTRATE}$ = 900-1000 ° C / CH_4 = 10 sccm, NH_3 = 10 sccm and H_2 = 260 sccm. **In** Figures 1 and 2 some results of XRD and SEM analysis are shown. Diamond grown by this method shows a cubic structure and the nanocrystals hava rounded forms that correspond to a formation at a low substrate temperature. The authors would like to thank Eloisa Aparicio and Israel Gradilla from the Center of Nanoscience and Nanotechnology of the UNAM for help in the characterization of our samples.

P-046

ANALYSIS OF FOUCAULT CURRENTS IN INDUCTORS OF PLCS INFLUENCED BY MICRO CORROSION IN THE ELECTRONICS INDUSTRY

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Keywords: Foucalut currents, PLC, micro corrosion, electronics industry.

Inductive proximity sensors contain an internal coil. When a current flow through it, a magnetic field is generated, which has the direction of the electric currents involved in it, as electrical flow in the input or output area. The coil or winding of the inductive sensor induces Foucault currents in the material to be detected, that are originated by eddy currents. These electrical flows generate a magnetic field, which opposes to the sensor coil, causing a reduction in the inductance of micro inductors of electronic devices. This reduction of the internal inductance originates bad function in the micro inductors used in the Programming Logic Controller (PLC). This PLC is in the manufacturing processes of the electronics industry and reduces their operation yielding. Sometimes the actuators of these electronic systems not operate correctly, and causing stops in the activities of industrial equipments and machines, being a factor of economic losses. A study of micro evaluation of these inductors which are elements of the relays of PLC was made to determine the influence of corrosion in these components. The analysis showed micro corrosion in these devices with images obtained of the Scanning Electron Microscopy (SEM) and also was made a correlation of the climatic factors as relative humidity (RH) and temperature with the corrosion rate (CR). The evaluation was made in indoor of an industrial plant which fabricate microelectronic components in Mexicali city. The major factors, which causes an adverse effect in the operation of PLC of this industrial plant was the humidity and sulfurs, which originates the deterioration of components of PLC.

P-047

ELECTRICAL CHARACTERIZATION OF MOS STRUCTURES WITH MULTI-REGION GATE DIELECTRICS CONTAINING SILICON NANOCRYSTALS

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Keywords: MOS, Si nanocrystals, TEM, I-V, C-V.

Metal-Oxide-Semiconductor (MOS) structures with multi-region gate containing silicon nanocrystals (Si NCs) are promising for applications in optical and electronic devices. In this study, three region gate dielectrics were prepared by the following processes: oxidation of n-type crystalline silicon at 1000 °C in dry oxygen atmosphere; thermal evaporation of SiO_x films (x = 1.15 or 1.3, ~ 100 nm thick) in vacuum; and furnace annealing/oxidation at 1000 ºC. The high temperature process was carried out in two steps: first, annealing in N_2 for 40 min and then oxidation in $N_2 + O_2$ atmosphere for 20 min. During the second step the crystals grown close to the top surface and the remaining excess Si in the SiO_x matrix become oxidized. For electrical characterization MOS capacitors with area of 2×10^{-3} cm^2 were patterned after Al metallization. Cross-sectional Transmission Electron Microscopy proves formation of two regions in the SiO_x film: a region free of nanoclusters close to the top surface and a second one, with nanoclusters embedded in an amorphous matrix, underneath the first region. The obtained MOS structures were characterized electrically by I-V and C-V measurements. I-V measurements show that the top oxide has excellent insulating properties, close to that of thermal oxide. Hysteresis C-V measurements in various bias ranges prove that the nanocrystals can be charged negatively by injecting electrons from the top contact. The structures display good retention times of the trapped charge.

P-048

SYNTHESIS AND STUDY OF THE STRUCTURE, MICROSTRUCTURE AND FERROELECTRIC PROPERTIES OF $(BI_{0.5}K_{0.5})TIO_3$

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Keywords: Lead-free ceramics, Bismuth-potassium titanate $(Bi_{0.5}K_{0.5})TiO_3$, BKT.

The study of high performance lead-free ceramics is one of the most important research lines in ceramic investigation, arising from the necessity to avoid the use of lead in electromechanical devices, sensors, and other piezoceramic material applications. Due to international regulations regarding the

restrictions of lead usage in applications were lead zirconate-titanate (PZT) is the most widely used material, other candidate materials for high performance lead-free ceramics are being studied, mainly those based on perovskites, where the structure is obtained by iso-composition of bismuth and a monovalent cation. Bismuth-potassium titanate ($(Bi_{0.5}K_{0.5})TiO_3$, BKT), which crystallizes with tetragonal structure, belongs to this family, as does bismuth-sodium titanate ($(Bi_{0.5}Na_{0.5})TiO_3$, BNT), which crystallizes with romboedral structure. Furthermore a morphotropic phase boundary (MPB) composition range has been reported for the BNT-BKT binary system, the composition range of which is still under debate. One reason for the discrepancies is that the thermodynamic instability of Bi_2O_3 and K_2CO_3 at processing temperatures coupled with the kinetics of chemical reactions at such temperatures favors the formation of unstable oxides. There is a small window available for temperature tuning for the solid-state reaction that leads to a fully reacted BKT and avoids compositional variation and precursor loss. In this contribution the reaction temperature was varied from 600 to 750 ºC, and the high-energy milling time of reactants was varied from 1 to 4 h. The temperature window was defined based on TGA-DSC analysis carried out up to 900 ºC. Subsequently, the sintering temperature of BKT was studied by varying the temperature between 600 and 900 ºC. The objective was to obtain densified BKT ceramics and to study the effect of the experimental variations on the ferroelectric properties. Ferroelectric properties are measured by polarization-electric field hysteresis curves and piezoresponse force microscopy.

P-049

DEPOSIT AND MONITORING OF ULTRATHIN FILMS USING A QUARTZ CRYSTAL SENSOR

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Keywords: Nanoscale, Thin Films, ferroelectric.

Today, scientists are increasingly working on nanoscale materials characterization; this requires the use of higher accurate devices than existing to monitor thin-films thickness during deposit process. The quartz crystal sensor (QCM) provides a high sensitivity, operates using a piezoelectric sensor which is rugged, supports very high frequencies and is relatively immune to vibration. The purpose of this study is to demonstrate the ease and comfort that the device may provide, consist on to incorporate a quartz crystal microbalance function within the bell evaporation and thus, directly measure the spatial evolution of ultrathin films. In this work, we present results from deposits of ultrathin films coating on Periodically Poled Lithium Niobate and Lithium Tantalate crystals. These crystals are preferred choice to manufacture acoustic wave devices used commonly in nonlinear optics (e.g. laser frequency doubling, optical parametric oscillators and second harmonic generation.), Q-switching devices, optical switches for Gigahertz frequencies and optical waveguides among others. Particularly, we use these materials to manufacture mirrors with optical low-pass filters and optical filters for specific wavelengths.

2nd POSTER SESSION

P-050

FORMATION OF SULFUR ADLAYERS ON GOLD FROM DITHIOCARBAMATE SALTS

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Keywords: self assembled monolayers; scanning tunneling microscopy; X-ray photoelectron spectroscopy; nanoscience; surface science.

The knowledge of the adsorbed sulfur behavior on metals is important to understand the structure and dynamics of self assembled monolayers of thiols on metals. The sulfur on gold system is of interest because gold is the preferred substrate for the preparation of well-ordered self assembled alkanethiol monolayers (SAMs). Therefore, the study of sulfur adlayers on metals could be a way of discerning between the substrate-molecule and molecule-molecule interactions in SAMs on metals, which could help to elucidate the role of the weak intermolecular interactions for the formation of the assembled structures. Sulfur coverage is spontaneously formed by immersion of Au (111) in a solution of 0.1 g of Na2(DTC2-Pz) and 0.4 g of NaOH in 10 cm3 of H2O (pH = 14) at room temperature. The low and high sulfur coverages were obtained for 14 and 24 hours respectively. The gold modified substrates have been studied by Scanning Tunneling Microscopy (STM) and X-Ray Photoelectron Spectroscopy (XPS). XPS data show no evidence of ditiocarbamate salts. The transformation from sulfur atom adsorption on Au (111) to rectangular S8 surface structures is described. This process involves sulfur atom adsorption, the formation of rectangular octomerical surface structures, and the displacement of sulfur atoms to nearest hollow sites. The Au(111) 3x3□ sulphur structure is observed in the STM image by combining the √3 x √3 R30º and 3x3 structures for low coverages.

P-051

EFFECT OF THE ALUMINA SHELL-LAYER IN THE MAGNETIC AND DIELECTRIC PROPERTIES OF $YCrO_3$

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Keywords: multiferroics, core-shell, magnetism, capacitance.

The development of core-shell nanocomposites (CSNs) has attracted considerable attention and become an important research area at the frontier of advanced materials. CSNs are nanoscaled assemblies with a chemical composition that is different on the surface compared to the core region. This architecture has found versatile applications in many fields, such as chemical sensors, drug delivery, quantum dots, catalysis, dielectric capacitors, etc,. In ferroelectrics, the core-shell architecture acts as barrier layer localizing electronic and ionic space charges, increasing thus the capacitance density [1]. Recent studies in $YCrO_3$ thin films have found charge accumulation at the grain boundaries that are detrimental to their ferroelectric properties [2]. In order to concentrate the charge accumulation within the grains and thus decrease the dielectric loss and improve the capacitance density, we have prepared alumina shell-layers of 5, 30 and 90 nm to cover the $YCrO_3$ grains, using an atomic layer deposition (ALD) technique. Here we show preliminary studies based on XRD, XPS, SEM and TEM characterization as well as on magnetic and dielectric measurements. Thanks are due to P. Casillas, E. Aparicio, I. Gradilla, F. Ruiz for their technical assistance. The work has been supported by PAPIIT-UNAM IN103213, IN114209, CoNaCyT Proj. No.166286 and 83275.

P-052

A STUDY OF THE Li, La, Ta DOPED KNN SYSTEM

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Keywords: Piezoelectricity, 77.65.-j, Piezoelectric Ceramics, 77.84.Dy, Permittivity, 77.22.Ch

Lead free piezoelectric ceramics with composition $[(K_{0.5}Na_{0.5})_{0.94}Li_{0.06}]_{0.97}La_{0.01}(Nb_{0.9}Ta_{0.1})O_3$ were synthesized by the traditional ceramic method. The calcined powders were sintered in their own atmosphere and in open air. The sintering process was carried out at 1100^0C for 1.0, 1.5 and 2.5 h. Results from X-ray diffraction show that Li^+, La^{3+} and Ta^{5+} diffuse into the $(K_{0.5}Na_{0.5})NbO_3$ structure to form a perovskite-structured solid solution that is preponderantly orthorhombic for 1 h sintering or mostly tetragonal for the longer sintering times. A second minority phase is detected identified as a tungsten-bronze tetragonal phase. The lattice parameters of the obtained phases were determined using the FullProf software. Scanning electron microscopy micrographs show rectangular shaped grains with average size of 1.1 ± 0.2 μm. Some porosity and traces of liquid phase are also seen and attributed to Na_2O evaporation during the sintering step. An increase of the dielectric permittivity with the growth of the c-parameter is observed for the longer sintering times. The incorporation of Li into the structure is deducted from the modification of the transition temperature with respect to that reported for KNNLaTa by other authors. Using a modified Curie-Weiss law analysis it is found that the samples undergo a normal phase transition. The piezoelectric parameters k_p, Q_m, σ_p, s_{11}, d_{31} and g_{31} were determined and compared with those of commercial PZT samples. Thanks are also due to E. Aparicio, I. Gradilla, and P. Casillas for their technical assistance. This work was supported by

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P-053

STRUCTURAL AND OPTICAL CHARACTERIZATION OF GATE DIELECTRICS CONTAINING SILICON NANOCLUSTERS

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Keywords: XTEM, SE, Si nanoclusters, Gate dielectrics.

Thin dielectric films containing crystalline or amorphous silicon nanoclusters were fabricated by thermal oxidation of n-type c-Si wafer in dry oxygen, deposition of SiO_x films (x= 1.15, d ~ 100 nm) by thermal evaporation of SiO in vacuum, followed by a two-step annealing/oxidation (N_2/N_2+O_2) process. Two groups of samples were prepared: in the first one silicon nanocrystals (Si NCs) were grown by 40 min annealing in N_2 and 20 min oxidation in N_2+O_2 atmosphere at 1000 °C, while in the second one amorphous silicon nanoparticles (a-Si NPs) were formed at 700/800 °C keeping the same annealing/oxidation times. Cross-sectional Transmission Electron Microscopy (XTEM) proves the formation of two regions in the SiO_x film: a region free of nanoclusters close to the top surface and a second region with nanoclusters underneath the first one. Spectroscopic Ellipsometry (SE) was used to obtain the volume fraction of the pure Si phase in the oxide matrix, ~ 31 and 28 vol. % for the regions with nanocrystals and amorphous nanoparticles, respectively. The dependencies of refractive index and extinction coefficient on wavelength have similar behavior as that of silicon monoxide. A correlation between the thicknesses of the three regions determined by XTEM and SE was found.

P-054

STRUCTURE AND DIELECTRIC PROPERTIES OF Pr AND Ba DOPED $SrTiO_3$

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Keywords: ferroelectric, dielectric properties, capacitance, crystalline structure.

$SrTiO_3$ (STO) is considered an incipient ferroelectric material at low temperatures. At room temperature, it has a dielectric constant of about 300 and is not ferroelectric. In the last few years, many

investigations have been carried out trying to detect ferroelectricty at room temperature. Heani et al. measured ferroelectrictiy at room temperature in STO thin films and attributed it to the distortion produced by the lattice mismatch between the $DyScO_3$-substrate and the $SrTiO_3$ film [1]. Cation substitution is another way to distort the crystal and modify the dielectric properties. Recently, studies by our research group have found that Pr ion substitution in STO induces ferroelectricity at room temperature [2]. In this work we report the effect of Ba and Pr substitution as a means to increase and stabilize the ferroelectric properties in STO. XRD analysis is used to determine the solubility limit of the doping cations. Polarization and permittivity measurements of the Pr and Ba substituted STO ceramics are presented. Thanks are due to E. Aparicio, I. Gradilla, J. Peralta for their technical assistance. The work has been supported by PAPIIT-UNAM IN103213, CoNaCyT Proj. No.166286.

P-055

DESING AND MANUFACTURING OF THREE-ELECTRODE CELL

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Keywords: Three-Electrode Electrochemical Cell, Reactor, Characterization, Nanoparticles.

Here, we are reporting the design and manufacture of a three electrode electrochemical cell of stainless steel, which will be used as electrochemical reactor for characterization of nanoparticles Pt-M (M = Mn, Fe, Co and Ni) supported on multiwall carbon nanotubes (MWCNTs). The reactor will allow study the behavior of materials under operating conditions of a direct methanol fuel cell (3-5 bar and 60-100 ° C). The reactor will be used for characterization for the electrocatalysts by cyclic voltammetry, CO stripping, chronoamperometry and faradaic impedance techniques.

P-056

EFFECT OF SUBSTRATE IN SEGREGATION OF POLY(STYRENE)-*b*-POLY(*N*, *N*-DIETHYLAMINOETHYLMETHACRYLATE) BLOCK COPOLYMERS in THIN FILMS

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Keywords: block copolymer, spin-coating, self-assembly, films.

Linear AB block copolymers self-assemble when A and B are immiscible to form a variety of nanoescale periodic patterns as spheres, cylinders, lamellae with dimensions of 5-100 nm and has applications ranging from electronics to biomedicine [1]. In this contribution we report on the use of diblock copolymers of poly(styrene) (PSt), an hydrophobic polymer as first block; and poly(*N*,*N*-diethylaminoethylmethacrylate) (PDEAEM), an hydrophilic polymer as second block. Thin films were prepared by Spin-Coating over mica, clean glass surface and also over glass surfaces modified with silanes by using solutions in different solvents. Two copolymers were used: $PSt_{60\%}$-*b*-$PDEAEM_{40\%}$, (M_n = 88,200 g/mol, PDI = 1.2) and $PSt_{90\%}$-*b*-

PDEAEM$_{10\%}$(M_n = 58,400 g/mol, PDI = 1.15), According to the theoretical phase diagram reported by Matsen [2], different morphologies were expected depending on copolymer composition. AFM micrographs obtained right after spin-coating and also after annealing by heat-treatment for long times, showed the effect of the interactions of the surface with blocks. Good seggregation, was obtained in mica and in silanized surfaces as compared to clean glass but with different dimension of the domains depending on the substrate type. Furthermore, annealing with temperature did not improved the segregation, since long annealing times resulted in some cases in film detachment with formation of irregular shape structures.

P-057

BIMETALLIC Ag-Fe SYSTEMS SUPPORTED IN MORDENITE AND FERRIERITE ZEOLITES

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Keywords: Zeolite, Mordenite, Ferrierite, ion exchange, SCR.

The catalytic properties of zeolites are strongly related to their ability to stabilize a variety of species within the structure [1]. In this work, Ag-Fe species were prepared by ion exchange from aqueous solutions in the Mordenite (MOR) and Ferrierite (FER) zeolites. The crystal structure of the samples was determined from X-ray data, the chemical composition and morphology were studied by SEM and EDS, respectively; and the type of the metallic species was identified by UV-Vis spectroscopy. The potential of MOR and FER zeolite catalysts promoted by Ag-Fe species was evaluated in the SCR of NOx with mixture of CO and propene. Authors acknowledge technical assistance of E. Aparicio, I. Gradilla, J. Peralta, F. Castillón and E. Flores, and financial support from CONACYT 102907, 179619 and DGAPA 203813 grants.

P-058

CATALITYC ACTIVITY OF (Cu,Ni)/MORDENITE CATALYSTS IN NO REDUCTION BY CO AND PROPENE

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Keywords: Zeolite, ion exchange, NO reduction.

Mordenite type zeolites with different SiO_2/Al_2O_3 molar ratios (MR) were subjected to an ion exchange process an excess of $Ni(NO_3)$ and/or $CuSO_4$ at 0.1 N solutions at different Cu:Ni ratios and exchange temperatures. Obtained catalysts were characterized by XRD, EDS, UV-Vis and TPR techniques. XRD results showed that the zeolite structure remains unchanged after ion exchange procedure. Amount of Cu and/or Ni decrease in line with MR increase (13>20>90) acording EDS analysis. The UV-Vis spectra of obtained catalysts present absorbance at wavelengths of ~ 390-400 nm and a doublet at 650 and 720 nm belonging to Ni^{2+} hexahydrate[1] and an absorbance from 600 nm to 850 nm referring to Cu^{2+} in seudooctaedral symmetry. The catalytic activity of NO reduction was studied in CO and propene presence within wide range of temperatura (30-500 ºC). Authors acknowledge technical assistance of E. Aparicio, I. Gradilla, J. Peralta, C. Morales, F. Castillón and E. Flores, and financial support from CONACYT 102907, 179619 and DGAPA 203813 grants.

P-059

GTL CONVERSION OVER BIMETALLIC Co_XFe_Y/HMS CATALYSTS

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Keywords: FTS, HMS, bimetallic Fe-Co catalysts.

Fischer-Tropsch synthesis (FTS) is an attractive alternative that converts synthesis gas [1], into a wide range of ultra-clean, sustainable and renewable free-sulfur long chain hydrocarbons. Recently, mesoporous materials such as MCM-41, SBA-15 and HMS, have attracted widespread attention as supports for Fischer–Tropsch catalysts [2-6]. In the present work, cobalt and iron bimetallic catalysts supported on hexagonal mesoporous silica (HMS) were synthesized and studied. Support and catalysts were prepared by neutral S^0I^0 templating route [7] and by incipient wetness impregnation respectively, varying the metallic content to study their effect. Characterization techniques used were N_2 adsorption–desorption isotherms (S_{BET}), X-ray diffraction (XRD), temperature programmed reduction (TPR), transmission electron microscopy (TEM) and inductively coupled plasma–mass spectrometry (ICP-MS). To evaluate their performances, FTS was carried out at 20 bars of pressure in a fluidized packed bed reactor, at a fixed temperature of 220 ºC. All bimetallic catalysts reached 50-75% CO conversion interval. The products yields of FTS are showed in Figure 1. We can notice that an increment in Co-content favors selectivity towards lighter fractions (Fig. 1 (a)) while an increment in Fe-content shifts selectivity to heavy hydrocarbons fractions (Fig. 1 (b)). Generally, the catalysts exhibited 50% syngas conversion with selectivity to waxes fractions. Our materials achieve conversions above 50% and selectivity centered on liquid fractions.

P-060

RuS2 AND Ni/RuS2 NANOCATALYSTS FOR SULFUR REMOVAL

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Keywords: Ruthenium-Niquel sulfide catalyst dibenzothiophene hydrodesulfuration.

RuS_2 is one of the most active catalysts to eliminate sulfur from refractory compounds presents in hydrocarbon fuels. Through this, the transformation of organosulfur compounds occurs mainly by hydrogenation pathway. Pecoraro and Chianelli[1] reported that the excellent catalytic activity of bulk transition metals sulfides (TMS). They observed that a periodic trend, the first TMS row is relatively inactive, but the second and third TMS rows exhibit higher activity, being the RuS_2 catalyst the most active one[1-3]. In this work we report that the addition of Ni to RuS_2 to examine the effect of the Ni with respect to selectivity. The precursors of RuS_2 catalyst were prepared by a mixing of an aqueous solution of $RuCl_3$ and NH_4Cl. Then, the product like $(NH_4)_3RuCl_6$ was sulfided in atmosphere of H_2S/H_2 to produce RuS_2, next the Ni was added from $Ni(NO_3)_2$ by impregnation method to RuS_2. The catalysts were designed as Ni_xRuS_2 where X=0.2-0.6. From this study, it can be concluded that the effect of the addition of nickel leads to reduction of area and catalytic activity but changes the selectivity. Still, the presence of low content of ruthenium gives a favorable effect on the selectivity towards hydrogenation route; the selectivity observed could be associated with Ni_9S_8 nickel phase. RuS_2 and Ruthenium-Niquel sulfide nanocatalysts structure was observed by high resolution transmission electron microscopy (HRTEM). The authors acknowledge CONACyT for financial support (Project 155388) and the valuable technical assistance to J. Peralta, M. Sainz, F. Ruíz, E. Flores, I. Gradilla, and E. Aparicio.

P-061

EFFECT OF ZINC SOURCE ON THE PROPERTIES OF CHEMICAL BATH DEPOSITED ZNS THIN FILMS

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Keywords: Chemical bath deposition, ZnS thin films, Complexing agent.

In this work, we study zinc sulfide (ZnS) thin films prepared by chemical bath deposition with different zinc sources on Si_3N_4 substrate in an alkaline solution. The materials used are zinc acetate, zinc nitrate, zinc sulfate, tri-sodium citrate and thiourea at a pH close to 10.5, with tri-sodium citrate being used as complexing agent. The reaction was kept at 80 °C. The reaction led to a color change to pale white. The structural and morphological characteristics of the films and their composition have been investigated by scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD), X-ray

photoelectron spectroscopy (XPS), and UV–Vis spectroscopic analysis. SEM characterization showed that the surface of the samples is compact and uniform, with some pinholes in the surface depending on the zinc source. XRD studies revealed the formation of pure ZnS films with a hexagonal structure for the ZnAc deposition. AFM indicates that the ZnS film has a rough surface with a high root mean square (RMS) value of 35 nm when deposited with ZnAc. XPS shows binding energies of thin films of ZnS, revealing bonds of Zn-S and Zn-OH. The transmission spectrum indicates an average transmittance of 80 to 85 % in the spectra range from 300 nm to 800 nm, and the optical band gap of the samples was around 3.71 to 3.74 eV. The thickness of ZnS thin films was in the 30-60 nm range.

P-062

ANTIPROLIFERATIVE ACTIVITY OF NANOPARTICLES BUILT BY HYDROPHOBICALLY MODIFIED CHITOSAN

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Keywords: hydrophobic chitosan, nanoparticles, cancer cells, light scattering, AFM.

Cancer is one of the most important diseases in the world due to its high mortality index, probably because until now there is no exists adequate and secure treatments to lower such mortality. Recently many researchers have suggested and used new chemotherapeutic methods through controlled drugs release using nanoparticles as vectors. Biopolymers like chitosan are widely used in drug release due to its biocompatibility and non-toxicity for human cells. Chitosan is widely used with insulin and other drugs as nanoparticles carrier due to its antibacterial and antitumor properties. Chitosan nanoparticles can have intrinsic anticancer activity and in this work we show also that hydrophobically modified chitosan can also produce significantly antitumor activity. Chitosan was modified with 10 and 30 % of octylaldehide and nanoparticles (NP) were obtained with a known method (ionic gelation). NPs were characterized by AFM, DLS RMN and FTIR spectroscopies. Anticancer tumor activity was evaluated by using MDA MB231 cells with the MTT method. Size of NP were around 200-300 nm and the hydrophobically modified chitosan NP showed a slightly significantly higher antiproliferative activity in comparison with non- modified chitosan NP..

P-063

SYNTHESIS OF GALLIUM INDIUM NITRIDE NANOCRYSTALS THROUGH PYROLYSIS ROUTE

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Keywords: Synthesis, Pyrolysis, Nanopowders, InGaN.

Gallium-Indium nitride and has gained much attention due to their optoelectronic properties. The main applications consist on the elaboration of solar cells, LED light bulbs and solid state illumination. In this paper a pyrolysis route is presented for the synthesis of InGaN nanocrystals with a wurtzite structure. The procedure consists in a thermal decomposition of an organic-metallic gallium indium complex in a horizontal quartz reactor at 600°C in the presence of high purity ammonia. A range of compositions between 0 -1 mole fraction is expected to be reached by this method, which will be controlled by monitoring the stequiometry between the carbohydrazide and the indium and gallium nitrates. In order to achieve the nitrides synthesis, first the gallium indium organic-metallic complex must be synthesized, that is achieved by dissolving gallium indium nitrates in toluene, once the nitrates are dissolved, the solution is heated until boiling point (111°C), and then the carbohydrazide is dissolved in the toluene solution. The next step consists of continuing heating the solution until all of the toluene is evaporated. At this point a very viscous polymer is formed (the gallium-indium complex). Once the gallium-indium complex is synthesized, we proceed with the pyrolysis reaction which occurs at a horizontal quartz reactor under a high purity ammonia atmosphere at about 740 Torr pressure and 600°C. In this step the nanocrystals of gallium-indium nitride are formed, after that the crystals are left to cool. Once cooled, the crystals are grinded to homogenize the sample, after that the sample is stored in glass vials for its future analysis. Through this method InGaN nanocrystals were synthesized at different compositions by monitoring the stequiometry of the reagents. The x-ray diffraction graph will be shown at the presentation. This synthesis route will be used in future experiments.

P-064

Au-Pd@SiO_2 NANOREACTORS

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Keywords: Nanoreactors, bimetallic nanoparticles, Au-Pd, UV-Vis, TEM.

The nanoreactors (NRs) present a new generation of heterogeneous catalysts. This novel structure consists in the encapsulation of the active sites (commonly metallic nanoparticles (NPs)) offering a barrier to prevent the deactivation caused by the reaction conditions. Au-Pd bimetallic NPs have been deeply studied in the different catalytic reactions. Furthermore, studies show that the structure of these NPs may change under different thermal treatments and/or using several environments impacting their catalytic properties. However, till now the use of Au-Pd NPs as nuclei in NRs has not been studied. The present work was focused on the study of the main stages of Au-Pd@SiO_2 NRs synthesis: (i) synthesis of nuclei and (ii) encapsulation of nuclei into silica. Au-Pd nuclei obtained via the seed method were encapsulated by a modified Stöber method. The synthesis of Au-Pd@SiO_2 NRs was monitored by *in situ* UV-Vis spectroscopy, TEM and STEM. The analysis of position and maximum intensity of Au surface plasmon resonance (SPR) in UV-Vis spectra recorded *in situ* allows follow the steps of Au NPs nucleation and growth. Our data are in a good agreement with the results obtained using more sophisticated methods (*in situ* XANES and SAXS techniques). The formation of metallic Pd onto the Au seeds provoked shifts of the Au SPR to the blue zone starting from the first seconds of contact. Encapsulation of bimetallic Au-Pd NPs into the silica shell (see Fig.1) results in the shift of Au SPR position to the red zone. The presence of Au-Pd core-shell inside the silica shell was confirmed by STEM images (Fig. 1). The method allowed the encapsulation of Au-Pd bimetallic NPs into silica shell. Pd was homogeneously deposited onto the Au seeds according to STEM analy The authors would like to thank O. Callejas, E. Flores, F. Ruiz, J. Peralta and M. Sainz for technical assistance. This research project was supported partly by CONACyT (Mexico) and PAPIIT-UNAM (Mexico) through grants 179619 and 203813, respectively.sis. To the best of our knowledge, this is the first study of the Au-Pd encapsulation into silica.

P-065

DECORATION OF GOLD BY CERIA IN Au@ZrO2 NANOREACTORS

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Keywords: decoration, gold, ceria, nanoreactors.

The decoration of heterogeneous catalysts results in the formation of new contact points or interfaces between materials and in the improvement of their catalytic properties. It is well known that Au nanoparticles (NPs) being supported on ceria are highly active in the several reactions due to the presence of Au-ceria interface. Au NPs to be used as cores for Au@ZrO$_2$ nanoreactors were synthesized using the Turkevich method. Subsequently the Au NPs were encapsulated into silica shell by the Stöber method. The decoration of gold cores of Au@ZrO$_2$ nanoreactors has been performed via filling of nanoreactors with aqueous solution of ceria precursor with subsequent hydrolysis of it with a base. Finally the samples were thermaly treated at 500°C. The structures formed are characterized by a spherical zirconium shell. UV-Vis spectrum of decorated Au-Ce@ZrO$_2$ nanoreactor is characterized by a new peak at ~612 nm which was assigned to the gold cores decorated with ceria because similar peak was found for Au NPs supported on ceria. The presence of ceria on gold cores was confirned by STEM analysis as well. The Au@ZrO$_2$ nanoreactors decorated with ceria manifested improved catalytic activity in CO oxidation compared to that of none-decorated ones. The authors would like to thank O. Callejas, E. Flores, F. Ruiz, J. Peralta and M. Sainz for their technical assistance. This research project was supported partly by CONACyT (Mexico) and PAPIIT-UNAM (Mexico) through grants 179619 and 203813, respectively.

P-066

OPTICAL PROPERTIES OF METALLIC NANOPARTICLES WITH COMPLEX SHAPES

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Keywords: Scattering nonspherical nanoparticles, LSP resonance, DDA method, Si solar cells.

The scattering of light and other electromagnetic radiation by small particles have significant interest of science and engineering for the interesting physical analysis and they many applications in nanotechnology. The Mie electromagnetic scattering theory is used to study different kinds of nanoparticles with arbitrary shapes. For isolated particles with complex geometry, a number of different theoretical and numerical techniques have been used [1]. In this work we used the Discrete-Dipole Approximation (DDA) to model the nanoparticle as an ensemble of coupled dipoles approximating the actual target by an array of polarizable points [2]. We modified the nanoparticle geometries to complex shapes with the implementation of Gielis superformula [3] to DDA scattering codes [4] for analyze the dependence of the shape and dimensions of different metallic nanoparticles in the Localized Surface Plasmon (LSP) resonance. Figure 1 show an example of extinction curves of Ag and Au particles for different shapes. We compare experimental extinction curve in the visible spectra for Au hexagonal nanoparticle with the DDA calculations. We calculated near-field intensity maps for scattering electric field distribution on different shapes of Au nanoparticles at the wavelenght of LSP resonance in the extinction curve. We presents calculations for a nanostructure of Au nanoparticle over ITO substrate to show that the substrate modifies the position of the LSP resonance and can create more peaks. We carried out near-field calculations with DDA method for electric-field intensities within a solar cell composed by an Ag nanoparticle over Si substrate to show that the presence of a nanoparticle above a Si substrate can modify substantially the internal field and changing only the shape of the nanoparticle for cubic to star-shaped particle the electric-field distribution in the Silicon active layer changes drastically.

P-067

PLASMONS IN METALLIC SPHEROIDS

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Keywords: Plasmon. Metallic nanoparticle, Spheroid.

The nanostructuring of materials has been proven to introduce novel properties not known to bulk systems of the same composition. This is especially true for metallic nanostructures which have been shown to enhance electromagnetic fields and confine them to previously unsuspected lengths. Artificially engineering metallic structures in the nanometer range leads to control of the plasmon resonances that

appear. In principle the energy can be tuned by tailoring the nanostructure shape, size and composition. Application and uses for such systems are widespread in many fields such as catalysis, medical imaging, drug delivery, sensing, etc. In this work we study the electromagnetic response of a metallic nanoparticle with a particular shape: a spheroid. This cigar shaped structure is a good academic system to study since it is a first step in breaking simplicity of the sphere but still retains enough rotational symmetry to be analytically tractable. Furthermore a needle shaped metallic nanostructure is of interest in applications such as drug delivery due to its preferential direction of diffusion with respect to particle orientation. We study the system analytically within the long wavelength approximation and numerically using Finite Differences in the Time Domain (FDTD). We obtain electromagnetic spectra which reflect the plasmon resonances. We compare both schemes and analyze application range of each method with regards to particle size and perturbing field characteristics.

P-068

A THEORETICAL STUDY OF COPPER AND COOPER OXIDE CLUSTERS ON DEALUMINATED MORDENITE ZEOLITE

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Keywords: Zeolite; Mordenite; Cooper clusters; Density functional theory.

We present a theoretical study of the configuration of different composites, on terms of periodic-density functional theory method, obtained by the hosting of Cu_x ($x=2\text{-}5$) and Cu_2O_x ($x=1\text{-}4$) clusters within the main channel of completely dealuminated mordenite zeolite. Results shows that cooper clusters are adsorbed by side-pockets electrostatically, in contrast with cooper-oxide clusters that have a preference to being adsorbed to the walls of the main channel of zeolite. On addition, was found that for an even number of copper atoms on clusters, [Cu]3d is the main orbital contribution to the forbidden energy level, while for an odd number [Cu]4d dominates.

P-069

STUDY OF THE EFFECT OF AU-INTERCALATED INTO THE STRUCTURE OF COPPER NITRIDE

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Keywords: Copper nitride, XPS, Structure, Ab initio, Semiconductor.

Copper nitride (Cu_3N) is a semiconductor with anti-ReO_3 structure in which Cu atoms do not occupy perfectly the closely packed sites on (111) planes, it has been suggested as an interesting material for nano-electronic and nano-photonic devices [1, 3]. Recently, it was found that is possible to insert transition metal atoms into the Cu_3N structure to induce significant changes in the optical and electrical properties [2, 4]. Copper nitride intercalated with Au (Cu_3N:Au) films were grown by reactive DC magnetron sputtering on glass substrates. The films were deposited using copper target modified by the insertion of gold pellets. For all films, DC power was 30 W during the sputtering. The working gas and the reactive gas were 99.99% purity Ar and N_2, respectively. In this work, nitrogen flows were 2 to 8 sccm, and argon flow was kept constant at 5 sccm. The deposition time for each sample was 20 min and the pressure during the deposits was 20 mTorr. The composition of the samples was obtained *in situ* by X-ray Photoelectron Spectroscopy (XPS). Nitrogen and gold content in the films change with the nitrogen flow variation. The Cu_3N:Au structure was studied by X-ray diffraction (XRD) analysis and minimization of the total energy with respect to the unit-cell volume. The calculated lattice parameters were in excellent agreement with the experimental values. The theoretical and experimental results showed an increase in the lattice parameter when the Au is intercalated in the Cu_3N structure. The electronic properties were performed by *ab initio* total energy calculations using the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method; the results showed that the Au-intercalated modifies the electronic structure of Cu_3N, so it becomes fully metallic. The Cu_3N:Au samples had a resistivity of $1x10^{-3}$ Ωcm. The authors are grateful to D.A. Domínguez, E. Aparicio, J.A. Díaz A. Tiznado, E. Medina, P. Casillas, for valuable technical assistance. This work was partially supported by projects DGAPA IN106709 and IN103711-2. One of us (IPC) received a scholarship from CONACyT-Mexico.

P-070

FIRST PRINCIPLES STUDY ON THE ATOMIC ARRANGEMENT AT THE INTERFACE OF AlN(0001) ON Al /Si(111): CHARGE DENSITY

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Keywords: AlN, GGA, Charge, Density, arrangement, Si(111), surface.

First principles calculations were performed to study and determine the atomic arrangement at the interface of AlN(0001) on Al/Si(111) surface. The starting system was a Al bilayer on Si(111) to avoid a nitrogen diffusion into the Si substrate. One $\sqrt{3}\times\sqrt{3}$ periodicity, which is reported as the most stable for Al on Si (111), was used; finally, two layers of AlN were added one by one. It is observed that the AlN bilayer grows into the (0001) direction and the mismatch of the AlN with respect the substrate Al/Si(111) induced a stress on the AlN bilayer, this stress will produce stacking defects on the AlN film if continue to grow. Charge density was obtained and compared with the experimental results reported in the literature. Calculations were performed within the periodic density functional theory as implemented in the PWscf code of the Quantum

ESPRESSO package. The exchange and correlations energies are treated according to the generalized gradient approximations (GGA) with the gradient corrected Perdew, Burke and Enzerholf (PBE) functional.

P-071

STUDY OF THE THERMOELECTRIC PROPERTIES OF ReCN

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Keywords: Thermoelectric material, thermopower, Seebeck coefficient, electrical and thermal conductivity.

With combining first principles band structure calculation with semi classical model analysis; we obtained the Seebeck coefficient as well as the electrical conductivity as a function of the relaxation time for the electrons. We used the linearly augmented plane wave code WIEN2k[1] to calculate the band structure and the BoltzTrap[2] code to calculate the thermoelectric properties. In this work we present results of our study that predict that hexagonal ReCN would be a good thermoelectric material at low temperature region.

P-072

RASHBA MODELS FOR Q1D AND Q2D SEMICONDUCTOR HEAVY HOLE SYSTEMS

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Keywords: Spintronics for holes. Rashba spin-orbit interaction.

One of the biggest challenges in Spintronics is the ability to efficiently manipulate spin currents in semiconductors systems without externals magnetic fields. Rashba spin-orbit interaction (SOI-R), is the more recurrent mechanism for achieving this, because its coupling parameter could be tuned via external electric fields. SOI-R for the heavy holes (hh) case is very different to the electrons or light holes (lh) case [1]. Starting from a (8 x 8) Kohn-Lüttinger Hamiltonian and using the Quasi-Degenerate Perturbation Theory (Löwdin partition scheme), we obtain an effective SOI-R Hamiltonian, for a Q2D hh system, with atypical cubic dependence on the wave number reported by Winkler et al. [2], and an expression for the coupling parameter which clarify the anomalous behavior [1] through the dependence on the difference of the hole levels energy. Comparisons with experimental data and previous models are shown. An effective SOI-R Hamiltonian for a Q1D hh system is also obtained. Despite the lack of previous models to compare with, we find an expected linear term [2] as well as a cubic one. In the framework of our theoretical modeling, we conclude that coupling SOI-R parameter diminishes as a function of the hh density for most semiconductors in both Q1D and Q2D cases. We acknowledge financial support from the research project Papiit DGPA-UNAM No.IN109911, México.

P-073

CONDUCTANCE QUANTUM OSCILLATIONS IN QUANTUM RINGS TUNED BY 2D QUANTUM POINT CONTACTS

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Keywords: Spintronics for holes. Transport in quantum rings and spin-orbit interaction.

In this report we study the influence of the Aharonov-Bohm (AB) and the Aharonov-Casher (AC) phases on the interference mechanism in a semiconducting quantum ring (QR), under the presence of Rashba type of spin-orbit interaction. A particular subject of investigation is the role of the upper- together with lower-arm two-dimensional (2D) quantum point contacts (QPCs) to the transparency of the quantum device setup. We additionally consider another 2D QPCs, allocated symmetrically at the ring periphery, thus conforming a different lead-to-ring interface junction [1]. Consistent with the AB-AC effects, expected coherent conductance oscillations are obtained, and its behavior is analyzed as the opacity in the QPC changes. It is shown that manipulating electrostatically the confinement strength at each QPC, as well as the AB and the AC phases, results into new harmonic patterns for the conductance. These phenomenology may be of utility to implement a novel way to modulate spin interference effects in semiconductor quantum rings, providing an appealing test-platform for spintronics applications [2,3].We acknowledge financial support from the research project Papiit DGPA-UNAM No.IN109911, México.

P-074

BACTERICIDAL EFFECT OF SILVER NANOPARTICLES AGAINST ENTEROPATHOGENIC BACTERIA

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Keywords: Bactericidal effect, *Salmonella spp*., EPEC, EHEC, *E. coli*, nanosilver.

Nowadays, the emergence of bacteria multi-resistant to antibiotics is a big challenge for health scientific research. Nosocomial infections and epidemic outbreaks of respiratory and gastrointestinal diseases coupled with antibiotic multi-resistant strains, convey us to explore new alternatives for treatment and control. In this research, we evaluated silver nanoparticles (Argovit) against enteric bacteria: commensal *Escherichia coli*, enteropathogenic and enterohaemorragic *E. coli*, as well as *Salmonella typhimurium*, were tested with different concentrations of Argovit. Lethal concentration of Argovit was determined and bacteriostatic/bactericidal effect of silver nanoparticles was evaluated. Bactericidal effect of Argovit was time-dependent and also concentration-dependent. Pathogenic bacteria survived to higher concentrations of Argovit compared to *E. coli* commensal strain, being *S. typhimurium* the most concentration-resistant bacteria tested. In regard of bactericidal/bacteriostatic effect of Argovit, we determined that silver nanoparticles have bactericidal but no bacteriostatic effect among tested bacteria. Very low concentration of silver nanoparticles had toxic effects on bacterial cultures, whereas animal and cell-culture exposition to Argovit showed no toxic effects at the same concentrations. Isogenic mutants' strains altered in detoxifying systems, efflux-pumps and multi-resistant antibiotic pathways will be challenge with Argovit to get insights about mechanisms of action.

P-075

APPLICATION OF ELECTRO STIMULATION TECHNIQUE FOR INCREASE OF BLOOD CIRCULATION IN DIABETIC FOOT TREATED WITH ARGOVIT SILVER NANOPARTICLES

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Keywords: silver nanoparticles, diabetes, ulcer, leg amputation, electrostimulation.

Diabetes is the number one cause of death in Mexico and the diabetic foot syndrome that results in numerous amputations per year nationwide is a common complication. These are important reasons to look for innovative methods for the prevention and treatment of this disease. The results obtained by the interdisciplinary group developing new method of treatment for diabetic foot syndrome with Argovit silver nanoparticles are of great impact for public health. More than 70 patients having diabetic ulcers have avoided leg amputations during the project clinical tests. Currently this project is on the stage of clinical trials in the hospitals of ISSTECALI. Our results have showed that in all cases, in which a negligible circulation was observed, application of silver nanoparticles cannot lead to positive results and amputation was unavoidable. Therefore the medical innovative group under leadership of doctor Dr. Cesar Alejandro Almonaci Hernández continues to look for complimentary methods, which could significantly improve blood supply and circulation. Electrostimulation technique is one of the prospective methods, which could be applied in the previously mentioned cases. In the present work the first results of the application of electro stimulation to improve blood circulation; perspective and discussion are presented.

P-076

GENOTOXICITY OF ARGOVIT NANOSILVER PARTICLES IN HUMAN LYMPHOCYTES IN *IN VITRO* CULTURE

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Keywords: Nanosilver, genotoxicity, citoxicity.

The objective of this study was to determine cytotoxic and genotoxic effects of Argovit silver nanoparticles over human lymphocytes in vitro cultures using the micronucleus assay by blocking of cytokinesis (MNBC). All three healthy subjects that participated in the study after signing informed consent, were normocytic and showed normal values in all parameters after SMAC-33 and standard blood cell counts. Each donor provided 10 mL of venous whole blood. The experiment consisted of a control and four treatments with 21 □L of 20% Argovit nanosilver (n-Ag) diluted at $2.5\text{x}10^{-4}$, $2.5\text{x}10^{-3}$, $2.5\text{x}10^{-2}$ and $2.5\text{x}10^{-1}$, adding to the culture 0.5 mL of blood, 6.2 mL RPMI and 0.3 mL of phytomeglutinina. Cultures were incubated at 37^{o}C in darkness, after 48 hours, cytokinesis was blocked with cytochalasin-B and incubated for 24 hours. Lymphocytes were fixed with 3:1 methanol-acetic acid, mounted on slides and stained with eosin and methylene blue. The cell proliferation index and the number of micronuclei per thousand of binucleated cells were determined by microscopic counts. The proliferation index showed normal values as in healthy subjects and compared with the control slide. The number of micronuleus in those treatments where n-Ag was added showed no statistically significant differences with the control. Experimental findings and evidence suggest that Argovit silver nanoparticles do not exhibit genotoxic nor cytotoxic effects over human lymphocytes, although further studies are necessary.

P-077

HISTOLOGICAL STUDIES OF DIABETIC FOOT SAMPLES OBTAINED FROM PATIENTS TREATED WITH ARGOVIT NANOSILVER

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Keywords: Argovit silver nanoparticles, histological studies, diabetic foot.

Diabetic foot is one of the more visible problems related to diabetes. It is characterized by the presence of ulcers and necrotic tissues, which may lead to the loss of the full leg and develop relative illness. This problem is difficult to attend adequately, mainly because the necrosis, the poor blood flux and the presence of pathogenic microbial agents. In the present work, tissues, obtained from patients with diabetic foot, silver nanoparticles were prepared and analyzed with standard histological techniques. The samples were obtained from 8 clinical patients of different physiological characteristics before and after Argovit silver nanoparticles treatment, and additionally after treatment of mixture of Argovit with tropoelastin. In total 291 histological samples were prepared and then were stained with two different techniques: Hematoxylin-Eosin, Gram stain and other were left unstained in order to perform further studies. The samples were studied with light microscopy. In preliminary studies, necrotic and infected areas in samples untreated with Argovit were investigated. In post-treatment samples, the epidermal layers showed a normal morphology and structure, as well as absence of microorganisms. On the other hand, samples treated with nanosilver and elastin apparently did not show an antimicrobial effect.

P-078

REGIONAL DEVELOPMENT IN BAJA CALIFORNIA, MEXICO: IMPORTANCE OF TECHNOLOGICAL DEVELOPMENT AND INNOVATION IN THE APPLICATION OF SILVER NANOPARTICLES (ARGOVIT) FOR BIOMEDICINE AND VETERINARY

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Keywords: regional development, Baja California, México, importance, silver nanoparticles, Argovit, biomedicine and veterinary.

Our group is a multidisciplinary team committed to the development of strategic projects within the areas of nanotechnology and biotechnology, focusing in economics and management aspects of these fields. This team has participated and/or developed The Science and Technology Special Program of Baja California, The Business Development Policy of Baja California, among others projects. Currently it is responsible for analyzing the potential for the formation of the Biotechnology Cluster in Baja California, and the search of new markets for the application of Argovit. This work presents the analysis of the potential of the technological sector of UNAM CNyN "Application of silver nanoparticles Argovit in Healthcare and Agriculture" for regional development in Baja California, Mexico. The results of this multidisciplinary study in the areas of economics, management, business models, marketing and more are described.

P-079

STUDY IN DIABETIC FOOT SYNDROME WITH APPLICATION OF ARGOVIT SILVER NANOPARTICLES IN PATIENTS AT ISSSTECALI MIRADOR HOSPITAL IN TIJUANA, BAJA CALIFORNIA, MEXICO

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Keywords: diabetic foot, nanosilver, ISSSTECALI, clinical study.

The Research Department Team at ISSSTECALI is currently negotiating and willing to compromise with CNyN-UNAM and other prestigious institutions in collaborating and implementing a comprehensive pre-clinical and clinical study, applying the innovative treatment of diabetic foot syndrome with the use of Argovit silver nanoparticles. This collaboration effort of ISSSTECALI is based on the need to look for better treatments in one of the most adverse consequences of diabetes, the diabetic foot syndrome; which in many cases leads to amputation. Is well known that diabetes is the leading cause of death amongst the Mexican population. In accordance with its institutional mission, ISSSTECALI is willing to contribute with its infrastructure to the fight against diabetes and its consequences. Currently we are consolidating an enthusiastic research medical team composed of surgeons, nurses, psychologists, social workers and undergraduate intern medics that had shown their interest in innovative methods of treatment. It is important to mention that ISSSTECALI highly recommends that a group of medical specialist in integral attention of diabetic patients is closely involved to advise and monitor the study progress at all times. Initially, subjects of study will be patients from the Mirador Tijuana Hospital, and later from the Ensenada and Mexicali ISSSTECALI Hospitals. Also, this valuable team is undergoing the necessary training by Dr. Cesar Alejandro Almonaci Hernández to handle with professionalism, those cases in which amputation is medically recommended. ISSSTECALI is also following thru with the formal paperwork deem necessary to initiate the study.

P-080

ADSORPTION OF nitrogenous organic BASES ON NATURAL MONTMORILLONITE AND SYNTHETIC NANO MONTMORILLONITE IN WATER TREATMENT

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Keywords: Organic nitrogenous compounds removal, montmorillonite adsorption, clay water treatment.

Advances in nanoscience and nanotechnology permit that many of the current problems related to water quality could be solved or improved with the use of nano materials that allow the removal of undesirable substances. This work presents the results of using natural montmorillonite and synthetic nano montmorillonite for the adsorption of nitrogenous organic bases from water solutions, which can be applied in the development of new processes for water treatment, drug delivery, etc. Furthermore, it is contemplated the potential use of natural and synthetic clays in the removal of toxic metal ions, soluble organic and inorganic substances with environmentally acceptable processes. The sample of natural clay (montmorillonite) was obtained from Tijuana UABC campus by digging 30 cm deep. The sample was sieved, thermally activated and decarbonated. The adsorption experiments of nitrogenous organic bases were carried out with samples of natural clay and synthetic nanoclay. Adsorption efficiency determined by means of adsorption isotherms using guanidine and uric acid solutions showed that nitrogenous organic base removal from aqueous solution was 70-85%. Additionally, the crude fraction and thermally activated montmorillonite shows a high adsorption capacity for aqueous H_2S and trace metals (Cu, Ni, Cr and Co) in solutions.

P-081

APPLICATION OF ARGOVIT SILVER NANOPARTICLES FOR TREATING PNEUMOENTERITIS

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Keywords: nanosilver, calf pneumonia, calf enteritis.

The raising calves in a dairy farm represent the future replacement of cows which are currently in production. Appropriate management decisions can increase significantly herd productivity. Pneumoenteritis is a very common problem in newborn animals, hence the concept drifts to "neonatal" one (usually occurs in species under 15 days and sometimes up to 35 days). It is characterized clinically by excretion of diarrheal stools, watery and profuse, dehydration, acidosis and death within a few days or hours. Although the term "pneumoenteritis" is grouped by both "pneumo" and “enteritis" words, the main draw is the enteric and that is where we should focus. A complex suffering calves from pneumoenteritis is causing important economic losses. All tools we now have at our disposal, including effective management techniques and advanced biological innovations should be applied to prevent pneumoenteritis. The aim of this study is to study the conditions of application of Argovit silver nanoparticles for treatment of calve pneumoenteritis. A totally 40 Holstein females fed newborn calves with colostrum at birth. 12 calves were selected (considering corporal condition and weight), and three groups were formed according to the methodology described by Cortes and Lara. The experimental groups (B and C), received two daily doses of silver nanoparticles solution in milk. Nanoparticles represent a liquid (20% of nanosilver containing 1.2% of metallic silver) and were prepared in a 1:66 dilution in milk. The application of treatment was at a dose of 1ml (sol. nanosilver)/kg (calf). The treatment time was seven consecutive days. The control group (A) received conventional therapy consisting in bismuth subsalicylate application with a dose of 5 ml sol / weight (kg). The dose was given 2 times a day in milk. The obtained results will be discussed.

P-082

THE DEVELOPMENT OF INNOVATIVE METHOD OF TREATMENT OF DIABETIC FOOT WITH ARGOVIT SILVER NANOPARTICLES

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Keywords: --------.

In the present work, the results of the application of a new method of treatment for diabetic foot with Argovit silver nanoparticles are presented. This innovative approach for the treatment of diabetic foot syndrome was successfully applied in more than 70 patients. The ethics committee of the General Hospital of Tijuana, B.C., Mexico approved the protocol of treatment with the developed method. From March to June of 2012 clinical studies were carried out in the General Hospital of the city of Playas de Rosarito. It is important to mentio that the application of Argovit silver nanoparticles resulted in the prevention of leg and foot amputation in diabetic foot syndrome patients, and that this prevention is of high social value. Currently the medical group under the leadership of Dr. Cesar Alejandro Almonaci Hernámedez is responsible for the training of medical staff of ISSSTECALI hospitals. The group is in constant search of improvements to all stages of the treatment of diabetic foot patients which exhibit different associated diseases.

P-083

DISTRIBUTION KINETICS AND TOXICITY OF ARGOVIT SILVER NANOPARTICLES

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Keywords: Argovit silver nanoparticles, distribution kinetics and toxicity.

Nanotechnology offers a wide range of therapeutic products for human use. Silver nanoparticles have been used as a potential medicine against virus and bacteria. But little is known about silver nanoparticles toxicity and their distribution patterns inside complex living organisms. Further efforts need to be accomplished to evaluate their safe use on humans. The present work has the following goals:

1. Evaluate the median lethal dose (LD50) of Argovit silver nanoparticles for Winstar rats.
2. Evaluate the distribution kinetics of Argovit silver nanoparticles in Winstar rats.
3. Evaluate toxicity of silver nanoparticles for cell culture. Cell viability assays (MTT, Bradford, neutral red).

Ten Winstar rat groups (10 rats in each group) were studied. Five groups were investigated for peritoneal and five groups for oral administration. A daily 50 uL dose of 40%, 20%, 10%, 5% and 2.5% solutions of Argovit silver nanoparticle were administered, than the procedure was reproduced. After 45 days of Argovit application measurement of silver content in different organs was performed. Blood samples were taken before Argovit administration, and 15th, 30th and 45th day of Argovit administration. Oral and peritoneal administration of silver nanoparticles had no mortality effect, even at 40% concentration, proving that LD50 is over this concentration. Blood analysis showed no significant changes of normal parameters. Evaluation of distribution kinetics and cell culture toxicity is being performed and soon will be finished.

P-084

EVALUATION OF ARGOVIT SILVER NANOPARTICLES AS ANTIMICROBIAL TREATMENT FOR DIABETIC FOOT ULCERS ON MEXICAN POPULATION AT ROSARITO GENERAL HOSPITAL

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Keywords: Nanotechnology, silver nanoparticles, diabetic foot.

The World Health Organization stated that there are 220 million people suffering diabetes (80% of that lives in underdeveloped countries such as Mexico) and 3.4 million people died due to high plasma glucose levels. Diabetes is the first cause of death among Mexicans. During the year 2008 the mortality rate was 71/100 thousand Mexicans. In the border Baja California state the disease had the 7th place in morbidity and the 3rd in mortality. Diabetic ulcer infections are hard to control because of the vascular troubles and the high rate of poli-microbiological and drug resistant infections presented by patients. The aim of the present work was to evaluate the effect of Argovit silver nanoparticles on treatment of diabetic foot ulcers. 15 patients

(not responding to conventional antibiotic treatment) with diabetic foot ulcers were treated with solution of Argovit silver nanoparticles. Antibiotic treatment of these patients was stopped and clinical tests with Argovit were conducted. 90% of the patients fully recovered in 3 months. Recovery time in case of Argovit application was shorter than in the cases of conventional antibiotic treatments.

P-085

ARGOVIT: APPLICATION PROSPECTS IN TREATMENT OF LIVESTOCK AND POULTRY IN CENTRAL MEXICO

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Keywords: nanosilver, alternative to antibiotics, feed conversion.

It has been 25 years since the last antibiotic for veterinary use was discovered, consequently as a result of using it every day, early signs of bacterial resistance begin to come to light. Veterinary clinicians are looking for an alternative to antibiotic treatments in order to replace them. Integración y Comercio company has been active in the establishment of protocols and marketing of a wide range of antibiotics for farm and companion animals. Since the founding of our company in 1997, our primary interest is focused on the development and linking with new technologies aimed to health and wellbeing of animals. Since some years ago we have been cooperating with CNyN-UNAM in implementing disruptive technologies (Argovit silver nanoparticles) in the field of animal health in Mexico. The goal of our collaboration with this institution has been to facilitate the transfer of these technologies to the production areas, farms producing eggs, broilers, pork and dairy producers, as well as promoting healthy farms. We know about the great achievements that nanotechnology products have had in the past, such as Argovit from Vector-Vita. The benefits of Argovit application in dairy calves have been proven in the field; we have also begun a trial with calves and broilers. We hope to demonstrate the benefits of using of Argovit in: reduction of mortality, decrease in the use of antibiotics, as well as higher animal growth compared to the control group that was treated with a mixture of antibiotics (Bacitracin and Colistin). Our main objective is to determine optimal concentration, treatment duration, zootechnical feed conversion effects, daily gain, weight obtained at a given age, mortality in the period, residual effect, rejecting consumerism and biological effects: intestinal integrity, effect on bacterial population, effect on other organisms, mainly fungi. Our aim is to show that Argovit is a real alternative to the use of antibiotics in disease prevention and therapy.

P-086

THE MOLECULAR EPIDEMIOLOGY OF HUMAN IMMUNODEFICIENCY VIRUS ON THE MEXICO-UNITED STATES OF AMERICA FRONTIER: APPLICATION OF SILVER NANO PARTICLES TO HIV RESEARCH

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Keywords: HIV, silver nanoparticles, molecular epidemiology.

The world's public health has been hardly hit by the HIV epidemic since the first HIV cases in the early 1980s. It's been more than 3 decades since its appearance and despite all the great scientific advances in discovering the nature of the HIV, and the factors influencing its population spread, we are long from being able to stop the epidemic. New and improved efforts must be applied to HIV research if we are to do it one day. Estimation reveals that there is one HIV positive person per every 125 people living in Tijuana, Mexico (population of Tijuana is over 3 million). The number of infections seems to have settled during the last decade due to the introduction of universal treatment and our efforts on improved prevention strategies. But, there are still around 15-25 new infected people per month in Tijuana. The impact of the HIV's high genetic variability is still unknown. There are more than 40 clusters spreading the epidemic and some of them have been related to a faster morbidity and mortality. Silver nanoparticles are well known by their anti-microbial properties. They inhibit bacterial, virus, and oncotic pathogens. The first stage of our study focuses on the discovery of the genetic HIV variants present on the northern part of Mexico. And in a second stage we will determine the nature of the interaction of our silver nanoparticles with the variants we find. Our main goal is to analyze if our silver nanoparticles can be used as a new HIV treatment.

P-087

DIABETIC FOOTWEAR WITH NANO-SILVER APPLICATION

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Keywords: diabetic footwear, preventive infections in the feet, nanosilver lining for footwear.

Nanopartículas Aplicadas, S.A. de C.V." is developing the special footwear for diabetic foot with nano-silver nanoparticules, to propose a new offer of diabetic footwear with more benefits in injuries prevention and protection of the common infections in the feet, comparing with another shoes availed in the actual market. This development involves at first, the investigation, evaluation and selection of the adequate materials free of restricted substances approved by the Leather Working Group Environmental Stewardship , and all the technical requirements established for the standard proposal of special footwear , in order to certificate the footwear with the MEDICARE in EUA, and finally to offer a reliable product to the patients. An independent and multidisciplinary team has been integrated considering designing area, modeling, product engineering, prototype review and production implementation. It has also invested in machinery and equipment for the exclusive production of pullovers. At the same time, feasibility studies have been conducted to assess market potential and profitability, as well as locate potential customers and sales establishment specialized in diabetic footwear. We also conducted surveys to receive feedback from the potential customers, and sales abroad strategies for United States, Central and South America, finding good opportunities for sale in Guatemala, El Salvador, Costa Rica, Panama, Chile, Colombia and Brazil. A unique trademark with the name of Nanofit® has been created to represent the line of Nano-silver diabetic footwear, which was registered in the IMPI and is currently in the process of registration in USPTO (United States Patent and Trademark Office), USA. This technology innovation is linked with the project: "Applications of nano-silver footwear lining for diabetic patients and sensitive feet, to protect from pathogens microorganisms", developed by CNyN-UNAM and CIATEC, A.C., supported by the IMPI patent application folio MX/E/2012/071886.

P-088

ELECTRICAL CHARACTERIZATION OF MICRO AND NANO SIZED STRUCTURES USING NOVEL DESIGN MANIPULATORS

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Keywords: manipulators, electrical measurements, nanostructures.

Advances in fabrication and synthesis of nanometer size materials and devices have created a demand for high resolution positioning mechanisms and manipulators. In a traditional measurements, the material (a nanorod, nanowire, nanotube) to be electrically measured is deposited on pre-fabricated micro electrodes on a substrate, relying on chance that the material touches the desired electrodes, or using the tip of an atomic force microscope to reposition the nanostructure. Another method consists of fabricating metal electrodes on both ends of the material previously deposited on a substrate. These methods are time consuming and require the availability of sophisticated equipment. In this work we report the use of novel nanopositioning devices with three DOF specially design to be used as electrical probes inside a SEM. At the end of the probes, fine metal tips make contact with sub-micro size structures. With this approach, electrical characterization is greatly simplified. We report examples of electrical measurements of carbon nanotubes and zinc oxide nanostructures, and discuss other applications in material characterization, such as using an optical fiber as a localized probe for optical characterization of light emitting materials.

P-089

MESOPOROUS MATERIALS AS SUPPORTS OF CATALYSTS AND BIOCATALYSTS

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Keywords: Nanorods, bio refinery, hydrodesulfurization.

Nanocatalysis encompasses chemical and biological catalysis, and bring together advances in nanotechnology and bionanotechnology such as the immobilization of biocatalyst on mesoporous materials used in heterogeneous catalysis. These materials hold important properties that make them excellent candidates to serve as a chemical catalyst supports for various applications in petrochemistry and biorefinery. Herein we present the synthesis, characterization and usage of Alumina Nanorods (AN-P123-1) as catalysts and as support material for enzyme immobilization. Alumina Nanorods are self-supported within a mesoporous Al_2O_3 with a well-defined unimodal pore size distribution; this material has shown a high surface area alumina (415 m^2 g^{-1}) in comparison with the commercial alumina (245 m^2 g^{-1}). Because of this, our research group has used them as supports for the immobilization of the enzyme Chloroperoxidase (CPO) from the black mold *Caldariomyces fumago* and to prepare catalysts based on Ni and W for desulfurization of refractory molecules such as dibenzothiophene (DBT) and 4,6'-dimethyl dibenzothiophene (4,6' DMDBT) by oxidative desulfurization or hydrodesulfurization respectively. Preliminary tests with the catalyst NiW-AN-P123 in sulphide phase, showed higher catalytic properties than the commercial catalyst NiW-HR-354 made in France. To use AN-P123-1 as support material for biocatalyst, we have calcinated the material at higher temperatures (700 and 900 °C) to obtain a larger pore size, according to these results, the best material for immobilizing the CPO-enzyme was the AN-P123-1 calcinated at 700°C. Immobilized CPO on AN-P123-1-700°C, shown a better halogenase activity when compare with the “free-enzyme”, suggesting that the material provides to the enzyme with a nanoenviroment that favors and improves its catalytic activity. Currently various techniques are being used for the complete characterization of this catalysts and verify the effect of the catalytic activity of AN-P123-1-700 in biodesulfurization process.

AUTHOR INDEX

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