

Tetrahedral motifs in the amorphous networks of Phase Change Materials

Flores-Ruiz Hugo M.^{1*}, Micoulaut M.², Pradel A.³ and Piarristeguy A.³

 ¹ Departamento de Ciencias Naturales y Exactas. CUValles, Universidad de Guadalajara, Carretera Guadalajara-Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México.
 ² Sorbonne Université, Laboratoire de Physique Théorique de la Matière Condensée, CNRS UMR 7600, 4 Place Jussieu, 75252 Paris Cedex 05, France
 ³ ICGM, Université de Montpellier, CNRS, ENSCM, 34095, Montpellier Cedex 5, France * hugo.flores@academicos.udg.mx

The binary amorphous telluride $GeTe_2$ is analyzed by first principle molecular dynamics simulations, in order to obtain structural information in the real and reciprocal space [1]. The structure properties from simulations are compared with X-ray diffraction experiments and finding a very good concordance [1]. It is found that base geometrical motif of the germanium atoms can be either tetrahedral or defected coordination involving pyramidal units [1], and the concentration of these tetrahedral geometries are quantified [1]. Also, the structure properties of amorphous GeTe₂ are compared with other systems like GeSe₂, GeS₂ and GeO₂ [1]. Additionally, it is found that Ge rich materials GeTe₂ and GeTe have soft tetrahedra in comparison with GeSe₂ or GeS₂ [1].

Key Words: tetrahedral, amorphous, phase change materials, abinito simulations.

References

[1] M. Micoulaut, Flores-Ruiz H. M., A. Pradel and A. Piarristeguy, *Physica Status Solidi* 15, 1-9, (2021).



EXPERIMENTAL EVIDENCE OF ELECTROCHROMISM IN ITO AND FTO AND AB INITIO STUDIES

Israel Pérez^{1*}, Víctor Sosa², Fidel Gamboa², José Luis Enríquez-Carrejo³ y Juan Carlos Mixteco Sánchez⁴

¹National Council of Science and Technology (CONACYT)-Department of Physics and Mathematics, Institute of Engineering and Technology, Universidad Autonoma de Ciudad Juarez, Av. del Charro 450 Col. Romero Partido, C.P. 32310 Juarez, Chihuahua, Mexico
²Applied Physics Department, CINVESTAV Unidad Merida, km 6 Ant. Carretera a Progreso, A.P. 73, C.P. 97310 Merida, Yucatan, Mexico

³Department of Physics and Mathematics, Institute of Engineering and Technology, Universidad Autonoma de Ciudad Juarez, Av. del Charro 450 Col. Romero Partido, C.P. 32310 Juarez, Chihuahua, Mexico

⁴Department of Natural and Exact Sciences, CU Valles, Universidad de Guadalajara, Carr. a Guadalajara km. 45.5, C.P. 46600 Ameca, Jalisco, Mexico

*Corresponding author e-mail: israel.perez@uacj.mx

Electrochromism is the effect of changing the optical properties of a material due to the intercalation/deintercalation of ions promoted by the action of an electric field. Electrochromic devices (ECDs) are made up of five layers in a sandwich arrangement: in the center is the electrolyte layer (liquid or solid), on one side of the electrolyte is an ion storage layer made up of an oxide of a metal of transition; on the opposite side, another transition metal oxide acting as electrochromic active material and as electrical contacts on the edges, two transparent conductors, usually ITO or FTO. In this work we show experimental evidence of electrochromism in transparent ITO and FTO conductors that were embedded in a LiCiO4/PG+EG solution bath. Transmittance and cyclic voltammetry tests were performed to estimate the electrochromic properties. ITO was found to have a respectable coloration efficiency of 33.4 cm2/C, while FTO has a coloration of 47.9 cm2/C (@ 637 nm). Ionic insertion was evaluated with X-ray photoelectron spectrometry (XPS) studies. To support the experiments, first principles calculations of lithium ion intercalation in the two systems were performed and the effects on the electronic properties were studied. Li enters as interstitial in FTO and as substitutional at vacant In/Sn sites in ITO. Valence band spectra were calculated and contrasted with XPS measurements. The results are in agreement with the observations. The findings are presented as evidence of electrochromism in transparent conductors, which can reduce the number of layers, as well as production times and costs in DECs [1,2].

References

- [1] I. Perez et al. J. Chem. Phys. 156, 094701 (2022); doi: 10.1063/5.0085531
- [2] I. Perez et al. To be published in Electrochimica Acta, 2022



DESIGN AND CHARACTERIZATION OF HIGHLY DIFFUSIVE NANOSTRUCTURED SURFACES BY SOFT COLLOIDAL LITHOGRAPHY

Jesus Gerardo Guerrero-Felix_{1,2}*, Javier Lopez-Miras₁, Carmen Lucia Moraila-Martinez_{2,3}, Miguel Angel Fernandez-Rodriguez₁.

Department of Applied Physics, University of Granada, 18071 Granada, Spain.
 Biology faculty, Autonomous University of Sinaloa, 80010 Culiacan, Sinaloa, Mexico.
 Department of Electronics and Computer Technology, University of Granada, 18011 Granada, Spain.

*gerardogf@correo.ugr.es

Nanostructuring of surfaces can enhance their optical, mechanical, magnetic, catalytic, and other properties. The optical enhancement in photovoltaic devices results into a higher energy efficiency by decreasing the reflectivity and increasing the amount of light that the device can harvest [1]. Currently, there are different techniques to fabricate these nanostructures; one of them is the Soft Colloidal Lithography. This technique consists in the self-assembly of a monolayer of microgels, nanoparticlescomposed of hydrogel, at the water/air interface using a Langmuir trough. After that, this monolayer is deposited on a solid substrate, in our case on a silicon wafer [2]. This deposited monolayer acts as a template when the substrate is immersed in a dispersion of inorganic nanoparticles. The nanoparticles are deposited between the microgels. With this technique, several structures can be created by double depositions of microgels on the substrate. The first microgel monolayer acts as a template where themicrogels of the second monolayer rearrange to occupy interstitial positions [3]. In this work, we show the results obtained using titanium dioxide nanoparticles (TiO₂) with a diameter of 78 nm with the Soft Colloidal Lithography technique (see Figure 1). We characterized the surfaces by means of Atomic Force Microscopy and performing diffuse reflectance measurements in order to find if they are able to enhance the diffusivity of the substrates, with potential impact on the energy harvesting of photovoltaic devices.



Figure 1–AFM images of a. Microgel monolayer with nanoparticles occupying interstitial positions b. Same substrate after the incineration of the microgels c. Nanostructure of microgels by double deposition.

References

- [1] Matthew C Beard et al. Nature nanotechnology 9.12 (2014), pp. 951–954.
- [2] Miguel Angel Fernandez-Rodriguez et al. Nanoscale 10.47 (2018), pp. 22189–22195.
- [3] Fabio Grillo et al. Nature 582.7811 (2020), pp. 219–224.



HYPERBOLIC PLASMONS IN MASSIVE TILTED DIRAC MATERIALS

Miguel Abraham Mojarro Ramírez₁*, Ramón Carrillo Bastos₂, Jesús Alberto Maytorena Córdova₃

¹ Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701, USA. ² Facultad de Ciencias, Universidad Autónoma de Baja California, Apartado Postal 1880, 22800 Ensenada, Baja California, México ³ Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Apartado Postal 2681, 22800 Ensenada, Baja California, México *mm232521@ohio.edu

We explore topological transitions in the type of propagation of surface electromagnetic modes in massive anisotropic tilted two-dimensional (2D) Dirac systems [1]. The presence of tilting and mass gives rise to an indirect band gap that strongly modifies the joint density of states compared to the gapless system [2]. New Van Hove singularities appear, and the interplay between intra- and interband transitions leads to an anisotropic optical conductivity with imaginary parts acquiring opposite signs in orthogonal directions, opening the possibility of having hyperbolic propagation of plasmons. Isofrequency contours and low plasmon losses, as obtained from the dispersion relation, show that transitions between purely anisotropic quasielliptical and well-defined, highly directional, hyperbolic modes are attainable only when tilt and mass coexist via frequency and Fermi level variation. This behavior could be probed in massive tilted 2D Dirac materials like the organic-layered compound α -(BEDT-TTF)₂I₃ [BEDT-TTF = (bis-(ethylenedithio)tetrathiafulvalene)] [3] or WTe₂, in which hyperbolic plasmons were recently observed [4], through far-infrared absorption, optical nanoscopy, and similar current tools in graphene plasmonics.

Key Words: Optical conductivity, plasma oscillations, two-dimensional systems.

References

[1] Mojarro, M. A., Carrillo-Bastos, R., & Maytorena, J. A. (2022). Hyperbolic plasmons in massive tilted two-dimensional Dirac materials. *Physical Review B*, *105*(20), L201408.

[2] Mojarro, M. A., Carrillo-Bastos, R., & Maytorena, J. A. (2021). Optical properties of massive anisotropic tilted Dirac systems. *Physical Review B*, *103*(16), 165415.

[3] Uykur, E., Li, W., Kuntscher, C. A., & Dressel, M. (2019). Optical signatures of energy gap in correlated Dirac fermions. *npj Quantum Materials*, *4*(1), 1-8.

[4] Wang, C., Huang, S., Xing, Q., Xie, Y., Song, C., Wang, F., & Yan, H. (2020). Van der Waals thin films of WTe2 for natural hyperbolic plasmonic surfaces. *Nature communications*, *11*(1), 1-9.



Berry-phase effect in single molecule magnets: Analytical and Numerical Results

Fco. Javier Anaya-García¹, Daniel Salgado-Blanco³ and <u>Gabriel González^{1,2*}</u>

¹ Coordinación para la Innovación y la Aplicación de la Ciencia y la Tecnología, Universidad Autónoma de San Luis Potosí, San Luis Potosí, 78000 MEXICO

² NanoScience Technology Center, Department of Physics, University of Central Florida, Orlando, FL

32826, USA

³ Instituto Potosino de Investigación Científica y Tecnológica, Camino a la Presa San José 2055, 78216, San Luis Potosí, MEXICO

*gabriel.gonzalez@uaslp.mx

We theoretically and numerically investigate transport signatures of quantum interference on the current through a single molecule magnet transistor tunnel coupled to oppositely polarized leads in the presence of a local transverse and longitudinal magnetic field. Our calculations are based on a density matrix approach where we treat the ground state energy splitting induced by tunneling of the spin between different paths with the aid of perturbation theory. Using this approach we show that it is possible to use an effective Hamiltonian which describes the Berry phase interference as a function of the transverse magnetic field which completely blocks the current flow when we place the single molecule magnet between oppositely polarized leads. Finally, we use this effective Hamiltonian in an open source Python software (QmeQ) that allows us to calculate the current through the single molecule magnet with oppositely polarized leads tunnel coupled to the single molecule magnet. The analytical results are well reproduced by our numerical simulations.



Figure 1 – Schematic of the proposed experiment to experimentally detect the Berry-Phase quantum interference effect in single electron transport across a single molecule magnet transistor.

Key Words: Single Molecule Magnets; Berry-Phase Interference; Single Electron Transport

References

[1] W. Wernsdorfer, M. Soler, G. Christou, and D. Hendrickson, "Quantum phase interference (berry phase) in single-molecule magnets of [mn 12] 2-," Journal of applied physics, vol. 91, no. 10, pp. 7164–7166, 2002.

[2] G. Gonzalez and M. N. Leuenberger, "Berry-phase blockade in single-molecule magnets," ' Physical review letters, vol. 98, no. 25, p. 256804, 2007.

[3] G. Kirsanskas, J. N. Pedersen, O. Karlstr * om, M. Leijnse, and A. Wacker, "Qmeq 1.0: An open-source python package for calculations of " transport through quantum dot devices," Computer Physics Communications, vol. 221, pp. 317–342, 2017.



Electronic structure and optical response of coordination polymers based on transition metal cyanides

Hebert Rodrigo Mojica Molina^{1*}, Ana Elizabeth Torres Hernández², Edilso Reguera Ruíz¹

 ¹ Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada, Instituto Politécnico Nacional, Calzada Legaria No. 694, Col. Irrigación, Del. Miguel Hidalgo, Cp 1500, Ciudad de México, México.
 ¹ Instituto de Ciencias Aplicadas y Tecnología, Universidad Nacional Autónoma de México, CU, Del. Coyoacán, Cp 04510, Ciudad de México, México
 *hmojicam1900@alumno.jpn.mx / rodrigo1993mx@gmail.com

Bidimensional coordination polymers based on transition metal cyanides and nitropusside ion were synthesized and studied by means of combined spectroscopic techniques (IR, raman, UV-Vis, XPS) and periodic DFT computations with GGA, meta-GGA and hybrid density functionals[1]. For the studied materials it was found that they correspond to wide band gap semiconductors with potential applications in photochemistry[2,3]. The influence of their dimensionality and the incorporated transition metals from groups XI and XII on the electronic structure and optical response is discussed. The mechanisms that dominate the HOMO-LUMO electronic transitions is studied according to the computed band dispersion, the density of states (Figure 1) and UV-Visible spectroscopy. It is found that metal-ligand charge transfer is responsible of their optical behavior through the π -back donation mechanism occurring in metal atomic orbitals is taken into account [3]. The exciton properties formed through indirect electronic transitions and the quantum confinement is also discussed. New band gap values are proposed, as well as methodologies that accelerate the computations of periodic coordination polymers obtaining accurate results at a reasonable computational cost.



Figure 1 – Projected density of states from Gold cyanide (AuCN) system.

Key Words: Cyano-based coordination polymers, wide band gap semiconductor, density



functional theory, electronic structure.

References

- [1] A. Cano, Y. Avila, M. Avila, E. Reguera., J. Solid State Chem. 339–344, (2019).
- [2] A.M. Chippindale, S.J. Hibble, E.J. Bilbé, E. Marelli, A.C. Hannon, C. Allain, R. Pansu, F. Hartl., J. Am. Chem. Soc, 16387–16400, (2012).
- [3] C.A. Bayse, J.L. Ming, K.M. Miller, S.M. McCollough, R.D. Pike., Inorganica Chim. Acta, 47–52, (2011).



DFT Study of the Structural, Electronic, and Chemical Properties Cun (n=3-20) clusters by grown pattern

José Aminadat Morato-Marquez (1)*, Carlos López-Castro (2), Gilberto Torres-Torres (1), Gabriel Merino (2), Filiberto Ortíz-Chi (3)*

 Universidad Juárez Autónoma de Tabasco, Centro de Investigación de Ciencia y Tecnología Aplicada de Tabasco, C.P. 86690, Cunduacán, Tabasco, México.
 Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados, Unidad Mérida. Km 6 Antigua Carretera a Progreso, Apdo. Postal 73, Cordemex, 97310 Mérida, Yucatán, México.

(3) Investigador por México, División Académica de Ciencias Básicas, Universidad Juárez Autónoma de Tabasco, C.P. 86690, Cunduacán, Tabasco, México.

*Corresponding author e-mail (aminadatmarquez@gmail.com, fortiz@conacyt.mx).

Transition metal clusters possess many exceptional properties and have been the subject of numerous experimental and theoretical studies, due to its wide range of applications in materials research. In the context of catalysis, small copper clusters have been found active for different reactions due to the high concentration of active sites and a favorable metal-support interaction. Several previous works have reported some small cupper clusters structures, and exits a trend to find them in other structures of bigger sizes, Due this, in this work a systematic computational study is presented for the determination of the minimum energy geometries of the clusters Cu_n (n=1-20) through grown pattern method. We determined a number of initial populations agree with the number "*n*" of atoms by "*i*" isomers of the "*n*" previous cluster (*n*-1). Then, the structures are carried out using methods based on the functional density theory (DFT) framework implemented in the Gaussian computer package 16. The structural information of copper clusters is in agreement with previous reports in the literature, and the energetic, electronic and chemical properties show a trend to the bulk cupper phase.





Figure 1 – Global minimum of Cu_n (n=3-20) clusters. **Key Words:** DFT, Clusters, Copper, Grown Pattern. **References**

[1] J. A., Morato-Márquez et al., Chem. Phys. Lett. (2020). DOI: 10.1016/j.cplett.2020.137677

[2] P. L. Rodríguez-Kessler, et al., J. Phys. Chem. C (2019). DOI: 10.1021/acs.jpcc.9b03637

[3] P. Calaminici et al., Comput. Theoret. Chem. (2013). DOI: 10.1016/j.comptc.2013.06.014



UNVEILING THE G4-PAMAM CAPACITY TO BIND AND PROTECT ANG-(1-7) BIOACTIVE PEPTIDE BY MOLECULAR DYNAMICS SIMULATIONS

L. América Chi^{1*}, Somayeh Asgharpour², José Correa-Basurto¹, Cindy Rodríguez Bandala¹, and Marlet Martínez-Archundia¹

¹ Laboratory for the Design and Development of New Drugs and Biotechnological Innovation, Escuela Superior de Medicina, Instituto Politécnico Nacional, Plan de San Luis y Díaz Mirón, Ciudad de México 11340, Mexico

²IAS-5/INM-9, Computational Biomedicine, Forschungszentrum Jülich, Wilhelm-Johnen-Strae, 52428 Jülich

* chiamerika@hotmail.com

New therapies that allow natural healing processes are required. Such as the endogenous peptide called Angiotensin-(1-7), a safe and effective drug, which is able to re-balance the Renin-Angiotensin system affected during several pathologies, including the new COVID-19; cardiovascular, renal, and pulmonary disease; diabetes; neuropathic pain; Alzheimer and cancer¹. However, one of the limiting factors for its application is its unfavorable pharmacokinetic profile. In this work, we propose the coupling of Angiotensin-(1-7) to PAMAM dendrimers in order to evaluate the capacity of the nanocarrier to improve isolated peptide features and to gain insight into the structural as well as the energetic basis of its molecular binding. The In Silico tests were performed in acidic and neutral pH conditions as well as amino-terminated and hydroxylterminated PAMAM dendrimers. High-rigor computational approaches, such as molecular dynamics and metadynamics simulations were used. We found that, at neutral pH, PAMAM dendrimers with both terminal types are able to interact stably with 3 Angioteinsin-(1-7) peptides through ASP1, TYR4 and PRO7 key aminoacids, however, there are some differences in the binding sites of the peptides. In general, they bind on the surface in the case of the hydroxylterminated compact dendrimer and in the internal zone in the case of the amino-terminated open dendrimer. At acidic pH, PAMAM dendrimers with both terminal groups are still able to interact with peptides either internalized or in its periphery, however, the number of contacts, the percentage of coverage and the number of HBs are lesser than at neutral pH, suggesting a state for peptide release. In summary, amino-terminated PAMAM dendrimer showed slightly better features to bind, load and protect Angiotensin-(1-7) peptides².

Key Words: Dendrimer, Nanocarrier, Peptide, Ang-(1-7), Metadynamics, Molecular Dynamics.

References

[1] Chi, L.A., et al. J Comput Aided Mol Des, 1-23, (2022).
[2] Shylesh CM, S., & VS, A. Clin. Exp. Hypertens., 44(1), 1-10, (2022).



ELECTRONIC STRUCTURE OF BENDING 2H-MoS₂ by TEM

Manuel Ramos^{1*}, Oscar A. López-Galán¹, Javier Polanco¹, Miguel José Yacamán²

1) Departamento de Física y Matemáticas, Instituto de Ingeniería y Tecnología, Universidad Autónoma de Ciudad Juárez, Edificio G-301A, 450 Avenida del Charro, Ciudad Juárez, Chihuahua, MX. Email: oscar.lopez@uacj.mx (OALG); javier.polanco@uacj.mx (J.P.); manuel.ramos@uacj.mx (M.R.)

2) Applied Physics and Materials Science Department and Center for Material Interfaces Research and Applications (MIRA), Northern Arizona University, Flagstaff, AZ, USA. E-mail: miguel.yacaman@nau.edu (M.J.Y.) *Correspondence: manuel.ramos@uacj.mx (M.R.); Tel.: +52 (656) 688-4887

Abstract

A systematically study using DFT methods to estimate electronic structure for bending 2H-MoS₂ layers up to 75°, motivated by *in-situ* TEM experiments is presented in here. Our results indicate that HOMO/LUMO and density of states reveal a semiconducting to metallic state transition at Fermi energy level (E_F) when slabs are bend. That is attributed due to stretching and contracting of sulfur-sulfur chemical bonds located over basal (001)-plane. The molybdenum ions play a major role in such transition due to reallocation of its metallic *d*-character orbitals inducing *"free electrons"* over 2D-layer causing an overlap between Mo_{-dx}²-y² and Mo_{dz}² orbitals. The metallic transition allows us to understand catalytic activity for onion-like MoS₂ nanostructures as reported in the literature.

Keywords: MoS₂, Band Structure, Isosurface, DFT, HOMO, LUMO

References

[1] G. Casillas, U. Santiago, H. Barrón, D. Alducin, A. Ponce, and M. José-Yacamán, "Elasticity of MoS₂ Sheets by mechanical de-formation observed by in situ electron microscopy," The Journal of Physical Chemistry C, vol. 119, no. 1, pp. 710–715, (2015).

[2] M. A. Ramos, R. Chianelli, J. L. Enriquez-Carrejo, G. A. Gonzalez, and G. Berhault, "Metallic states by angular dependence in 2H-MoS₂ slabs," Computational Materials Science, vol. 84, pp. 18–22, Mar. 2014, doi: 10.1016/j.commatsci.2013.11.038.



SCHEELITE TO FERGUSONITE PHASE TRANSITION IN CdMoO4: A FIRST-PRINCIPLES STUDY

Pricila Betbirai Romero Vázquez*1 Sinhué López-Moreno2

¹Instituto Potosino de Investigación Científica y Tecnológica, División de Materiales Avanzados, Camino a la Presa de San José 2055, Lomas 4ta Secc, 78216 San Luis, S.L.P,México.

² CONACYT - Instituto Potosino de Investigación Científica y Tecnológica, División de Materiales Avanzados, Camino a la Presa de San José 2055, Lomas 4ta Secc, 78216 San Luis, S.L.P, México.

pricila.romero@ipicyt.edu.mx sinhue.lopez@ipicyt.edu.mx

First-principles calculations based on Density Functional Theory (DFT) were performed on cadmium molybdate (CdMoO₄) under high pressure up to 20 GPa. Calculations under hydrostatic conditions reveal a second-order phase transition at 12.2 GPa from scheelite to fergusonite. This structural transition driven by pressure was already observed on other scheelite-type molybdates (AMoO₄) and tungstates (AWO₄) [1-3]. In order to understand the crystallographic changes of CdMoO₄ under pressure, we analyze the pressure evolution of volume (V), lattice parameters (a, c), polyhedral volume (V_{CdO8} , V_{MoO4}), and interatomic distances (d_n). Our results show no volume reduction at transition pressure, a consequence of the second-order phase transition. However, lattice parameter *a* split into *a* and *c*, while *c* becomes *b* without discontinuity at transition pressure. Also, the angle changes from 90° to 90.35° at 12.2 GPa and increases with pressure up to 90.4 at 20 GPa. On the other hand, we observe that V_{CdO8} and V_{MoO4} do not suffer a discontinuity at transition pressure. following a smooth continuity in the scheelite-fergusonite transition. Finally, we analyzed the distortion parameters of polyhedral with pressure; our results show that MoO₄ undergoes a more significant distortion than CdO₈ in the high-pressure phase due to symmetry reduction.





Fig. 1. Crystal structure of (a) scheelite and (b) fergusonite phases of CdMoO₄. **Key Words:** Second-order phase transition; First-principles calculations; Scheelite-fergusonite transition.

References

[1] D. E., *Mater. Res. Bull.* 44 807–811 (2009).
[2]D. E., *J. Appl. Phys.* 109 043510–043510–5 (2011).
[3]J. L.-S., *Phys. Status Solidi.* B 244 325–330 (2007).



A FIRST-PRINCIPLES STUDY OF THE PREFERENTIAL LOCATION OF THE OXYGEN GROUPS ON ZIGZAG GRAPEHENE NANORRIBBONS

Olga L. Ramírez-Ramírez^{1*}, Sinhué López-Moreno^{2,3}

¹División de Materiales Avanzados, IPICYT, Camino a la presa de San José 2055 Col. Lomas 4a seccion, San Luis Potosí 78126, México
 ²CONACYT - División de Materiales Avanzados, IPICYT, Camino a la presa de San José 2055 Col. Lomas 4a seccion, San Luis Potosí 78126, México
 ³Centro Nacional de Supercómputo, IPICYT, Camino a la presa de San José 2055 Col. Lomas 4a seccion, San Luis Potosí 78126, México
 ³Centro Nacional de Supercómputo, IPICYT, Camino a la presa de San José 2055 Col. Lomas 4a seccion, San Luis Potosí 78126, México

We performed first-principles calculations to study graphene oxide nanoribbons' (GONR) energetic stability, geometric structure, and magnetization. Our work is focused on the analysis of the oxygen functional groups (OFg) location in the antiferromagnetic zigzag graphene nanoribbon (GNR) to build the GONR. In this study, the OFg considered were: O (epoxy), OH (hydroxyl), CO (acvl), and carboxyl (COOH). In order to investigate the change of properties and determine the most stable structure, the OFgs were arranged at different sites on the layer. Our observations indicate that the structural deformation of GNR strongly depends on the OFg location, proximity to the edge, and the relative location of the OFg. These factors were followed to find the lowest energy configurations for specific configurations. For CO and COOH, the adsorption is favored when these OFg are adsorbed at the edge of carbons replacing H atoms. In the case of epoxy and hydroxyl groups, the preferential location is close to other groups and near the border. For all cases, it was observed that by decreasing the distance between the groups and the distance from the edge, the stability of the system increases, and adsorption is favored. Furthermore, we found that structural and electronic properties are modified depending on the OFg and their distribution on the layer [1-3]. While the magnetization behavior is itinerant, mainly affected by the OFg and the relative position in the GNR.

Key Words: Graphene oxide nanoribbons; first-principles calculations; electronic structure.

References

[1] E.A. Appl. Mater. Today., 8, 1-17, (2017).

[2] R.L., & B.B. Am. Chem. Soc. Div. Pet. Chem. Prepr., 47(2), 428-431, (2002).

[3] H. P. Stud Surf Sci Catal., 48, 145-157, (1989).



GREEN SYNTHESIS OF IRON OXIDE NANOPARTICLES USING BASIL EXTRACT (OCIMUM BASILICUM) BY CONVENTIONAL AND MICROWAVE ASSISTED HYDROTHERMAL METHOD

Beatriz Italia DE LA TOBA ACEVEDO1*, Mitchel Abraham RUÍZ ROBLES1, Eduardo Gerardo PÉREZ TIJERINA1, Francisco SOLÍS POMAR1, Jorge Luis HERNÁNDEZ PIÑERO2. 1 Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León, Pedro de Alba S/N, C.P. 66451, San Nicolás de los Garza, N.L, México. 2 Facultad de Ciencias Biológicas, Universidad Autónoma de Nuevo León, Pedro de Alba S/N, C.P.66451, San Nicolás de los Garza, N.L, México. *beatriz.dltobacv@uanl.edu.mx

In the present project, it is proposed two easy and green hydrothermal methodologies for the synthesis of iron oxide nanoparticles (IONPs) using aqueous basil extract (Ocimum basilicum) as reducing and stabilizing agent. The first methodology is a conventional hydrothermal method and the second one, is a hydrothermal method assisted by microwave. Thegreen-synthesized IONPs were characterized by scanning electron microscope (SEM), transmission electron microscope (TEM), UV-Vis spectroscopy and Fourier transform infrared (FT-IR) spectroscopy. The IONPs were synthesized with different ratios of precursor solution and basil extract and additionally with both hydrothermal methods. It was demonstrated that the size, morphology, and core-shell structures changed depending the conditions of synthesis. It was observed by TEM and FT-IR that the magnetic IONPs made a core and had a carbon layer as shell. The UV-Vis spectra results revealed a strong absorbance peak between 300 and 450 nm. The FT-IR spectra showed the characteristic peaks on 580, 526 and 436 cm-1 of the Fe-O bound, in addition it had been found a coincidence on the peak 1596 cm-1 that represent the presence of C=C bound and in peaks of the region between 3388 and 3178 cm-1 which indicate the OH groups. At least, due the nanometric size it was observed a peak in 900, 695 and 691 cm-1 which indicates FeO(OH) bounds.



Figure 1. Green synthesis methodologies. **Figure 2.** FT-IR, UV-Vis Spectra, SEM and TEM images.



ZnONPs DEGRADATION AS A FUNCTION OF pH AND TIME

Luis Eduardo Miranda Domínguez₁, Luis Hernández-Adame₁*, Thelma Rosa Castellanos Cervantes₁, Luis Guillermo Hernández Montiel₁, Abraham Loera Muro₁, Arturo Ponce Pedraza₂

¹ CONACYT-Centro de Investigaciones Biológicas del Noroeste (CIBNOR), Av. Instituto Politécnico Nacional 195, Playa Palo de Santa Rita Sur, La Paz, Baja California Sur, 23090, México. ² Department of Physics, University of Texas San Antonio, TX 78249, USA. *ladame@cibnor.mx

Nanotechnology is an interdisciplinary field that can help agricultural production using nanofertilizers and nanofungicides. Some systems based on Ag, CeO₂, CuO, MnO and ZnO nanoparticles (NPs) have been evaluated as agroproducts, with ZnO being one of the most outstanding systems [1]. In the degradation of ZnONPs, Zn2+ has been used by plants as a micronutrient, which is why it is so widely used in producing nanofertilizers. The degradation rate of ZnONPs as a function of pH and time is an important issue for the development of agrochemicals because the pH of the plant cell is slightly alkaline (pH 7.5), except for vacuole, Golgi apparatus and thylakoids (light phase) which have a mainly acidic pH [2]. In this sense, the present work evaluated the degradation rate of ZnONPs as a function of pH and time. For this, a set of ZnONPs was synthesized by microwave technique (90 °C, 2 min) using two precursor salts (sodium acetate and sulfate). The results show NPs with a size distribution of 10 and 30 nm, respectively. Those of sulfate have a quasi-spherical shape, while acetate samples have a rosette shape. For the degradation tests, a solution of 800 ppm of ZnONPs in sodium citrate (0.05 M) was prepared for pH 3 and 5, while sodium phosphate (0.05 M) was used for pH 7 and 9. The suspensions were kept under stirring constant, taking 50 mL aliguots at 0, 3, 6, 15, 30 and 60 min, which were later centrifuged at 5000 rpm for 30 s, analyzing the supernatant by Atomic Absorption Spectroscopy. The results show that at acidic pH the degradation rate of ZnONPs is more significant than those suspended in basic solutions, highlighting that greater degradation was produced by acetate precursor salt (Fig. 1).

Key words: Agronanotechnology, Kinetic degradation, Nanofertilizers, ZnO





Figure 1. ZnO NPs degradation as a function of pH and time

References

- S.A. *et al.*, J Mater Sci **1**, 185-201, (2018).
 I.K. Plant Cell Monogr. **1**, 59-74, (2013).



EFFECT ON CHITOSAN STRUCTURE, CONCENTRATION AND pH ON CHITOSAN-MALTODEXTRIN NANOGELS CHARACTERISTICS

Estefanía DOMÍNGUEZ-FONSECA1*, Brianda María GONZÁLEZ MARTÍNEZ1, Edgar FIGUEROA OCHOA2, Alberto GUTIÉRREZ BECERRA1, Julien ROSSELGONG3, Lourdes Mónica BRAVO-ANAYA3**

1CUTonalá, Departamento de Ciencias Básicas y Aplicadas, Universidad de Guadalajara, Nuevo Periférico # 555, C.P.45425, Ejido San José Tateposco, Jalisco, México. 2Universidad de Guadalajara, Departamento de Química. Blvd. M. García Barragán #1451, C.P. 44430, Guadalajara, Jalisco, México. 3Université de Rennes 1, Institut des Sciences Chimiques de Rennes, CNRS, UMR 6226, Campus de Beaulieu, Bat 10C, 35042 Rennes Cedex, France. *estefania.dominguez8282@alumnos.udg.mx **lourdes-monica.anaya@univ-rennes1.fr

Nanogels are 3D networks formed by crosslinked polymers with sizes in the nanometric scale [1]. They represent one of the most relevant applications of biopolymers, such as polysaccharides, in drug delivery. Nanogels based on biopolymers are characterized by their stimuli responsiveness, biodegradability, biocompatibility, stability, and non-toxicity [2]. In this project, pH sensitive nanogels were synthesized for drug delivery applications by combining chitosan and maltodextrins. For this purpose, a crosslinking reaction of chitosan with partially oxidized maltodextrins was carried out through a reductive amination reaction. Three chitosan samples with different degrees of acetylation (DA) and molecular weights (MW) were selected, and two oxidation degrees were pursued for maltodextrins (9 and 47%). Chemical reactions and the resulting products were followed through IR and 1H NMR spectroscopies. Nanogels were characterized by DLS, SEM and
-potential to determine their size, PDI, charge and morphology. The impact of chitosan structure, concentration, pH and % oxidation of the maltodextrins on nanogels characteristics (size and charge) was studied. It was found that nanogels present sizes ranging from 73 to 300 nm, depending on the selected parameters. Nanogels with smaller particle sizes were obtained when using greater % oxidation (47%), lower pH (3.5), chitosan with lower DA (DA=0.05) and medium MW (160 kg/mol), and a chitosan concentration equivalent to 1/10 its overlap concentration (c*/10).

Key Words: Nanogels; biopolymers; reductive amination.

References

[1] Ekkelenkamp, A. E.; Elzes, M. R.; Engbersen, J. F.J.& Paulusse, J. M.J., *J. Mater. Chem. B* 6(2), 210-235, (2018).
 [2] Kost, B., Brzeziński, M., Socka, M., Baśko, M., & Biela, T, *Molecules* 25(15), 3404, (2020).



Synthesis of Copper Oxide Nanoparticles From Extract of Neem Leaves and Chrysocolla Ore

Eleazar GÁNDARA MARTINEZ¹*, Nora ELIZONDO VILLAREAL¹

¹ Universidad Autónoma de Nuevo León ,Pedro de Alba S/N, Niños Héroes, Ciudad Universitaria. C.P. 66451,San Nicolás de los Garza, Nuevo León, México. *Corresponding author e-mail (ele-gr@hotmal.com).

The synthesis of nanoparticles (NPs) derived from plants is part of the technological development of ecological synthesis methods at affordable costs, being one of the recent trends in the field of materials science. According to this context, in the present work, copper oxide (CuO) nanoparticles are synthesized following a green approach [1], using the extract of Neem leaves (Azadirachta indica), this was obtained from 5.5gr of leaves, was added dropwise to the solution made up of deionized water and 0.01 gr of copper hydroxynitrate, this salt was obtained manually from stones extracted from a copper oxide mine (Chrysocolla), which were crushed and using nitric acid formed crystals of copper. The biosynthesis was stopped when the color change to a light green occurred, it was taken to an ultrasonic bath, later it was characterized by UV-Vis spectroscopy confirming the formation of CuO nanoparticles.

Key Words: CuO nanoparticles nanoparticles, copper oxide mine, green chemistry, Neem leaves

References

[1] Chakraborty, N., Banerjee, J., Chakraborty, P., Banerjee, A., Chanda, S., Ray, K., ... & Sarkar, J. (2022). Green synthesis of copper/copper oxide nanoparticles and their applications: a review. Green Chemistry Letters and Reviews, 15(1), 187-215.



SELF-ASSEMBLY OF GALLIUM ARSENIDE NANOWIRES DOPED WITH TWO SILICON DELTA DOPING BY MOLECULAR BEAM EPITAXY TECHNIQUE AND DETERMINATION OF ITS OPTICAL PROPERTIES

<u>Elihu Hazel Sánchez Martínez^{1*}</u>, Reyna Méndez Camacho^{1,2}, Cristo Manuel Yee Rendón³, Esteban Cruz Hernández¹

 ¹Coordinación para la Innovación y Aplicación de la Ciencia y Tecnología, Universidad Autónoma de San Luis Potosí, Av. Sierra Leona 5502, Lomas 2a de San Luis, 78210, San Luis Potosí, S.L.P. 78210, México.
 ²Facultad de Ciencias, Universidad Autónoma de San Luis Potosí, Av. Parque Chapultepec 1570 Priv. Del Pedregal, 78210, San Luis Potosí, S.L.P. 78210, México.
 ³Physics Department, Center for Research and Advanced Studies of the National Polytechnic Institute, Apartado Postal 14–740, Mexico, D.F. 07000, Mexico.

*elihuhazels@yahoo.com.mx

In recent years, guantum systems have been of great interest due to the opportunities that it can generate to explore physical phenomena or to be used in potential technological applications. In particular, we are interested in 1D systems, where the formation of a Wigner crystal occurs, which is a topic of current scientific interest [1]. In this work we report the self-assembly of nanowires using a GaAs substrate with crystallographic orientation (631), where the substrate acts as a template for the growth of nanowires [2]. The growths were based on a GaAs/AlGaAs heterostructure, the surface morphology was studied using atomic force microscopy for a series of samples grown at a different temperature. For the sample grown at a temperature of 690°C it was confirmed the presence of nanowires. A two-dimensional autocorrelation function analysis was performed to quantitatively determine the uniformity of the nanowires on the surface. In addition, the results obtained in the study of photoluminescence spectroscopy and photoreflectance spectroscopy are presented, where the emission energy of the nanowires and the electric field generated by silicon delta doping are determined. In order to carry out a comparative study, the results are also reported for a sample grown at a temperature of 690°C but using a GaAs substrate with crystallographic orientation (100).

Key Words: Nanowire, MBE, PL

References

[1] R.M.C., Physical Review B **102**, 035403-1-035403-8, (2020).
[2] E.C.H., Appl. Phys. Lett. **101**, 073112-1-073112-4, (2012).



LUMINESCENT TERBIUM DOPED YTTRIA SYNTHESIZED BY THE SOL-GEL PROCESS

Alan Daniel ALCANTAR MENDOZA¹*, Antonieta GARCÍA MURILLO¹, Felipe de Jesús CARRILLO ROMO¹

¹ Centro de Investigación e Innovación Tecnológica (CIITEC), Cerrada de Cecati, Santa Catarina, C.P. 02250, Azcapotzalco, CDMX, México. *Corresponding author e-mail: a_daniel_am@outlook.com

Rare earth oxides (REO) are frequently used as catalysts or phosphors due to their high efficiency for the transfer energy between the electronic orbitals [1]. Typically, sol-gel process uses a rare earths metallic salt as the precursors in an ethanolic solution, which upon the addition of an organic epoxide forms a gel [2]. Although, there have been attempts to use salts, such as metal nitrates, as the precursor, to obtain high purity materials [3]. Therefore, the synthesis of contaminant-free, REO materials via epoxide-assisted sol-gel method remains a significant challenge. In the current work, yttrium oxide (Y_2O_3) powders doped with the terbium ion (Tb^{3+}) were synthesized by the sol-gel process. Terbium-doped Y₂O₃ xerogels were synthesized at different molar ratios (0, 2, 5, 8, 10, 20, 30, 40, and 50 mol%) and heat-treated at 1073 K in order to yield ceramic powders. Terbium-doped Y₂O₃ ceramic powders were characterized by infrared spectroscopy (IR), x-ray diffraction (XRD), and photoluminescent studies were performed to establish the relationship between their structural and luminescent properties. After the 1073 K heat treatment, infrared spectra revealed the characteristic absorption band for the M-O-M bond located around 560 cm⁻¹. Also, all the Y₂O₃ powders in presence of Tb³⁺ present well-defined reflections characteristic of a cubic-type crystalline structure. Finally, according to luminescence studies, the emission bands around 490, 550, 590, and 620 nm were due to the ${}^{5}D_{4} \rightarrow {}^{7}F_{6}$, ${}^{5}D_{4} \rightarrow$ ${}^{7}F_{5}$, ${}^{5}D_{4} \rightarrow {}^{7}F_{4}$ and, ${}^{5}D_{4} \rightarrow {}^{7}F_{3}$ transition levels of the Tb³⁺, respectively.

Key Words: Rare earths, luminescence, sol-gel.

References

[1] C.R.C., "Luminescence in Rare Earth Ion-Doped Oxide Compounds" in *Luminescence – An outlook on the Phenomena and Their Applications*, 33-66, (2016).

[2] U.S., "Chemistry and Fundamentals of the Sol-Gel Process" in *Part One Sol-Gel Chemistry Methods*, 1-27, (2015).

[3] M.A.W., "Chlorine-free, monolithic lanthanide series rare earth oxide aerogels via epoxide-assisted sol-gel method" *J. of S. S. T.*, 1-13, (2018).



NUMERICAL CHARACTERIZATION OF THE REFLECTANCE OF A SENSOR BASED ON A COMPOSITE SYSTEM OF POROUS SILICON BRAGG MIRRORS AND A THIN SILVER FILM

Andrea Citlalin Ramírez-Zúñiga^{1*}, Jacinto Sandoval-Lira¹, Arturo Santos-Gómez¹.

¹ Instituto Tecnológico Superior de San Martín Texmelucan, Camino a Barranca de Pesos S/N, San Lucas Atoyatenco, C.P. 74120, San Martín Texmelucan, Puebla, México. *L18060017@smartin.tecnm.mx

Tamm resonance is a collective oscillation of electrons coupled with electromagnetic waves that, unlike surface plasmons, can be excited at normal incidence of light, which makes them ideal for the design of sensors or other devices in embedded circuits [1, 2]. In this work we present the results of the numerical simulation of the reflectance of a device based on a photonic crystal of porous silicon Bragg mirrors and a silver nanolayer using the transfer matrix method [3], considering the cavities of the silicon with air and atrazine, which is a pesticide used in vegetable crops. The proposed configuration allows exciting Tamm resonances which, according to the results, the resonance wavelength depends on the porosity of the layers, as well as on the concentration of the chemical inside the pores.

Key Words: Photonic crystal, Sensor, Tamm resonance.

References

- [1] Kaliteevski, M., et al. Physical Review B 76, 165415, (2007).
- [2] Zaky, Z. A., et al. Photonics and Nanostructures-Fundamentals and Applications 49, 100995, (2022).
- [3] Orfanidis, S. J. Electromagnetic waves and antennas. (2002).



PHOTOCATALYTIC ACTIVITY OF Bi₂WO₆@PbMoO₄ FOR THE DEGRADATION OF CIPROFLOXACIN

Ángel Daniel González Guzmán¹, Diana Berenice Hernández Uresti^{1*}, Daniel Sánchez Martínez²

 ¹Universidad Autónoma de Nuevo León, Facultad de Ciencias Físico Matemáticas, Ave. Universidad S/N, Cd. Universitaria, San Nicolás de los Garza N.L. México, C.P. 66455.
 ²Universidad Autónoma de Nuevo León, Facultad de Ingeniería Civil – Departamento Ecomateriales. Ave. Universidad S/N, Cd. Universitaria, San Nicolás de los Garza N.L. México, C.P. 66455 .*Corresponding author email: diana.hernandezrt@uanl.edu.mx

 $Bi_2WO_6@PbMoO_4$ heterostructures were synthesized by sonochemical method. The composite was characterized by X-Ray Difraction (XRD), Diffuse Reflectance Spectroscopy (DRS), BET method and Scanning Electron Microscopy (SEM). The photocatalytic activity was evaluated by the degradation of ciprofloxacin (CIP) under simulated solar irradiation. 25% $Bi_2WO_6@PbMoO_4$ sample showed the highest photocatalytic activity reaching 99% degradation under a half-time life of ~29 minutes. The predominant oxidizing species in the photocatalytic reaction was analyzed using species scavengers, concluding that the photogenerated holes are the predominant species in the photocatalytic reaction.

Sample	Eg (eV)	Cristallyte Size (nm)	Web <u>Distortion</u> (%)
PbMoO ₄	3.11	10.7	1.57
5Bi	3.05	11.1	1.566
10Bi	3.01	11.1	1.566
15Bi	2.91	11.4	1.569
20Bi	2.91	11.1	1.575
25Bi	2.87	12.5	1.541
30Bi	2.67	12	1.545
Bi_2WO_6	2.69	20.3	1.287

Table 1 – Physical properties of $Bi_2WO_6@PbMoO_4$ heterostructures



Figure 1 – Photocatalytical activities of $Bi_2WO_6@PbMoO_4$ heterostructures

Key Words: Ciprofloxacin, Heterogeneous Photocatalysis, Bi₂WO₆@PbMoO₄

References

[1] He,Z., Fuel, 294, (2021)

[2] R.M., Physica B: Condensed Matter, 620, (2021).

[3] S.S., Catalysts, 437, (2021)

[4] W.Z., Science Of The Total Environment, 764, (2021).



Hybrid solutions used in the conservation of quarry monuments

Moreno Rodríguez César ¹, Silva Gutiérrez César Habbib ¹, Bobadilla Valencia Ana Karla¹, Martínez Piñeiro Esmeralda Lizet ², Álvarez Guzmán Gilberto ², Cervantes Jáuregui Jorge ², Guerra Contreras José Antonio ²

 ¹ Facultad de Ciencias, UNAM, México, 04510 Ciudad de México, CDMX, Coyoacán, C.U.
 ² Departamento de Química, Cuerpo Académico de Química y tecnología del Silicio, División de Ciencias Naturales y Exactas, Universidad de Guanajuato, Noria Alta s/n 36050, Universidad de Guanajuato *cesarmoreno7066@ciencias.unam.mx.

In the search of other silicon derivatives with potential use in the field of historical building stone conservation, we have suggested the use tetrakis(2-hydroxyethyl)silane (THEOS) as precursor because they are water-soluble [1]. Additionally, it is already known that THEOS is compatible with different natural polysaccharides as chitosan, obtaining a homogeneous film formation [2,3,4,5]. The present report is related to evidence the interaction of different solutions of THEOS-chitosan with four different quarry stones. These hybrid solutions are applied for the conservation of siliceous stones from historical building in Guanajuato. Mechanical tests, FT-IR spectroscopy, SEM, and colorimeter test evidence that no esthetic change was produced, but the hardness was increased until 20%, indicating that these treatments can be used as conservation of THEOS-chitosan. Acknowledgments to CONACYT-México (Proyecto 284510, CVU 132061), Fondo Sectorial de Investigación para la Educación and Universidad de Guanajuato – DAIP (Guanajuato, México) y al Proyecto LANCIC LN315853 y LN 314846, CICORR, UAC.

Key Words: conservation treatment, cultural Heritage, film

References

[1] R.C. Mehrotra, R.P. Narain. Indian J. Chem. 1967, 5, 444.

[2] Y.A. Shchipunov, T.Y. Karpenko, A.V. Krekoten. Composite Interfaces. 2005, 11, 8-9, 587-607.

[3] I. Bravo-Flores, M. Meléndez-Zamudio, A. Guerra-Contreras, E. Ramírez-Oliva, G. Álvarez-Guzmán, R. Zárraga-Núñez, A. Villegas, J. Cervantes. Macromolecular Rapid Communications. 2021, 45, 5,

2000612.

[5] M. Meléndez-Zamudio, et al. Molecules. 2021, 26(4), 938.



Hybrid solutions and nanoparticles treatments used in the conservation of marble monuments

<u>Silva Gutiérrez César Habbib</u>¹, Moreno Rodríguez César ¹, Bobadilla Valencia Ana Karla¹, Martínez Piñeiro Esmeralda ², Álvarez Guzmán Gilberto ², Cervantes Jáuregui Jorge ², Guerra Contreras José Antonio ²

 ¹ Facultad de Ciencias, UNAM, México, 04510 Ciudad de México, CDMX, Coyoacán, C.U.
 ² Departamento de Química, Cuerpo Académico de Química y tecnología del Silicio, División de Ciencias Naturales y Exactas, Universidad de Guanajuato, Noria Alta s/n 36050, Universidad de Guanajuato *habbibs@ciencias.unam.mx.

The conservation of historical building stone is essential for protect our identity. In Mexico City there are a lot of monuments as Bellas Artes or the Hemiciclo a Juárez created with marble. Regrettably, these buildings have a lot of deterioration problems for the acid rain caused by the high pollution of the city. In the present research, we have tested different formulations in order to avoid the degradation of the marble. Some are water-solubles solutions as tetrakis(2-hydroxyethyl)silane (THEOS) and tris(2-hydroxyethyl)methyl silane (MeTHEOS) [1,2] and other are based in nanoparticles of lime (diameter of 4 nm) and hydroxyapatite (20 nm) produced from egg shell waste. Additionally, there was synthetized some solutions of THEOS-chitosan and MeTHEOS-chitosan with hydroxyapatite nanoparticles to increase the film formation properties. There were performed different test (mechanical test, colorimeter, SEM) to demonstrates that these treatments don't produce changes in the visual appearance of the marble but increases the cohesion and the hardness of the stone, showing that can be used as stone preservation treatment. Regarding the application in the conservation of different building stones from historical monuments with calcareous composition, recently we have reported initial results using the glycolalkoxysilanes-chitosan as consolidant and hydrophobic formulations [3].

Acknowledgments to CONACYT-México (Proyecto 284510, CVU 132061), Fondo Sectorial de Investigación para la Educación and Universidad de Guanajuato – DAIP (Guanajuato, México) y al Proyecto LANCIC LN315853 y LN 314846, CICORR, UAC

Key Words: hydroxyapatite, nanomaterials, conservation cultural Heritage

References

[1] R.C. Mehrotra, R.P. Narain. Indian J. Chem. 1967, 5, 444.

[2] I. Bravo-Flores, M. Meléndez-Zamudio, A. Guerra-Contreras, E. Ramírez-Oliva, G. Álvarez-Guzmán, R. Zárraga-Núñez, A. Villegas, J. Cervantes. Macromolecular Rapid Communications. 2021, 45, 5,

2000612.

[3] M. Meléndez-Zamudio, et al. Molecules. 2021, 26(4), 938.



Nanoparticles treatments conservation treatment for the protection of caliche archaeological monuments

Martínez Piñeiro Esmeralda ¹, Álvarez Guzmán Gilberto ¹, Cervantes Jáuregui Jorge ¹, Guerra Contreras José Antonio ¹

¹ Departamento de Química, Cuerpo Académico de Química y tecnología del Silicio, División de Ciencias Naturales y Exactas, Universidad de Guanajuato, Noria Alta s/n 36050, Universidad de Guanajuato *esmeraldamartinez@ciencias.unam.mx.

The conservation of historical building stone is essential for protect our identity. Comonfort, Guanajuto has an archaeological site that was unique in the world because is built from caliche, a calcareous stone. This material is susceptible to deterioration problems by pollution and climate changes. In the present research, we have tested nanoparticles of lime (diameter of 4 nm) and hydroxyapatite (20 nm) synthesized from eggshell waste [1,2] in order to preserve the stone materials. There were performed mechanical test to demonstrates that the nanoparticles increase 400% cohesion and hardness of the caliche without changing the original color of the stone, something that was looking for conservation treatments. Lime nanoparticles presented different kinds of carbonation structures that can be controlled with the synthesis process, something that influence the conservation efficiency.

Acknowledgments to CONACYT-México (Proyecto 284510, CVU 132061), Fondo Sectorial de Investigación para la Educación and Universidad de Guanajuato – DAIP (Guanajuato, México), Laboratorio de Microscopía Electrónica del Laboratorio Nacional de la Universidad de Guanajuato, Dra. Ma. Del Carmen Salazar Hernández, del Instituto Politécnico Nacional, Campus Silao, Unidad Profesional Interdisciplinaria de Ingeniería Campus (UPII-GTO) de Silao, Guanajuato del Grupo de Investigación en Materiales y Termofluídos

Key Words: hydroxyapatite, nanomaterials, conservation cultural Heritage

References

Gergely, G., Wéber, F., Lukács, I., Tóth, A. L., Horváth, Z. E., Mihály, J., & Balázsi, C. (2010). Preparation and characterization of hydroxyapatite from eggshell. *Ceramics International*, *36*(2), 803-806.
 Rivera, E. M., Araiza, M., Brostow, W., Castano, V. M., Diaz-Estrada, J. R., Hernández, R., & Rodriguez, J. R. (1999). Synthesis of hydroxyapatite from eggshells. Materials Letters, *41*(3), 128-134.
 2000612.



STUDY OF NUCLEIC ACID-BASED COMPLEXES DESTABILIZATION IN PRESENCE OF GLYCOSAMINOGLYCANS

Paulina Alejandra MONTAÑO GONZÁLEZ^{1*}, Fabienne GAUFFRE¹, Sylvain TRANCHIMAND², Lourdes Mónica BRAVO ANAYA^{1**}

¹ Institut des Sciences Chimiques de Rennes (ISCR), 217 Avenue du Général Leclerc, 35042 Rennes Cedex, France.

² École Nationale Supérieure de Chimie de Rennes, 11 All. de Beaulieu, 35708 Rennes, France *paulina-alejandra.montano@univ-rennes1.fr, ** lourdes-monica.anaya@univ-rennes1.fr

Natural or synthetic polycations are used as complexing agents which interact electrostatically with nucleic acids, condense them into nanoparticles, protect them and control their entry into cells [1]. Although the formation of these particles is well documented [2], fewer studies focus on the physical-chemistry behind the disassembly and nucleic acids release after the endosomal escape, especially under physicochemical conditions found in an intracellular environment. Glycosaminoglycans (GAGs) are negatively charged biomacromolecules that are necessary for the regulation of different biological functions. In the presence of polyelectrolyte complexes, the GAGs that are present in the cells are expected to compete with nucleic acids and dissociate the complexe if polycation-GAG association is thermodynamically favored. This research project aims to study the colloidal stability of DNA/chitosan and DNA/PEI complexes in presence of GAGs (heparin and hyaluronic acid) through Dynamic Light Scattering (DLS) measurements. It was found that the colloidal stability depends on the charge ratio [N⁺]/[P⁻] of the complex. The aggregation onset of nucleic acid-based complexes after different GAGs addition was found to be dependent on the charge density of the GAG.



Image 1 – Schematic representation of GAGs addition to nucleic acid- based complexes (left) and evolution of particle size as a function of added GAG.

Key Words: Colloidal stability, Synthetic vectors, Polyplexes, Polyelectrolytes. **References**

[1] V. S. Meka, et al., Drug Discov. Today, vol. 22, no. 11, pp. 1697–1706, 2017.

[2] A. D. Kulkarni et al., Artif. Cells, Nanomedicine Biotechnol., vol. 44, no. 7, pp. 1615–1625, 2016.



First principles calculation of physical properties of LiFe_xMn_yPO₄ electrochromic batteries

Jose Alan BARRAZA VILLAVERDE¹ Israel Omar PÉREZ LÓPEZ²

Authors' Affiliations, with complete postal address (Arial, size 11, italics, single space) ¹ Universidad Autónoma de Ciudad Juárez, Manuel Díaz H. No. 518-B Zona Pronaf Condominio, 32315 Cd Juárez, Chih, México. alan_barrazaa@hotmail.com

² Universidad Autónoma de Ciudad Juárez, Manuel Díaz H. No. 518-B Zona Pronaf Condominio, 32315 Cd Juárez, Chih, México. israel.perez@uacj.mx

The electrochromic devices consist of materials capable of changing their color and optical transmittance under the influence of a potential difference (Figure 1). The project purpose is the simulation via first-principles calculations to see if it's an optimal material for the task. The simulation of the materials is critical to saving money and time for experimental scientists developing these materials and optimizing the research and evolution of the electrochromic devices[1]–[3].

Calculations were made with the aid of the software WIEN2k. This software provides the density of states of the material and all its atoms, band structure, optical properties, and energy formation



from the material[4]-[6].

Figure 1 – (a) An image of a working electrochromic device (b) A graph representing the transmittance of the device with respect to time[2].



Key Words: Electrochromic, simulations, batteries, and WIEN2k.

References

- [1] E. L. Runnerstrom, A. Llordés, S. D. Lounis, and D. J. Milliron, "Nanostructured electrochromic smart windows: traditional materials and NIR-selective plasmonic nanocrystals," *Chem. Commun.*, vol. 50, no. 74, pp. 10555–10572, 2014, doi: 10.1039/c4cc03109a.
- [2] P. Yang, P. Sun, and W. Mai, "Electrochromic energy storage devices," *Mater. Today*, vol. 19, no. 7, pp. 394–402, 2016, doi: 10.1016/j.mattod.2015.11.007.
- [3] J. Yang and J. S. Tse, "Li ion diffusion mechanisms in LiFePO 4: An ab initio molecular dynamics study," *J. Phys. Chem. A*, vol. 115, no. 45, pp. 13045–13049, 2011, doi: 10.1021/jp205057d.
- [4] P. Blaha, *WIEN2k*, vol. 1. 2021.
- [5] C. Ambrosch-Draxl and J. O. Sofo, "Linear optical properties of solids within the full-potential linearized augmented planewave method," *Comput. Phys. Commun.*, vol. 175, no. 1, pp. 1–14, 2006, doi: 10.1016/j.cpc.2006.03.005.
- [6] S. Cottenier, *Density Functional Theory and the Family of (L)APW-methods: a step-by-step introduction*, no. L. 2013.



MAGNETO-CONTROLLED REENTRANT SUPERCONDUCTIVITY EFFECT IN YBCO@TO CORE-SHELL HETEROSTRUCTURES

<u>Rodolfo Ezequiel López Romero^{1*}</u>, Dulce Yolotzin Medina Velázquez¹, and Roberto Escudero Derat²

¹ División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana-Azcapotzalco, Av. San Pablo No 180, Col. Reynosa-Tamaulipas, C.P. 02200 México, D.F., México.

² Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, A. Postal 70-360 México, D.F., México.

*roleze86@gmail.com

The superconducting spin valve effect has been proposed as a viable mechanism to manipulate and control the superconducting transition temperature (T_c) in Ferromagnet/Superconductor/Ferromagnet (F/S/F) heterostructures. Research in this field establishes than T_c can be decreased or increased, or eventually suppress, when the ferromagnetic layers are parallel (P) or antiparallel (AP) magnetized [1,2]. However, since the variation ΔT_c is smaller than the width of the superconducting transition itself. it has not been possible to establish an optimal temperature at which the system is in the normal state in the P configuration and becomes completely superconducting in the AP configuration [3]. In this work, we propose to explore an alternative variant to the superconducting spin-valve effect, which consists of studying the influence of the antiferromagnetic order in the superconducting state in heterostructures formed by an YBa₂Cu₃O₇- Δ (YBCO) superconducting core and a Terbium Oxalate (OT) heptahydrate antiferromagnetic shell in order to promote a magneto-controlled reentrant superconductivity effect in the heterostructure, and thus lead in the same way to a possible switchable effect between normal and superconducting states below the T_{c2} through the application of small magnetic fields. Different heterostructures were made varying the weight ratio between superconducting core and antiferromagnetic shell. These heterostructures were analyzed by both, structural and magnetically, in order to study the reentrant superconducting effect.

Key Words: Heterostructures, Reentrante superconductivity, Spin-valve effect.

References

- [1] L.R. Tagirov. Physical review letters, 83 2058, (1999).
- [2] Sangjun Oh, D. Youm, and M.R Beasley. Applied physics letters, 71 2376-2378, (1997).
- [3] J.Y Gu, et al. Physical review letters, 89 267001, (2002).



Kekulé Induced Valley Birefringence and Skew Scattering in Graphene

Elias Andrade Amezcua_{1,*}, Ramon Carrillo Bastos₂, Mahmoud M. Asmar₃ and Gerardo García Naumis₄

 ¹ Posgrado en Ciencias Físicas, Instituto de Física, Universidad Nacional Autónoma de México (UNAM). Apdo. Postal 20-364, 01000 México D.F., México.
 ²Facultad de Ciencias, Universidad Autónoma de Baja California, Apdo. Postal 1880, 22800 Ensenada, Baja California, México.
 ³Department of Physics, Kennesaw State University, Marietta, Georgia 30060, U.S.A.
 ⁴Depto. de Sistemas Complejos, Instituto de Física, Universidad Nacional Autónoma de México (UNAM). Apdo. Postal 20-364, 01000 México D.F., México.

*eandrade@estudiantes.fisica.unam.mx

In graphene, a Kekulé-Y bond texture modifies the electronic band structure generating two concentric Dirac cones with different Fermi velocities lying in the Γ-point in reciprocal space [1]. The energy dispersion results in different group velocities for each isospin component at a given energy. This energy spectrum combined with the negative refraction index in p-n junctions, allows the emergence of an electronic analog of optical birefringence in graphene [2]. We characterize the valley birefringence produced by a circularly symmetric Kekulé patterned and gated region using the scattering approach. We found caustics with two cusps separated in space by a distance dependent on the Kekulé interaction and that provides a measure of its strength. Then, at low carrier concentration we find a non-vanishing skew cross section, showing the asymmetry in the scattering of electrons around the axis of the incoming flux. This effect is associated with the appearance of the valley Hall effect as electrons with opposite valley polarization are deflected towards opposite directions.



Figure 1 – Schematic of the system, graphene with a circular region of Kekulé-Y bond texture of radius R. We consider an incoming flux of electrons with wavenumber k.



Figure 2 - Probability density (in log₁₀ scale) for an incoming flux of valley polarized electrons into a circular patch of a) pristine graphene where one caustic appears, b) Kekulé-Y graphene where the two group velocities produce two wavefronts. c) and d) show the components that preserve and flip the valley respectively.

Key Words: Graphene, Kekulé, Scattering, Birefringence, Valleytronics.

References

[1] Gamayun, O. V., et al. New Journal of Physics 20.2 (2018): 023016.

[2] Cserti, József, András Pályi, and Csaba Péterfalvi. Physical review letters 99.24 (2007): 246801.



Kekulé-modulated α - T_3 model

Luis Eduardo Sánchez-González^{1*}, Ramón Carrillo-Bastos².

¹ Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Coahuila, Edificio A, Unidad Camporredondo, 25000, Saltillo, Coahuila México. ²Facultad de Ciencias, Universidad Autónoma de Baja California, Apartado Postal 1880, 22800 Ensenada, Baja California, México *Corresponding author: luis-sanchez@uadec.edu.mx

Graphene has interesting electronic transport properties and has inspired the search for similar Dirac-like systems [1]. Among those systems are the Kekulé-distorted graphene [2, 3], with a tripled unit cell, and the α -T₃ model [4], where the honeycomb lattice has an extra atom in the center of each hexagon. In this work, we present a hybrid model of these two, consisting of Kekulé modulated α -T₃ model, i.e., the atom in the center of the hexagon appears with Kekulé periodicity. This system is obtained if atoms are deposited with Kekulé periodicity on a hexagonal lattice with sublattices displaced in the z-plane (like in silicene [5]). Using a tight-binding model for nearest-neighbor and considering small α , we calculate an analytical expression for the dispersion relation. As a result, we find a flat band with a double cone structure.



Fig 1. (Left) Dispersion relation for small α . (Right) Dispersion relation for large α .

Key Words: Kekulé distortion, α - T_3 model, Dirac materials

References

[1] T.O. Wehling, et al., Dirac materials. Advances in Physics, 63, 1–76, (2014).

[2] C. Gutierrez, et al., Imaging chiral symmetry breaking from Kekulé bond order in graphene. *Nature Physics*, **12**, 950–958, (2016).

[3] O. Gamayun, et al., Valley-momentum locking in a graphene superlattice with y-shaped kekulé bond texture. *New Journal of Physics*, **20**, 023016, (2018).



[4] A. Raoux, et al., From dia-to paramagnetic orbital susceptibility of massless fermions. *Phys. Rev. Lett.*, **112**, 026402, (2014).

[5] M.A.K., *et al.*, Review-Silicene: From Material to Device Applications, *ECS J.S.S. Sci. Tech.*, **9**, 115031, (2020)



Green synthesis of zinc oxide nanoparticles mediated by coffee extract

<u>J. León-Flores^{1*}, E. Melo-Uscanga², S. Tehuacanero-Cuapa¹, R. Escamilla³, J. Arenas¹.</u>

¹ Instituto de Física, Universidad Nacional Autónoma de México, Coyoacán, Ciudad Universitaria, C.P. 04510, Ciudad de México, México.

² Facultad de Ingeniería, Universidad Nacional Autónoma de México, Coyoacán, Ciudad Universitaria, C.P. 04510, Ciudad de México, México.

³ Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Coyoacán, Ciudad Universitaria, C.P. 04510, Ciudad de México, México.

*jleon86@fisica.unam.mx

The green chemistry, generally understood as the definition proposed by Anastas and Warner as *"the utilization of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design, manufacture and application of chemical products"* is under considerable attention from the scientific community due the environmental pollution achieved when new materials are produced [1]; in the is sense, providing new eco-friendly synthesis protocols are of interest.

At the present work, it is presented a scalable green synthesis protocol for the production of ZnO nanoparticles with a particle size d < 100 nm. The ZnO nanoparticles were characterized by SEM, TEM microscopy as well as XRD and UV-Vis spectroscopy. The effect of the concentration of coffee extract also was analyzed.

Key Words: Transmission electron microscopy, X-Ray diffraction, Green synthesis, Scanning electron microscopy.

Acknowledgments: This research was partially supported by the UNAM-DGAPA-PAPIIT Program IN112422. J. León-Flores acknowledge the postdoctoral-scholarship granted by CTIC-DGAPA-UNAM. The authors also thank to Phys. Roberto Hernández Reyes, M. Sc Jorge Barreto and Ar. Diego Quiterio for the technical support.

References

[1] Green Chemistry: Theory and Practice, P T Anastas and J C Warner, Oxford University Press, Oxford, 1998.



SIMULATING MICROGELS IN SOLID-LIQUID INTERFACES

Rodrigo RIVAS-BARBOSA1*, Xhorxhina SHAULLI2, Maxime Jolisse BERGMAN2, Nicoletta GNAN11,3, Frank SCHEFFOLD2, and Emanuela ZACCARELLI1.3

¹ Department of Physics, Sapienza University of Rome, Piazzale Aldo Moro 2, 00185 Roma, Italy ² Department of Physics, University of Fribourg, Chemin du Musée 3, 1700, Fribourg, Switzerland ³ CNR Institute of Complex Systems, Uos Sapienza, Piazzale Aldo Moro 2, 00185, Roma, Italy *rodrigo.rivasbarbosa@uniroma1.it

Microgels are cross-linked polymer networks that present a reversible size transition at a critical temperature: the microgel changes from a swollen to compact state as temperature is raised from below to above the so-called volume phase transition temperature. The on-demand response to external cues makes microgels a system of interest both for applications such as drug delivery purposes, and for addressing fundamental questions like jamming [1,2]. A realistic numerical description of microgels has been developed [3,4], tested and used to explain new observations such as microgels placed in liquid-liquid interfaces and the swelling of charged microgels [5,6]. Here, we numerically investigate the volume phase transition of similarly assembled microgels in solid-liquid interfaces, in particular, we study microgels on hydrophilic and hydrophobic surfaces and compare them to super-resolution measurements. The volume phase transition of microgels on hydrophilic surfaces is insignificantly perturbed with respect to the bulk case. On the other hand, on hydrophobic surfaces, microgels spread over the interface in order to decrease the liquid-solid contact area; as temperature is increased, a competition between the self-collapse of the microgel and

the expansion over the interface is seen.

References

- [1] J. Polym. Sci. Part A: Polym. Chem., 51, 2013, 3027-3043.
- [2] Science Advances, 2017, 3, e1700969.
- [3] Macromolecules, 2017, 50, 8777-8786.
- [4] Macromolecules 2019, 52, 20, 7584–7592.
- [5] ACS Nano 2019, 13, 4548-4559
- [6] Soft Matter, 2019, 15, 8113-8128



SYNTHESIS AND FUNCTIONALIZATION OF NANOMATERIALS FOR BIOMEDICAL APPROACHES

Maria Antonieta Ramírez-Morales_{1,2*}, Elisa De Luca₃, Giuseppe A. Mele₂, Pier Paolo Pompa₄, Maria Ada Malvindi₁

¹HiQ-Nano s.r.l., Arnesano. Lecce, IT. ²Dipartimento di Ingegneria dell'Innovazione, Universitá del Salento. Lecce IT. ³CNR NANOTEC, Institute of Nanotechnology. Lecce. IT. ⁴Istituto Italiano di Tecnologia, Nanobiointeractions&Nanodiagnostics. Genova, IT, <u>*maryarmzm@gmail.com</u>

In recent years, multiple nanotechnological tools have been developed for them use in biomedical applications such as drug delivery, biomarkers, sensing, imaging and others. Being the compatibility and toxicity parameters of high importance. Focusing on imaging, the quantum dotsand dye-loaded nanoparticlesare among the most used nanomaterials. But some materials tend to agglomerate, to reduce this problem different surfactants can be added in the solution by two common approaches: surface absorption and covalent attachment. Using biomolecules such as proteins, enzymes, polymers, ligands, DNA strains and drugs.

Biotin, also known as vitamin H or B₇, is used not only in the role of dispersant and stabilizer but also as a fundamental part of the bioapproach. Some types of cancer, such as breast cancer, over express biotin receptors. Taking this affinity as an advantage, we are proposing a tailored synthesis to obtain monodisperse and well-defined fluorescent coreshell nanosystems(from 25 to 500 nm), capable of interacting directly with the cancer cells and facilitating future diagnostic and therapeutic therapies such as imaging and drug delivery.



Figure 1. Schematic representation of two-cycle Stöber method



The core-shell nanosystems present two different dyes (Green and far-red) trapped in different silica matrices. Nanosystems were functionalized by two approaches: simple biotinylationand carboxylic acid groups (-COOH) activation using biotin-hydroxysuccinimide ester (NHS).

Different mass ratios between the nanoparticle suspensions and biotin were prepared (1:1, 3:1, and 5:1 by a bath sonicator for 30 minutes. Stability and dispersion were measured by means of Z-potential by DLS technique. Size, morphology and composition by Transmission Electronic Microscopy (JEM-2200FS) and FT-IR spectroscopy. The emission fluorescence was investigated using TECAN dispositive (200 PRO NanoQuant) and by Confocal microscopy.



Figure 2. TEM images and size distribution of obtained nanoparticles. A) 50 nm, B) 90 nm and C)120 nm.

For the evaluation of biotin-conjugation Z-potential measurement was carried out, having a control without any type of biotin, this control yields a negative potential value that is expected by the negative charges on the surface related with silica oxide nanoparticles. In both cases, the excess of nanoparticles gives a better distribution compared to the equal proportion. For simple biotinylation the optimum ratio corresponds to 3:1 while for biotin-NHS the ratio 5:1 obtains better results. FT-IRspectras are compared with silica-oxide nanoparticles, biotin solution and our biotin-nanosystem, to confirm the presence of each



material in the suspension. Fluorescent emission spectra and confocal images show individual and dual-colored nanoparticles as potential tools in diagnosis and therapeutics for that, additional studies are in progress to identify both the behavior and the toxicity in plant and animal cells.

Key Words: Nanoparticles, synthesis, functionalization, bioapproaches, imaging.

References

- 1. Jiang, W. et al., Int J nanomed, 14, 5611-5622. 2019.
- 2. Shahrzad, D., et al., Chim Acta, 1030, 142-147. 2018.
- 3. Chen, G. et al., Dyes and Pigments, 93:13, 1532-1537. 2012.
- 4. Ma, K., et al., Chem Mat, 25:5, 677-691. 2013.

The authors would like to thank the Project 860914 financed through Maria Sklodowska Curie, Innovative Training Networks. Call: H2020-MSCA-ITN-2019



PIEZORESPONSE IN NANOVOID-RICH WO3 THIN FILMS

Pamela M. Pineda Domínguez1, Torben Boll2, José Luis Enríquez Carrejo1, Abel Hurtado Macías3, John Nogan4, Martin Heilmaier2, Manuel Ramos1*

1 Universidad Autónoma de Ciudad Juárez (UACJ), Av. del Charro 450 N, Juárez 32310, México

² Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-WK), Institute of Nanotechnology (INT) and Karlsruhe Nano Micro Facility (KNMFi), Engelbert-Arnold-Strasse 4, Karlsruhe 76131, Germany

³Laboratorio Nacional de Nanotecnología, Centro de Investigación en Materiales Avanzados S.C. (CIMAV), Miguel de Cervantes 120, Chihuahua 31109, México

⁴ Sandia National Laboratories, Center for Integrated Nanotechnologies (CINT), 1101 Eubank Bldg. SE, Albuquerque, NM 87110, USA

* manuel.ramos@uacj.mx

We report a piezoresponse in WO₃ thin films fabricated by RF-sputtering and subjected to post-deposit annealing treatments under a forming gas (3% H₂ in N₂), related to the presence of oxygen vacancies and ionic charge dynamics [1], rather than to a non-centrosymmetric structure. The film processed at 400 °C shows piezo active domains (Fig. 1a) and hysteresis loops ($d_{33} = 35\pm5$ pm/V) by switching spectroscopy – piezoresponse force microscopy (SS-PFM) technique (Fig. 1b) [2]. X-ray diffraction (XRD) and transmission electron microscopy (TEM) show a mixture of WO₃ phases [3]. Atom probe tomography (APT) (Fig. 1c) reveals nanovoids filled with constituents of the forming gas, indirectly causing the piezoresponse.

Key Words: WO3, nanovoids, piezoresponse, APT, non-piezoelectric effects



Figure 1. WO₃ thin film exposed at 400°C shows a) topography by SS-PFM before (up) and after (down) the measurement, b) hysteresis loops and c) microstructure obtained by APT.



References

- [1] Park *et al.*, *Science*, no. 6581, 653–657, (2022)
 [2] Gruverman, *et al.*, *Nat. Commun.*, 1661, (2019)
 [3] Kim *et al.*, *Appl. Phys. Lett.*, 032904, (2010)



Exploring the structure and reactivity of Pt_nCu_n (n = 1–7) alloy clusters

P. L. Rodríguez-Kessler¹*, A. R. Rodríguez-Domínguez², Alvaro Muñoz-Castro³

¹Centro de Investigaciones en Optica A.C., Loma del Bosque 115, Col. Lomas del Campestre, C.P. 37150, Leon, Guanajuato, Mexico.

²Instituto de Física, Universidad Autonoma de San Luis Potosi, San Luis Potosi 78000, Mexico. ³Facultad de Ingenieria, Arquitectura y Diseno, Universidad San Sebastian, Bellavista 7, Santiago,8420524, Chile.

*Corresponding author e-mail: plkessler@cio.mx

In this work, we investigate the structure, electronic and reactivity properties of PtnCun (n = 1-7) clusters by using density functional theory (DFT) calculations. The equilibrium structures of the most stable clusters are obtained by a structure search procedure based in simulated annealing. The results show that the PtnCun cluster alloys adopt layered structure motifs with segregation of the Cu and Pt species. The total magnetic moments of the clusters adopt the low spin configuration. The bimetallic cluster reactivity is investigated by using the ionization potential, electron affinity, and the d-band center, respectively. The results show that the PtnCun clusters with (n = 5-7) have similar vIP and vEA parameters compared to the unary Pt clusters, but the d-band center molecular electrostatic potential shows that the Cu species increase the available active sites on the cluster surface. The data on the infrared spectra of the clusters is also provided. These results are useful to understand the fundamental properties of Pt–M bimetallic alloys in the subnanometer region. Most importantly, these clusters are active catalysts according to their properties and features provided.



Figure 1 – The molecular electrostátic potential [Vs(r)] for PtnCun (n=1-7) clusters. **Key Words:** First Principles, Cu-Pt, Clusters, Alloys



References

[1] Phys Chem. Chem. Phys. 23 (12), 7233-7239 (2021) DOI: 10.1039/d1cp00379h



A COMPARATIVE MOLECULAR DYNAMIC STUDY FOR PLATINUM POTENTIALS

Arturo Jáuregui Díaz¹*, Sergio Mejía Rosales^{2†}

¹ Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León, Av. Universidad S/N, Ciudad Universitaria C.P. 66455, San Nicolás de los Garza, Nuevo León, México.

*arturojd@outlook.com, *sergio.mejiars@uanl.edu.mx

Platinum is an important material with great applications in fields like biomedical, energetics, and textile, due to its thermal, catalytic and mechanical properties. The use of Pt in the composition of nanaoalloys also opens the possibility for novel applications[1]. Molecular dynamics simulation is a tool that allows us to predict the behavior of a material without the necessity to synthesize it [2], but in order to assure robust results, the interaction potential used in the simulations must be properly characterized. This work presents a comparative study for important aspects of an interatomic potential for Pt, obtaining the lattice constant, surface energies (100), (110) and (111), stiffness constants, and state equation, and a comparison of these results are made against the ones obtained in the simulations of Padilla [3]. Comparing newer potentials with some potentials used in the past allows us to take decisions on its use depending on the relation between prediction capability of the potential and its computational efficiency. The results obtained show that the potential studied [4] has some limitations for modeling the behavior of the platinum at bulk, but it also is an important incentive to develop a better potential.

Key Words: Molecular Dynamics, Platinum

References

X.-M. Z. R. Huang, G.-F. Shao and Y.-H. Yen, Journal of Saudi Chemical Society 25, 101297 (2021).
 D. C. M. R. A. C. T. v. D. T. J. Carlos F. Sanz-Navarro, J. Phys. Chem. A 112, 1392 (2008).
 A. M. I. Padilla, T. Jacobs, J. Chem. Theory Comput. 141, 633 (2021).
 A. C. T. F. H. W. Sheng, M. J. Kramer and M. W. Chen, PHYSICAL REVIEW B, 83, 134118 (2011)



SELF-DIFFUSION OF SOME BUCKMINSTERFULLERENE DERIVATIVES IN AQUEOUS MEDIA: A MOLECULAR DYNAMICS APPROACH

Alexis Tepale-Luna^{1*}, Minerva González-Melchor¹⁺

¹ Instituto de Física "Ing. Luis Rivera Terrazas", Benemérita Universidad Autónoma de Puebla, Av. San Claudio s/n, Cd. Universitaria, La Hacienda, C. P. 72592, Puebla, Puebla, México. *atepale@ifuap.buap.mx,⁺minerva@ifuap.buap.mx

Fullerenes are molecules composed of carbon atoms joined by covalent bonds, which can take geometric shapes such as ellipsoids or spheres, among others. They were discovered in 1985 in an experiment designed by H. W. Kroto and collaborators [1], and some years later, fullerenes have drawn the attention of the scientific community due to their interesting properties which can be exploited in medical and pharmaceutical applications, as well as in the treatment of wastewater [2]. We focus our attention on the fullerene C₆₀. This molecule is highly stable and poorly soluble in water; which has been a challenge for its biomedical applications. To tackle this complication, we can substitute some of the carbon atoms in the fullerene surface with another chemical species with the purpose of enhancing its physicalchemical properties, for instance its solubility in water. These new molecules are called heterofullerenes. Although there are no synthesis methods for industrial scale production yet, and therefore experimental research has been limited, molecular simulations are a powerful tool to gain insight into these systems, in this work we perform molecular dynamics simulations. In this presentation we shall talk about the behavior of C₆₀ derivatives: C₅₇N₃, C₆₀F₁₈, C₆₀(OH)₁₂ (see example of figure 1) when they are dispersed in water. We analyze the mean squared displacement, and by means of the Einstein relation we compute the fullerene self-diffusion coefficient D, we emphasize on their behavior in terms of the mass and geometry of the diffusing molecules, as well as the system temperature (see table 1).

Table 1 – *D* as function of temperature for several heterofullerenes immersed in SPC/ ϵ water in units of 10⁻⁵ cm²/seg.

T (K)	C ₅₇ N	$C_{60}F_1$	C ₆₀ (OH)
280	0.202	0.100	0.035
320	0.567	0.388	0.312
360	2.337	1.574	0.296



Figure 1 – Simulation visualization of $C_{57}N_3$ and water molecules.

Key Words: Fullerenes, Self-diffusion, Molecular Dynamics.



References

H. W. Kroto, et al., Nature **318** 14, 162-163 (1985).
 S. Goodarzi, et al., Materials Today **20** 8, 460-480 (2017).



MULTILAYERED HYPERBOLIC MATERIAL FOR NONLINEAR OPTICS

<u>Fernando-Arturo ARAIZA-SIXTOS¹</u>*, Fernando SOLORIO-SOTO², Hugo TIZNADO², Eder LIZARRAGA MEDINA³, Ramón CARRILES-JAIMES⁴, Raúl RANGEL-ROJO¹

¹Centro de Investigación Científica y de Educación Superior de Ensenada, Carr. Tijuana-Ensenada 3918, Zona Playitas, 22860 Ensenada, B.C. ²Centro de Nanociencias y Nanotecnología, Carr. Tijuana-Ensenada km107, C.I.C.E.S.E., 22860 Ensenada, B.C. ³Facultad de Ciencias de la Ingeniería y Tecnología, Universidad Autónoma de Baja California, Valle de las Palmas, Mexico. Blvd. Universitario #1000, Unidad Valle de las Palmas, 22260 Tijuana, B.C. ⁴Centro de Investigaciones en Óptica, Lomas del Bosque 115, Lomas del Campestre, 37150 León, Gto. *araizaf@cicese.edu.mx

In this work we present the design and fabrication of a multilayered hyperbolic material to enhance the third-order nonlinear response. The multilayer structure consists of a metal (ruthenium) and a dielectric (titanium dioxide), and the width of the layers is being manipulated in order to obtain a point of Epsilon Near Zero (ENZ) around 800 nm.

In order to check if the third-order nonlinearity is being enhanced around 800nm, the nonlinear response was studied in different wavelengths using an Optical Parametric Amplifier and the z-scan technique. In Figure 1 we can observe the nonlinear refractive index n_2 measured at different wavelengths, it is clearly seen that the nonlinear signal is being enhanced at 800 nm.



Figure 1 – Measured nonlinear refractive index as a function of wavelength. It is clear that the nonlinear response is being enhanced at 800 nm.

Key Words: ENZ, nonlinear optics, hyperbolic materials, multilayered structure



DFT AND EXPERIMENTAL STUDIES ON ELECTRONIC AND STRUCTURE PROPERTIES OF PBSE_{1-X}S_X ALLOYS

Sergio Jahir MONTIEL PERALES¹*, Cesia GUANEROS AGUILAR², Felipe CABALLERO BRIONES¹

 ¹ Instituto Politécnico Nacional, Materiales y Tecnologías para Energía, Salud y Medio Ambiente (GESMAT), CICATA Altamira. Km 14.5 Carr. Tampico- Puerto Industrial Altamira.89600, Altamira, México.
 ² CONACYT- Instituto Politécnico Nacional, Materiales y Tecnologías para Energía, Salud y Medio Ambiente (GESMAT), CICATA Altamira. Km 14.5 Carr. Tampico- Puerto Industrial Altamira.89600, Altamira, México.

*Corresponding author e-mail: smontielp2100@alumno.ipn.mx

In this study, density functional theory has been used to investigate the structural and electronic properties of lead selenide (PbSe) and lead sulfide (PbS) semiconductors and their alloys PbSe_{1-x}S_x using the virtual crystal approximation and random alloy generations. The generalized gradient approximation (GGA) has been used to obtain lattice parameters which are compared with theory and experimental results. The generalized gradient approximation (MGGA) of TB09LDA has been used to calculate the electronic bands, and the electronic bands have been obtained for different sulfur compositions ($0 \le x \le 1$, $\Delta x=0.1$). It has been observed that the transition from the valence band to the conduction band takes place at the L point, which agrees with previous theoretical investigations. It has been observed that both the forbidden bandwidth and lattice parameters of the alloys obey Vegard's law.

Key Words: Alloys, lead chalcogenides, DFT



SYNTHESIS AND CHARACTERIZATION OF CATALYSTS FOR THE OXIDATION OF METHANE USING ELECTROCHEMICAL PROCESSES

Laura Juliana CORTÉS CHACÓN1*, Marlene GONZÁLEZ MONTIEL2

1 Instituto Politécnico Nacional, CICATA Unidad Legaria 2 CONACYT-Instituto Politécnico Nacional, CICATA Unidad Legaria Calz Legaria 694, Col. Irrigación, Miguel Hidalgo, 11500 Ciudad de México, CDMX <u>*laurajulianacorteschacon@gmail.com</u>

Currently, a high percentage of methane resources are burned to produce electricity or provide heating, contributing significantly to carbon dioxide emissions. However, methane through an oxidation process can produce methanol, an alcohol whose annual demand has grown driven by emerging energy applications [1-3].

This work proposes the synthesis and characterization of materials through two pathways, one hydrothermal and one rapid precipitation, these materials will be tested in an H-type electrochemical cell to evaluate their performance oriented to methane oxidation under mild reaction conditions.

Initially, nickel chloride (Cl_2Ni) was used for both synthesis processes, then 10% sodium metavanadate (NaO_3V) and 10% hydrated sulfate oxide (O_9SV) for the hydrothermal process and 10% vanadium chloride (Cl_3V) for the rapid precipitation process, obtaining with both processes a dark green powder in the case of the nickel oxide precursor that contains nickel chloride and a powder between green and yellow in the precursors that contain vanadium as can be seen in figures 2a and 3a. Those precursors were calcined at 325°C and 500°C to obtain nickel oxide.

For the characterization of the synthesized materials, X-ray diffraction, infrared spectroscopy and scanning electron microscopy have been performed.



Figure 1 – 1) Illustration hydrothermal method, 2) Nickel oxide precursor a) after hydrothermal synthesis; b) calcined at 325° C; c) calcined at 500° C; 3 Nickel oxide precursor doped with 10% of metavanadate a) after hydrothermal synthesis; b) calcined at 325° C; c) calcined at 500° C



Key Words: methane oxidation, metal oxides, vacancies.

References

[1] Prajapati, A., Collins, B. A., Goodpaster, J. D., & Singh, M. R., Fundamental insight into electrochemical oxidation of methane towards methanol on transition metal oxides, Proceedings of the National Academy of Sciences, 118(8), 2021.

[2] Jang, J., Shen, K., & Morales-Guio, C. G., Electrochemical direct partial oxidation of methane to methanol. Joule, 3(11), 2019, 2589-2593.

[3] Fornaciari, J. C., Primc, D., Kawashima, K., Wygant, B. R., Verma, S., Spanu, L. & Weber, A. Z., A perspective on the electrochemical oxidation of methane to methanol in membrane electrode assemblies. ACS Energy Letters, 5(9), 2020, 2954-2963.



WOOD/PLASTIC NANOCOMPOSITE FOR PRODUCT DESIGN

Alejandra MONTES-VILLAGRAN¹, Santos-Adriana MARTEL-ESTRADA^{1,*}, Laura-Elizabeth VALENCIA-GÓMEZ², Hortensia REYES-BLAS², César-Omar BALDERRAMA-ARMENDÁRIZ², David CORTES-SÁENZ²

Authors' Affiliations, with complete postal address (Arial, size 11, italics, single space) ¹ Instituto de Arquitectura, Diseño y Arte, Universidad Autónoma de Ciudad Juárez, Av. Del Charro No. 450 Norte. C.P. 32310, Ciudad Juárez, Chihuahua. ² Instituto de Ingeniería y Tecnología, Universidad Autónoma de Ciudad Juárez, Av. Del Charro No. 450 Norte. C.P. 32310, Ciudad Juárez, Chihuahua.

*mizul@yahoo.com

Wood and plastic composites are any compounds containing plant fibers (such as wood) and thermosets or thermoplastics [1]. The ability to manipulate matter at the nanoscale promises enormous potential for various applications and innovations involving new materials for different areas [2]. One of the most used particles is zinc oxide, which is conferred on materials such as resistance to mechanical abrasion, antimicrobial, stain and dust repellent, and water repellent, among others [3]. This research use this nanoparticle to improve the properties of the wood/plastic composite material. One of the most used particles is zinc oxide, which is conferred on materials such as resistance to mechanical abrasion, antimicrobial, stain and dust repellent, and water repellent, among others [3]. This research elaborated a nanocomposite of wood/plastic improved with nano zinc oxide to produce a filament for its use in additive manufacturing. The thermal properties of the composites were investigated through TGA. The filament morphology was assessed using a scanning electron microscope (SEM). The crystallography of the samples was evaluated through X-ray diffraction (XRD), and the physicochemical properties were confirmed by Fourier-Transformed. Also, it was estimated the antibacterial properties of the The cumulative results obtained from IR and X-ray diffraction spectra, TGA, and samples. antimicrobial test suggest that the material could be used in product design

Key Words: Nano zinc-oxide, wood-composite, additive manufacturing, nanocomposite.

References

[1] Ashori, A. (2008). Wood–plastic composites as promising green-composites for automotive industries. Bioresource Techonology, 99, 4661–4667.

[2] Almendárez-Camarillo, A., & González-Calderon, J. A. (2011). Nanomateriales: su crecimiento, caracterización estructural y tendencias. Ide@s CONCYTEG, 6(72), 772–787.

[3] Empa, T. T. S. (2011). Grundlagen und Leitprinzipien zur effizienten Entwicklung nachhaltiger Nanotextilien.



LOCAL AND STRUCTURAL ATUDY BY SPECTROSCOPY MÖSSBAUER OF ALLOYS AlxFe(1-x) (X=0,25; 0,5 and 0,75) OBTAINED BY ARC FURNACE

R. Rocha Cabrera^{1*}

1 Universidad Nacional Mayor de San Marcos, Facultad de ciencias físicas, Lima, Perú. <u>*rrochac@unmsm.edu.pe</u>.

The Fe-AI metallic alloys in the iron-rich regions are of great importance due to their interesting magnetic properties present in their nanocrystalline state, in which they are used in magnetic memory devices and magnetic sensors, while for aluminum-rich regions, These alloys are used in the automotive and space industries because of their low density and excellent corrosion resistance. In the present work the samples were synthesized by arc furnace technique (HA) and later foram treated at temperatures of 600°C, 950°C and 1000 °C for 48, 290 and 48 hours, respectively. After preparing the samples, they are characterized at room temperature (ST) as at 600°C, 950°C and 1000°C. See figure 1.



Figure 1 – Mössbauer spectrum of the compositions $Fe_{25}AI_{75}$, $Fe_{50}AI_{50}$ and $Fe_{25}AI_{75}$ at 600₀C. At these temperatures, for the compositions $AI_{25}Fe_{75}$, $AI_{50}Fe_{50}$, the intermetallic FeAI and the solid solution Fe(AI) rich and poor in iron with ferromagnetic and paramagnetic behavior are observed for the composition $AI_{75}Fe_{25}$, the intermetallic $AI_{13}Fe_4$ and the solid solution Fe(AI) are observed. rich in aluminium [1]. See table 1.

Temperaturas	Al25Fe75	Al ₅₀ Fe ₅₀	Al75Fe25
ST	Fe(Al)	FeAl	$\mathrm{Al}_{13}\mathrm{Fe}_4,\mathrm{Fe}(\mathrm{Al})$
600°C	Fe(Al)	FeAl, Fe(Al)	$\mathrm{Al}_{13}\mathrm{Fe}_4,\mathrm{Fe}(\mathrm{Al})$
$950^{0}C$	Fe(Al)	FeAl, Fe(Al)	Al ₁₃ Fe ₄ , Fe(Al)
$1000^{\circ}C$	Fe(Al)	FeAl, Fe(Al)	Al ₁₃ Fe ₄ , Fe(Al)

Table 1 – Crystal structures and solid solutions obtained.

Key Words: Mössbauer spectroscopy, X-ray diffraction, arc furnace.

References

[1] R. Rocha Cabrera. Revista de investigación de física 24(3), (2021).



DESIGN AND FABRICATION OF SEIRA SUBSTRATE BASED IN NANOANTENNAS TO DETECT DISASSES

JAVIER MENDEZ-LOZOYA^{1,2*}, FERNANDO SEBASTIAN CHIWO^{1,3}, <u>JUAN ROBERTO MORENO¹</u> DE LA ROSA ZAPATA-ARIEL^{2,} DÍAZ DE LEÓN ZAPATA-RAMÓN ²

¹ Universidad Marista de San Luis Potosí, Av. Beato Marcelino Champagnat 305, Villa Magna, 78183 San Luis, S.L.P.

²Instituto Tecnológico de San Luis Potosí, Tecnológico S/N, Col. Unidad, Ponciano Arriaga, 78436 Soledad de Graciano Sánchez, S.L.P.

³ Centro de Tecnología Avanzada, CIATEQ A.C., Eje 126 No. 225, Zona Industrial del Potosí, 78395, San Luis Potosí, México.

* javier.ml@slp.tecnm.mx.

The implementation of detector based in nanoantennas array takes a big importance in the medical diagnostic. The optical properties of nanoantenna are correlated with their morphology and efficiency heat-electric energy conversion of incident radiation. In this paper, we proposed a Bowtie Cross Nanoantenna (BCN). We study the reflection of incident infrared radiation by nanoantenna to analyze resonance frequency, the heat flux and the heat-electric energy conversion by Seebeck effect in COMSOL simulations. Fig. 1 shows a 3D plot of **E** field enhancement as function of frequency at three maximum absorbance values. Electric field enhancement presents a maximum value when v_{r1} =12.58 THz, v_{r2} =25.31THz, v_{r3} =36.87 THz and v_{r4} =49.37 THz [1]. The array of Silver-Nickel-Boron Silicon doped (Ag-Si:B-Ni) nanoantennas was fabricated by electron beam lithography (EBL) in Si/SiO₂ substrates [2]. We also study the optical properties with FTIR.

Key Words: Bowtie Cross Nanoantenna (BCN), Fourier-transform infrared spectroscopy (FTIR), resonance frequency (v_r), Seebeck effect.



Figure 1 –shows a 3D plot of E field enhancement factor as function of frequency observed in the simulation.

References

[1] S. H. Tang, P. P. Craig, and T. A. Kitchens, Seebeck Coefficient at the Curie Temperature: Specific Heat of Charge Carriers in Ferromagnets, Phys. Rev. Lett. **27**, 593 (30 August 1971).

[2] F. J. González, J. Alda, J. Simón, J. Ginn, and G. Boreman, The effect of metal dispersion on the resonance of antennas at infrared frequencies, Infrared Physics and Technology, vol. **52**, no. 1, p. 4, 2009.