SLAFES XXIV MORELIA

XXIV Latin American Symposium on Solid State Physics
November 7-11, 2022

Abstract Book

POSGRADO EN CIENCIA E INGENIERÍA DE MATERIALES

INSTITUTO DE CIENCIA, TECNOLOGÍA E INNOVACIÓN DEL ESTADO DE MICHOACÁN

Sociedad Mexicana de Física

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Acknowledgment

Instituto de Investigaciones en Materiales – UNAM
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Welcome

The XXIV Latin American Symposium on Solid State Physics (SLAFES), will be held in Morelia, Michoacán, from the 7th to the 11th of November 2022. SLAFES is one of the most important and traditional meetings in the area of the Solid State Physics in Latin America. The most recent editions were held in Colombia (Boyacá, 2013), Chile (Puerto Varas, 2015) and Argentina (Bariloche, 2018). The XXIV edition of SLAFES in Morelia will take place at the conference center (CSAM) of the Universidad Nacional Autónoma de México, Campus Morelia.

The main goal of the SLAFES is to provide scientists from Latin America and from around the world, the opportunity to exchange information, new results, new ideas and to be in a unique forum to discuss the latest developments in this strategic area of knowledge as it is the Solid State Physics.

Morelia is located around 320 km to the west of Mexico City, in the province of Michoacán. Morelia is a colonial city that was declared in 1991 by the UNESCO “Patrimonio Cultural de la Humanidad”, and is considered one of the most beautiful cities in México, and also one of the most important tourist destinations of our country.

The SLAFES is sponsored by the Instituto de Investigaciones en Materiales and the Posgrado en Ciencia e Ingenieria de Materiales, both from the Universidad Nacional Autónoma de Mexico (UNAM). The Instituto de Ciencia, Tecnología e Innovación of the State of Michoacán (ICTI). The ESIME-Culhuacán of the Instituto Politécnico Nacional. The Sociedad Mexicana de Física. We are also indebted to many people and members of the National and International Committee that sponsored and contributed to the organization of the SLAFES in various ways.

On behalf of the XXIV-SLAFES Organizing Committee we wish you an enjoyable and productive stay in Morelia, and hope that you benefit from both the academic event throughout the conference and the cultural experience at the city of Morelia.

General Information

Venue

The symposium will be held at the conference center (CSAM) of the Universidad Nacional Autónoma de México, Campus Morelia.

Registration

The registration desk will be located in the esplanade of the CSAM at the UNAM Campus and will be operate from Monday 7 to Tuesday 8, from 9:00 to 18:00

Oral Presentation

Plenaries, Invited Talks and Contribution will take place in the auditorium of the CSAM at the UNAM Campus Morelia. Plenary sessions will last 45 minutes plus 5 minutes for questions. Invited Talks will last 20 minutes plus 5 minutes for questions. Oral Contributions will last 12 minutes plus 3 minutes for questions.

Posters Presentation

There will be only one Poster session: Tuesday 8th from 16:00 to 18:00 hrs at the esplanade of the CSAM.

Proceedings

The proceedings of the SLAFES will be published as regular papers at the Revista Mexicana de Fisica (impact factor 1.7), following the review process already establish in his web page rmf.smf.mx Please submit the manuscript to the Solid State Physics Section. The deadline for manuscript submissions is December 2, 2022

SOCIAL PROGRAM

Morelia is located around 320 km to the west of Mexico City, in the province of Michoacán. Morelia is a colonial city that was declared in 1991 by the UNESCO “Patrimonio Cultural de la Humanidad”, and is considered one of the most beautiful cities in México, and also one of the most important tourist destinations of our country. Enjoy the city of Morelia.

Wednesday, 9th

15:00 -19:30 Conference excursion to Patzcuaro (pueblo mágico), this event is optional and the cost is not included in the registration fee
19:30 – 21:00 Cocktail at the Cultural Center of UNAM (downtown).

Monday 7th

9.00- 9.30 Opening

Chairman O. Navarro

9.30 -10.30 (Plenary Lecture 1) - Plasmonic response of nanoparticles arrays and its potential applications, Cecilia Noguez , UNAM/Instituto de Fisica, cecilia@fisica.unam.mx

10.30 - 11.00 (Invited Talk) Molecular symmetry protected topological phases, Joel Yuen-Zhou, Kai Schwennicke, University of California San Diego, Department of Chemistry and Biochemistry, La Jolla, joelyuen@ucsd.edu

11.00 - 11.30 (Invited Talk 1) - Role of geometry in hinge-states in second-order topological phases, Jose Eduardo Barrios-Vargas , Facultad de Química, UNAM, jebarrios@quimica.unam.mx

11.30 - 12:00 Coffee Break

Chairman M. Cruz Irisson

12.00 - 13.00 (Plenary Lecture 2) – Dynamical tuning of the thermal conductivity via electrophononic, magnetophononic and photophononic effects, Riccardo Rurali , ICMAB-CSIC, Barcelona, España, rrurali@icmab.es

13.00 - 14.00 (Plenary Lecture 3) - Growth of zinc-blende and wurtzite III-N heterostructures and nanostructures by molecular beam epitaxy, Maximo Lopez-Lopez , Centro de Investigación y de Estudios Avanzados del IPN, mlopezl@cinvestav.mx

14.00 - 16:00 Lunch
16.00 – 16.30 Coffee Break

Chairman B. Aguilar

16.30 - 17.00 (Invited Talk 2) - Electronic transport in phosphorene junctions, Karla Johana Lamas-Martínez, Sergio Molina-Valdovinos, José Alberto Briones-Torres, Isaac Rodríguez-Vargas , Universidad Autónoma de Zacatecas, isaac@uaz.edu.mx

17.00 - 17.15 (S1) - Surface lattice resonances of Ag nanoparticle honeycomb arrays, Alejandro Ramos Romero and Ana L. González , Benemérita Universidad Autónoma de Puebla, anagr@ifuap.buap.mx

17.15 - 17.30 (S2) - Strain engineering on the impurity-induced magnetism in graphene nanostructures, Lilia Meza-Montes, Juan Hernández-Tecorralco, Romeo de Coss , Benemérita Universidad Autónoma de Puebla, lilia@ifuap.buap.mx

17.30 - 18.00 (Invited Talk 3) - Disorder effect on transport, thermoelectric and magnetoresistance properties in a ferromagnetic superlattices based on 2D-Materials, Outmane Oubram; Eric Jovani Guzmán; Isaac Rodríguez-Vargas; Oracio Navarro Chavez , Facultad de Ciencias Químicas e Ingeniería/Universidad Autónoma del Estado de Morelos,, Oubram@uaem.mx

Tuesday 8th

Chairman M. López

09.00 - 10.00 (Plenary Lecture 4) - Coatings to improve magnesium alloys as orthopedic biomaterials, Benjamín Millán-Ramos, Daniela Morquecho-Marín, Phaedra Silva-Bermudez, José Victoria-Hernández, Dietmar Letzig, Argelia Almaguer-Flores, Sandra E. Rodil, Universidad Nacional Autonoma de Mexico, srodil@unam.mx

10.00 - 11.00 (Plenary Lecture 5) - Optical and Structural Characterization of High Crystalline Quality InGaAsSb Semiconductor Layers Grown by LPE for Near and Mid-Infrared Applications, J.G. Mendoza-Alvarez, Y.L. Casallas-Moreno, G. Villa-Martínez, M. Ramírez-López, M. Pérez-González, P. Rodríguez-Fragoso, M.L. Gómez-Herrera, J.L. Herrera-Pérez , Centro de Investigación y de Estudios Avanzados del IPN, juliogma1@gmail.com

11.00 - 11.30 (Invited Talk 4) - Size effects on the physical properties of superconductors and semiconductors, Luis A. Pérez , Instituto de Física, Universidad Nacional Autónoma de México, lperez@fisica.unam.mx

11.30 - 12:00 Coffee Break

Chairman R. Rurali

12.00 - 13.00 (Plenary Lecture 6) - Nanostructures made by sputtering for applications in magnetism, medicine, energy and aerospace industry, José Miguel García-Martín, CSIC (Spain), josemiguel.garcia.martin@csic.es

13.00 - 14.00 (Plenary Lecture 7) - Excitonic and structural properties of epitaxial subnanometric quantum dots and quantum wells of ii-vi semiconductors, Isaac Hernández-Calderón , CINVESTAV IPN, Isaac.hernandez@cinvestav.mx

14.00 - 16:00 Lunch

16.00 – 16.30 Coffee Break

16.30 – 18.00 Poster Presentation

Wednesday 9th

Chairman J. Miguel

09.00 - 10.00 (Plenary Lecture 8) - Some Strategies to Integrate 2D Materials into Functional Applications, Mildred Quintana, Universidad Autónoma de San Luis Potosí, mildred.quintana@uaslp.mx

10.00 - 11.00 (Plenary Lecture 9) - Surprises from electron-phonon interaction with chiral phonons in two-dimensional materials, Luis E. F. Foa Torres, Universidad de Chile, luis.foatorres@uchile.cl

11.00 11.15 (S3) - Search for atomic structures by ab initio methods and evolutionary algorithms for monatomic systems under hydrostatic pressure, Beatriz Cogollo, Javier Montoya , University of Cartagena, bcogolloo@unicartagena.edu.co

11.15 - 11.30 (S4) - Towards high-performance permanent magnets with reduced-rare earth content: The effect of Zr and Nd substitution on SmFe11V alloy, A.M. Schönhöbel, R. Madugundo, C. Echevarria-Bonet, L. Zamora, J. M. Barandiarán, G. C. Hadjipanayis , Universidad del Valle, ana.schonhobel@correounivalle.edu.co

11.30 - 12:00 Coffee Break

Chairman E. Barrios

12.00 - 13.00 (Plenary Lecture 10) - Dirac Equation in Solid State Systems, Alfredo Raya , IFM-UMSNH, alfredo.raya@umich.mx

13.00 - 14.00 (Plenary Lecture 11) - Atomic scale modelling of aperiodic heterostructures, Chumin Wang , Universidad Nacional Autónoma de México, chumin@unam.mx

14.00 - 18:00 Excursion

19.30 - 21:00 Cocktail/Centro Cutural UNAM

Thursday 10th

Chairman A. Raya

09.00 - 10.00 (Plenary Lecture 12) - Flat-bands and superconductivity in magic angle twisted graphene multilayers, Gerardo Naumis, Leonardo A. Navarro-Labastida, Abdiel Espinosa-Champo , PHOTOPHONONIC EFFECTS, naumis@fisica.unam.mx

10.00 - 11.00 (Plenary Lecture 13) - An analysis of different magnetometry protocols to determine dipolar interactions in particle assemblies, Armando Encinas , División de Materiales Avanzados, Instituto Potosino de Investigación Científica y Tecnológica, armando.encinas@ipicyt.edu.mx

11.00 - 11.30 (Invited Talk 5) - Steering the current flow in twisted bilayer graphene, Jesús Arturo Sánchez-Sánchez, Montserrat Navarro-Espino, Yonatan Betancur-Ocampo, José Eduardo Barrios-Vargas, Thomas Stegmann , Universidad Nacional Autónoma de México, stegmann@icf.unam.mx

11.30 - 12:00 Coffee Break

Chairman J. Arriaga

12.00 - 13.00 (Plenary Lecture 14) - Nonlocal optical response of metamaterials and metastructures, F. Pérez-Rodríguez, J. G. Medrano, P. L. Valdés-Negrin, F. J. Flores-Ruiz, N. M. Makarov , Benemérita Universidad Autónoma de Puebla / Instituto de Física, fperez@ifuap.buap.mx

13.00 - 13.15 (S5) - Effects of f and cl in the vibrational properties of porous silicon carbide with si and c-terminated pore surface., Ricardo Bermeo Campos, Alejandro Trejo Baños, Fernando Salazar Posadas, Miguel Cruz Irisson , ESIME Culhuacan - IPN, rick.berm.gin@gmail.com

13.15 - 13.30 (S6) - Generalized Hamiltonian for Kekulé graphene and the emergence of valley-cooperative Klein tunneling, Yonatan Betancur Ocampo, Santiago Galván y García, and Thomas Stegmann , Universidad Nacional Autónoma de México, ybetancur@fisica.unam.mx

13.30 - 13.45 (S7) - Incorporation of Mn into w-AlN nanostructures by MBE, Jesús Fernando Fabian-Jocobi, Raul Trejo-Hernández, Jorge Ivan Hernández- Martínez, Angel Leonardo Martínez-López, Yenny Lucero Casallas-Moreno, Salvador Gallardo-Hernández, Daniel Olguin-Melo, Máximo López-López , CINVESTAV, jesus.fabian@cinvestav.mx

13.45 - 14.00 (S8) - Tight-binding calculation of band-gap energy in a four-channel model DNA and its dependence on temperature, length, hydration, and basis sequence , Luis Gabriel Mesa Suárez and Carlos Jose Páez Gonzalez , Universidad Industrial de Santander, luis.mesa1@correo.uis.edu.co

14.00 - 16:00 Lunch

16.00 – 16.30 Coffee Break

Chairman J. Lemus

16.30 - 17.00 (Invited Talk 6) - Theoretical approach to the optical properties and vibrational spectroscopies of semiconductor nanostructures, Alejandro Trejo Baños, Miguel Cruz Irisson, Instituto Politécnico Nacional, alejandtb13@gmail.com

17.00 - 17.30 (Invited Talk 7) - Theoretical study of various noncovalent interactions in larger molecules, S. E. Perez-Figueroa, A. Trejo, A. Miranda, M. Cruz-Irisson , UNAM, sperezf@gmail.com

17.30 - 18.00 Conference meeting

Friday 11st

Chairman T. Soto

09.00 - 09.15 (S9) - Inverse band gap versus polarization relation in ferroelectric materials from first principles, Nicolás Forero, Nicolás Varas, Sebastián Reyes-Lillo , Universidad Andres Bello, nicolas.forero.cl@gmail.com

09.15 - 09.30 (S10) - Two particle wavefunctions and electron pairs in periodic and aperiodic systems., Uriel Alberto Díaz Reynoso, Ernesto Huipe Domratcheva, Oracio Navarro Chávez , IIM UNIDAD MORELIA, UNAM, udiazr@ciencias.unam.mx

09.30 - 09.45 (S11) - First-principles calculations of molecular adsorption on graphene, Omar Everardo Arroyo Miranda, Francisco Sánchez Ochoa, Cecilia Noguez. , Universidad Nacional Autónoma de México , arroyomirandaomar@ciencias.unam.mx

09.45 - 10.00 (S12) - Enhancement of parameters performance of an SPR optical biosensor based on bimetal - 2D materials structures, Jefte Ceballos Zumaya, Ireri Aydée Sustaita Torres, , José Samuel Pérez Huerta, Jesús Madrigal Melchor, Universidad Autónoma de Zacatecas, jceballoslumat@uaz.edu.mx"

10.00 - 10.15 (S13) - Nonreciprocal Linear Transmission of Sound in a Viscous Environment with Broken P Symmetry, J. Arriaga , Benemérita Universidad Autónoma de Puebla, arriaga@ifuap.buap.mx

10.15 - 10.30 (S14) - Spin wave localization in magnonic crystals with defects, Zorayda Lazcano-Ortiz, César L. Ordóñez-Romero, Guillermo Monsivais , Benemérita Universidad Autónoma de Puebla, zlazcano@ifuap.buap.mx

10.30 - 11.00 (Invited Talk 8) - Stability improvement of $CH_3NH_3PbI_3$ hybrid perovskite through tin and chlorine doping., Bertha Aguilar, Tania Soto, Kristell Sánchez, Oracio Navarro, Aranza Valdespino, Universidad Nacional Autónoma de México, baguilar@iim.unam.mx

11.00 - 11.30 (Invited Talk 9) - Perovskites, and chalcogenides for energy storage/conversion systems, E. Carvajal , Instituto Politécnico Nacional, ESIME-Cul., eliel.carvajal@gmail.com

11.30 - 12:00 Coffee Break

Chairman F. Estrada

12.00 - 12.30 (Invited Talk 10) - Structural, magnetic and electrical magneto-transport properties of nanowire networks, Joaquín de la Torre Medina , Univesidad Nacional Autónoma de México / Instituto de Investigaciones en Materiales - Unidad Morelia, delatorre@materiales.unam.mx

12.30 - 13.00 Closing

POSTER SESSION

Tuesday 8th

TUP01 - p-Wave superconductivity in nanostructured systems, Fernando Ruiz Gonzalez, Daniela Vieyra Rivera, Carlos Ramirez Ramos, Cesar Gabriel Galvan Peña , Universidad Autonoma De San Luis Potosi, cesar.galvan@uaslp.mx

TUP02 - A Bogoliubov de Gennes approach to chiral superconductivity, Efrain Ruiz Alvarado, Luis Antonio Perez, Cesar Gabriel Galvan Peña , Universidad Autónoma de San Luis Potosí, era.maya.98@gmail.com

TUP03 - Multifractal wavefunctions of charge carriers in graphene with folded deformations, ripples, or uniaxial flexural modes: Analogies to the quantum Hall effect under random pseudomagnetic fields, Abdiel de Jesús Espinosa Champo
Gerardo García Naumis , Instituto de Física, Universidad Nacional Autónoma de México, abdielespinosa@estudiantes.fisica.unam.mx"

TUP04 - Thermal evolution of equivalent sites in a gold-copper cluster from molecular dynamics., Alessio Palavicini, Diana E. Moreno, Guillermo I. Guerrero-García, José M. Cabrera-Trujillo, César G. Galván , Facultad de Ciencias, Universidad Autónoma de San Luis Potosí, alessio.palavicini@uaslp.mx

TUP05 - Synthesis and characterization of Fe nanoparticles, Azury Nava Guzmán, Mary Carmen Amador Meléndez , Enrique Sánchez Mora , Benemérita Universidad Autónoma de Puebla, anavag@ifuap.buap.mx

TUP06 - Ballistic transport in gated phosphorene superlattices including disorder effects. , Eric Jovani Guzmán Ortiz, Outmane Oubram, Oracio Navarro Chávez, Isaac Rodríguez Vargas , Facultad de Ciencias Químicas e Ingenieria, Universidad Autónoma del Estado de Morelos, eric.guzman@uaem.edu.mx

TUP07 - Adsorption of sarin nerve agent simulant by metal-decorated silicene: a DFT calculation, Francisco De Santiago, Álvaro Miranda, Miguel Cruz-Irisson, Luis A. Pérez , Instituto de Física, UNAM, fdesantiago@fisica.unam.mx

TUP08 - Charge transfer in twisted TiS2-G heterostructure, Francisco Hidalgo , No Institution, fhidalgo76@gmail.com

TUP09 - ELECTRONIC STRUCTURE FOR 2D GaAs DOPED WITH Si AMPHOTERIC IMPURITIES: A DFT STUDY, G.J. González-Loera, K.A. Rodríguez-Magdaleno, F.M. Nava-Maldonado, J.C. Martínez-Orozco , Universidad Autónoma de Zacatecas, gerardojafet.gonzalez@fisica.uaz.edu.mx

TUP10 - Analysis of performance parameters of a SPR optical sensor based in 2D Materials for CO_2 detection, Ireri Aydée Sustaita Torres, Jefte Ceballos Zumaya, David Ariza Flores, José Samuel Pérez Huerta, Jesús Madrigal Melchor , Universidad Autónoma de Zacatecas, ireri.sustaita@uaz.edu.mx

TUP11 - Optical Properties of heterostructures based on twisted bilayer graphene , J. Madrigal-Melchor, G. A. Navarro-López, J. S. Pérez-Huerta, D. Ariza, I. A. Sustaita-Torres , Universidad Autónoma de Zacatecas, jmadrim@uaz.edu.mx

TUP12 - Low-dimensional thermoelectricity in bilayer graphene superlattices, José Alberto Briones Torres, Rolando Pérez Álvarez, Sergio Molina Valdovinos, Isaac Rodríguez Vargas , Universidad de La Ciénega del Estado de Michoacán de Ocampo, jabriones@ucemich.edu.mx

TUP13 - Dipole matrix elements and absorption coefficient for GaAs/AlGaAs QCL-like potential profile., J. A. Sánchez-Reyna, K. A. Rodríguez-Magdaleno, J. C. Martínez-Orozco, F. M. Nava-Maldonado , Universidad Autónoma de Zacatecas UAZ, jose.sanchez@fisica.uaz.edu.mx

TUP14 - Study of electronic proprieties of CSSNI3 nanowires: a DFT approach, Gonzalez Vazquez Julio Zuriel, Ornelas Cruz Ivan De Jesús, Trejo Baños Alejandro, Crisóstomo Reyes Margarita Clarisaila, Miranda Durán Álvaro, Salazar Posadas Fernando, Cruz Irisson Miguel , Instituto Politécnico Nacional-Escuela Superior de Ingeniería Mecánica y Eléctrica Culhuacan, zuriel.gov@gmail.com

TUP15 - Surface Li effects on the electronic properties of Ge nanowires: A first principles approach, Ricardo Jiménez Sánchez, Pedro Morales Vergara, Fernando Salazar Posadas, Jacqueline Rebollo Paz , Instituto Politecnico Nacional, rjimenezs1902@alumno.ipn.mx

TUP16 - Search and analysis of the most stable structures of small AgAu bimetallic clusters and their adsorption and reactivity properties., Sergio Jovany López Muñoz, Jorge Alberto Vargas Téllez , UAZ, Unidad Académica de Física, sergio.lopez@fisica.uaz.edu.mx

TUP17 - Effects of doping and vacancies on the structural and electronic properties of the SiC monolayer, Ranferi Cancino, Lucia G. Arellano, Francisco De Santiago, Álvaro Miranda, and Miguel Cruz-Irisson , Instituto de Física, UNAM, fdesantiago@fisica.unam.mx

TUP18 - DFT studies of the basic optoelectronic properties of borophene doped with Al and Ga., J. J. Alvarado-Goytia , F. M. Nava-Maldonado, K. A. Rodríguez-Magdaleno , J. C. Martínez-Orozco , Universidad Autónoma de Zacatecas, Unidad Academica De Física , jesus.alvarado@fisica.uaz.edu.mx

TUP19 - Magnetoelectric effect in composite of piezoelectric ceramics and Ni-Mn-Ga ferromagnetic shape memory alloy: design and measurement , A. M. Schönhöbel, P. Lázpita, I. Orue, J. M. Barandiarán, Jon Gutiérrez , University of Basque Country, ana.schonhobel@gmail.com

TUP20 - Micromagnetic simulations of magnetite nanoparticles, José Francisco Barrón-López, Guillermo Alvarez, Herlinda Montiel , Instituto de Ciencias Aplicadas y Tecnología- UNAM, jf.barron82@gmail.com

TUP21 - Magnetic anisotropy field detection in cobalt foil by means of a magnetoimpedance sensor, Carmen López-Ortega, José Francisco Barrón-López and Herlinda Montiel , Instituto de Ciencias Aplicadas y Tecnología, Universidad Nacional Autónoma de México, jf.barron82@gmail.com

TUP22 - Disorder effect on transport and magnetoresistance properties in a ferromagnetic superlattices based on phosphorene, Outmane Oubram; Eric Jovani Guzmán; Isaac Rodríguez-Vargas; Oracio Navarro Chavez, Luis Manuel Gaggero-Sager, J. Guadalupe Velásquez Aguilar , Facultad de Ciencias Químicas e Ingeniería/Universidad Autónoma del Estado de Morelos,, Oubram@uaem.mx

TUP23 - Electronic structure and magnetic properties of ARE_2X_4, A=Cd, Mg, RE=Ho, Er, Tm, Yb, Lu, X=S, Se spinels, Pablo de la Mora, Gustavo Tavizón, Esther Agacino , Universidad Nacional Autónoma de México, delamora@unam.mx

TUP24 - New materials with spin crossover phenomena for the harvest of residual thermal energy, Yosuan Avila García , Karla Scanda Raymundo Silva, Edilso Reguera Ruiz , Universidad Nacional Autónoma de México, yosuan.ag87@gmail.com

TUP25 - Sintering evaluation of CoCrMo powders by dilatometry , Armando Michel Garcia Carrillo, Luis Rafael Olmos Navarrete , José Lemus-Ruiz. , Universidad Michoacana de San Nicolas de Hidalgo , armando_121096@hotmail.com

TUP26 - Magnetic biochar from water lily as a route for the valorization of this invading species, Daniel Esteban Camacho Martínez, Armando Encinas , Instituto Potosino de investigación científica y tecnológica, daniel.camacho@ipicyt.edu.mx

TUP27 - Magnetic elastomers with reconfigurable properties controlled by temperature and external magnetic fields, Daniela Abigail Lopez Mireles, Daniel Esteban Camacho Martínez, Armando Encinas , División de Materiales Avanzados, Instituto Potosino de Investigación Científica y Tecnológica (IPICYT), daniela.lopez@ipicyt.edu.mx

TUP28 - Synthesis OF CuO nanoparticles of a copper ore cuprite using papaya, Eleazar Gándara Martínez , Nora Elizondo Villarreal, Dora Martínez Delgado, Francisco Vázquez Rodríguez, , Universidad Autónoma de Nuevo León, ele-gr@hotmail.com

TUP29 - Solid state transformations in hollow Fe spheres , Luis Béjar, Centli T. Guerrero, Ismeli Alfonso , Universidad Michoacana de San Nicolás de Hidalgo, ialfonso@unam.mx

TUP30 - Oxidation kinetics of Ti_6Al_4V alloy deposited by wire arc additive manufacturing using argon gas as processing atmosphere., J.E. Ordaz-Cervantes, R. Morales-Estrella, E. Reyes-Gordillo, R. Escudero , UMSNH, 2023446g@umich.mx

TUP31 - Production and characterization of micrometer α-Al2O3 powder produced by sol-gel method , Miranda-Hernández Quetzalmaflor, Lemus-Ruiz José, Zárate-Medina Juan, A. Contreras-Cuevas Antonio , UMSNH, ing.miher@gmail.com

TUP32 - Sintering analysis of the Ti-12.5Ta-12.5Nb composite by in-situ dilatometry , Ceylin Fernández Salvador, Rogelio Jr. Macias Ambriz, Luis Rafael Olmos Navarrete, Pedro Garnica González, Maria de Lourdes Mondragón Sánchez , TecNM/Instituto Tecnológico de Morelia, jr.cach1m@gmail.com

TUP33 - Effect of Nb on the mechanical and corrosion properties of Ti-xNb alloy fabricated by powder metallurgy, Leonardo Orozco Soria; Rogelio Jr. Macias Ambriz; Luis Rafael Olmos Navarrete; Pedro Garnica González , TecNM/Instituto Tecnológico de Morelia, jr.cach1m@gmail.com

TUP34 - Magnesium matrix composites produced by pressureless infiltration, I. I. López-López, A. Contreras, J. Lemus-Ruiz , Universidad Michoacana de San Nicolás de Hidalgo, i.ignacio.ll@hotmail.com

TUP35 - Specific energy and power measures of an electric battery configuration based on the graphene oxide electrodes, W. Hincapie, J. J. Prías-Barragán , Universidad del Quindío , wahincapie@uqvirtual.edu.co

TUP36 - Evolution of photoluminescence of porous silicon with thermal oxidation conditions, Estela Gómez Barojas, Guillermo Santamaría Juárez, Enrique Quiroga González, Enrique Sánchez Mora , Mayra Matamoros Ambrocio , Benemérita Universidad Autónoma de Puebla, egomez@ifual.buap.mx

TUP37 - Praseodymium-doped BiYO3 for the photocatalytic degradation of oxytetracycline, Ethel G. Méndez Vélez, Diana L. Hernández Arellano, Juan C. Durán Álvarez, Rodolfo Zanella, Rigoberto Juárez López , Universidad Nacional Autónoma de México- IIM-Unidad Morelia, et09gmv@gmail.com

TUP38 - Effects of annealing on InGaN optical and structural properties, Rubén Martínez Revuelta, Horacio Irán Solís Cisneros, Ángel Guillén Cervantes, Yenny Lucero Casallas Moreno, Salvador Gallardo Hernández, Carlos Alberto Hernández Gutiérrez, Máximo López López , Tecnológico Nacional de México/Instituto Tecnológico de Tuxtla Gutiérrez, D19270973@tuxtla.tecnm.mx

TUP39 - C-V model of CdS/CdTe thin films solar cells with the dependence of the applied voltage frequency, A. González-Cisneros, P. A. Hernández-León, F. L. Castillo-Alvarado, A. Durán-Ledezma , Instituto Politécnico Nacional, agc0@hotmail.com

TUP40 - Thyroxine quantification by means surface-enhanced raman spectroscopy substrates based on Au and Ag nanoparticles, Enrique Sánchez-Mora, Paulina De León Portilla, Ana Lilia González-Ronquillo , Benemérita Universidad Autónoma de Puebla, esanchez@ifuap.buap.mx

TUP41 - Surface-enhanced micro-raman scattering substrates based on Ag-nanoparticles and Ag-nanoparticles/poly (methyl methacrylate) composites, Mayra Matamoros Ambrocio, Enrique Sánchez Mora, Estela Gómez Barojas , Benemérita Universidad Autónoma de Puebla, mayra.matamoros@alumno.buap.mx

TUP42 - Surface-enhanced raman scattering (SERS) substrates based on Ag-nanoparticles and Ag-nanoparticles/poly (methyl methacrylate) composites, Mayra Matamoros Ambrocio, Enrique Sánchez Mora , Estela Gómez Barojas , Benemérita Universidad Autónoma de Puebla, mayra.matamoros@alumno.buap.mx

TUP43 - 2D SiGe as anchoring material for Li – S batteries: a DFT study, Brandom Jhoseph Cid, Luis Edgar Mora, Fernando Adán Serrano, Luis Antonio Pérez , Instituto Politécnico Nacional, bcidl1000@alumno.ipn.mx

TUP44 - Study of electronic correlation in a low dimensional system, E. Huipe-Domratcheva, U. A. Díaz-Reynoso, O. Navarro , UNAM, IIM-Morelia, ernesto.h.957@gmail.com

TUP45 - Doped silicon nanowires for the adsorption of urea: an ab-initio study, José Eduardo Santana, Ángel Ramón Montoya, María Isabel Iturrios, Miguel Cruz-Irisson , Instituto Politécnico Nacional, ESIME Culhuacan, eduardo.santana.gin.2017@gmail.com

TUP46 - NH3 adsorption on functionalized thin carbide monolayer: A DFT study, Kevin Jafet García, Sergio Leonel Rosas, Akari Narayama Sosa, Álvaro Miranda , Instituto Politécnico Nacional, ESIME-Culhuacán , kevin.garcia.gin2020@gmail.com

TUP47 - Preliminary Design Assessment of an 83 kW Electric Motorbike., García Romero Martín Felipe, Mondragón Escamilla Nancy, Araujo Vargas Ismael, Basurto Rios Viviana, Velázquez Elizondo Pedro Enrique, Cano Pulido Kevin , Instituto Politécnico Nacional, mgarciar2010@alumno.ipn.mx

TUP48 - Preliminary Design and Assessment of an 83 kW Electric Motorbike., Martín Felipe García Romero, Nancy Mondragón Escamilla, Ismael Araujo Vargas, Pedro Enrique Velázquez Elizondo, Kevin Cano Pulido , Instituto Politécnico Nacional, mgarciar2010@alumno.ipn.mx

TUP49 - Bound states in the continuum in nanoribbons with wider sections: a divide-and-conquer algorithm based on scattering matrices, Ricardo Y. Días, Mauricio J. Rodríguez, Carlos Ramírez, Departamento de Física, Facultad de Ciencias, UNAM, carlos@ciencias.unam.mx

Effects of annealing on InGaN optical and structural properties

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InGaN-based solar cells have the potential to increase conversion efficiency because by changing the In content, this alloy is suitable to absorb most of the solar spectrum ranging from 365 to 1771 nm (3.40 - 0.7 eV) [1]. Furthermore, due to the high InGaN absorption coefficient being around ~$10^5 cm^{-1}$, it is possible to employ thinner absorber layers [2]. Despite these unique properties, $In_xGa_{1-x}N$ solar cells have not shown any significant improvement in conversion efficiency, mainly due to the difficulty of incorporating high indium concentrations. It has been reported that if the Indium (In) molar fraction exceeds 0.20 (or if the InGaN layer thickness increases above a critical value), phase separation may occur [3,4] . In fact, one of the critical issues in obtaining high-efficiency solar cells is the phase separation.

Adequate indium incorporation in the InGaN ternary alloy is very important, therefore methods to prevent/eliminate phase separation are especially desirable. In this work, we prepared two series of InGaN samples by molecular beam epitaxy (MBE) employing a RF-nitrogen plasma source. The first series is comprised of InGaN layers grown in the stable hexagonal phase on Si (111) substrates. The other series comprised InGaN layers grown in the metastable cubic phase on GaAs (100) substrates. After the growth, in order to study the changes in the Indium incorporation in the films, the samples were annealed. Samples from both series were characterized by XRD, AFM, Raman spectroscopy, photoluminescence, EDS, SEM, and UV-VIS spectroscopy. We will present the effects on surface morphology, crystal structure and optical properties as a function of annealing temperature and annealing time.

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STABILITY IMPROVEMENT OF $CH_3NH_3PbI_3$ HYBRID PEROVSKITE THROUGH TIN AND CHLORINE DOPING.

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In recent years, the hybrid perovskite $CH_3NH_3PbI_3$ (MAPI) has been widely studied because of its potential application in the fabrication of high efficiency solar cells [1]. The main challenge is to avoid destabilization of this compound under working conditions. Indeed, the MAPI begins to decompose into the precursor phases, a few hours or days after being formed [2,3]. We reported a stability monitoring of doped compounds $CH_3NH_3Pb_{0.9}Sn_{0.1}I_{2.6}Cl_{0.3}$ and $CH_3NH_3Pb_{0.75}Sn_{0.25}I_{2.25}Cl_{0.75}$, obtained as films from solutions of the precursors in N–N dimethylformamide on chemically treated glass substrates. The monitoring was carried out using X-Ray diffraction and absorbance measurements in the UV–Vis region. The tetragonal symmetry initially determined for the compounds, remains almost unaltered for $CH_3NH_3Pb_{0.75}Sn_{0.25}I_{2.25}Cl_{0.75}$ even after 600 days, under environmental conditions. The bandgap value for this doped perovskite is 1.44 eV (Figure 1), close to ideal value, 1.34 eV [4].

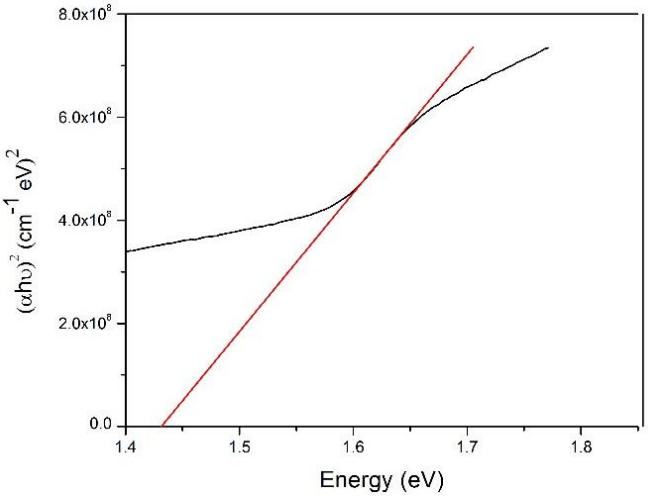

Figure 1. Extrapolation of the linear portion of $(\alpha h\nu)^2$ *Versus hv,* to find the bandgap value for a) x = 0.1 and b) x = 0.25.

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DFT STUDIES OF THE BASIC OPTOELECTRONIC PROPERTIES OF BOROPHENE DOPED WITH Al AND Ga.

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Currently, two-dimensional materials are widely studied theoretically and experimentally, since these are promising for electronic application, photocatalysts and optoelectronic systems, just to mention some of the most important ones, without neglecting the interest in their properties from the basic science point of view. After the discovery of graphene, many investigations have been carried out to discover other two-dimensional allotropes of the several elements and their heterostructures, among them it is borophene, which due to its interesting physical and chemical properties, such as its exceptional structural complexity, extreme hardness, and high chemical stability, it has attracted a lot of attention of the scientific community. Therefore, in this work we will study borophene form the point of view its basic optoelectronic features. The properties of interest, such as the band structure and density of states, as well as the imaginary part for the dielectric function, is systematically calculated within the density functional theory methodology for a borophene monolayer and for a borophene layer with Al and Ga substitutional impurities to see the effect of them on the system. All this task using SIESTA (acronym for “Spanish Initiative for Electronic Simulations with Thousands of Atoms”) which is a method and a computer program for electronic structure calculations. We performed the study with the LDA and GGA functionals and discuss their properties from the basic point of view.

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p-WAVE SUPERCONDUCTIVITY IN NANOSTRUCTURED SYSTEMS

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It has been demonstrated that the Cooper pairs present in the superconductivity phenomenon are found in singlet state, frequently associated with a superconducting gap with *s*-wave and *d*-wave symmetry in metals and cuprates respectively. However, it is believed that some systems could present Cooper pairs in a triplet state which leads to an asymmetric *p*-wave superconducting gap. One of the most interesting reasons to study *p*-wave superconductivity is that it could host Majorana zero modes which may be applied to quantum computation. Specifically, it has been shown that the Kitaev Hamiltonian for Majorana fermions can be obtained from the Hubbard Hamiltonian for a *p*-wave superconducting linear chain [1]. In this work we use the Hubbard Hamiltonian to study *p*-wave superconductivity for nanostructured periodic systems such as ribbons, wires, and tubes. We determine the variation of the local superconducting gap solving numerically the Bogoliubov-de Gennes (BdG) coupled self-consistent equations which have been used to study bidimensional nanoparticles [2]. Thermodynamic properties are calculated as a function of the temperature and size of the systems. Our preliminary results show that there are optimal parameters that increase the critical temperature with respect to the bulk one. Finally, we also analyze the energy spectrum and the probability density to find the conditions that allow Majorana zero modes. This work could set a precedent to study these modes in other superconducting systems like the magnetic vortex formed in type II superconductors which are good candidates to create qubits.

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DIPOLE MATRIX ELEMENTS AND ABSORPTION COEFFICIENT FOR GaAs/AlGaAs QCL-LIKE POTENTIAL PROFILE.

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Double and triple quantum wells in GaAs/AlGaAs are frequently used as basic elements for a quantum cascade laser (QCL) device [1,2], where asymmetry takes a fundamental role in the design of possible optoelectronic systems, because this permit the electron wavefunction localization to be manipulated. For this purpose, studies of the electronic structure and the dipole matrix elements associated with the conduction band states, gives significant information to compute physical properties such as the intraband absorption coefficient, in this case. Working in the effective mass approximation, in this work is reported the dipole matrix elements, as well as the absorption coefficient for asymmetric triple GaAs/AlGaAs quantum wells, which constitutes the active region of a quantum cascade laser system. We found that it can be tuned the absorption coefficient peaks by changing the values for electric and magnetic fields, and that the magnetic field can enhance significatively the absorption coefficient magnitude and the electric field can easily modify the absorption coefficient energy position.

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Dirac Equation in Solid State Systems

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Dirac equation emerges in the realm of high energy physics trying to reconcile the postulates of quantum mechanichs and the special theory of relativity. Nevertheless, it also emerges as the low energy effective equation of motion in several solid state systems. In this talk we review some scenarios in which Dirac equation, its modifications and extensions play a core role in the description of elementary excitations in solids of different dimensionalities.

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DISORDER EFFECT ON TRANSPORT, THERMOELECTRIC AND MAGNETORESISTANCE PROPERTIES IN A FERROMAGNETIC SUPERLATTICES BASED ON 2D-MATERIALES

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The inevitable structural disorder associated with fluctuation of barrier and well widths, as well as barrier heights in superlattices of 2D materials, can greatly affect electron transport and related phenomena. In this talk, we discuss the impact of structural disorder on electron transport, thermoelectric and Tunneling Magnetoresistance (TMR) properties of Gated Ferromagnetic Superlattices based on 2D-materiales (GFS2Ds). An effective low-energy Hamiltonian has been used to describe the electrons in 2D-materiales. To obtain the transport, TMR and thermoelectric properties, the transfer matrix approach, the Landauer-Büttiker formalism and the Cutler-Mott formula have been implemented. The obtained results show that the disorder has a destructive effect on the thermoelectric and transport properties as well as has a benefit effect on the TMR properties. Our investigation indicates that the magnitude of impact of disorder on such properties depends principally of the kind of structural disorder. Additionally, we will show that to have and preserve good electrical, thermoelectric and TMR properties on GFS2Ds, it is fundamental to determine the dominate disorder structural.

XXIV Latin American Symposium on Solid State Physics

Electronic structure and magnetic properties of ARE_2X_4, A=Cd, Mg, RE=Ho, Er, Tm, Yb, Lu, X=S, Se spinels.

Pablo de la Mora, Gustavo Tavizón , Esther Agacino

In the ARE_2X_4 (A=Cd, Mg, RE=Ho, Er, Tm, Yb, Lu, X=S, Se) spinels the rare earth (RE) have a very localized 4f state that interacts very little with other atoms and in the Density of States one can see very narrow peaks. In the case that these peaks are at the Fermi energy (E_F) and there is another state from another atom also at E_F then the system will have Intermediate Valence, in the case that there are flat bands and not so flat bands at E_F, then the system will be a Heavy Fermion.

The electronic structure calculations show that for RE=Lu there is a Lu:4f below E_F, and the system is insulating. For RE=Yb a Yb:4f peak moves to the lower edge of the band-gap with E_F in this peak and there are states of X, therefore these systems are Intermediate Valent and the bands show that these systems are Heavy Fermion. For RE=Tm, Er, Ho the RE:4f moves above the band-gap and these systems are insulators, nevertheless for RE=Tm and Er, if they are electron doped then one obtains an Intermediate Valent system with a Heavy Fermion character.

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Surprises from electron-phonon interaction with chiral phonons in two-dimensional materials

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Since the early days of the quantum theory of solids, the interaction between electrons and lattice vibrations has provided a long list of exciting discoveries. Examples include the role played by electron-phonon (e-ph) interaction in the development of the theory of superconductivity and conducting polymers, where charge doping is used to circumvent the Peierls transition. In the last decade, the theoretical prediction [1] and observation of phonons with intrinsic chirality in two-dimensional materials [2] brought a new ingredient to this long standing problem. In this talk I will provide an overview on this field and present our recent results on the effects of the interaction between electrons and chiral phonons in two-dimensional materials [3-5]. By using a non-perturbative solution we show that chiral phonons introduce inelastic *Umklapp* processes resulting in copropagating edge states which coexist with a continuum. Our results hint on the possibility of having new electron-phonon states of matter.

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Multifractal wavefunctions of charge carriers in graphene with folded deformations, ripples, or uniaxial flexural modes: Analogies to the quantum Hall effect under random pseudomagnetic fields

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The electronic behavior in graphene under arbitrary uniaxial deformations, such as foldings or flexural fields, is studied by including it in the Dirac equation pseudoelectromagnetic fields. General foldings are thus studied by showing that uniaxial deformations can be considered pseudomagnetic fields in the Coulomb gauge norm. This allows one to give an expression for the Fermi (zero) energy mode wavefunctions. For random deformations, contact is made with previous works on the quantum Hall effect under random magnetic fields, showing that the density of states has a power law behavior and that the zero energy mode wavefunctions are multifractal. This hints at an unusual electron velocity distribution. Also, it is shown that a strong Aharonov–Bohm pseudoeffect is produced. For more general nonuniaxial general flexural strain, it is not possible to use the Coulomb gauge. The results presented here helps to tailor-made graphene uniaxial deformations to achieve specific wavefunctions.

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SURFACE LATTICE RESONANCES OF Ag NANOPARTICLE HONEYCOMB ARRAYS

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Plasmonic lattices have a wide range of applications [1,2], one of the most exploited is as sensors of gases or to detect molecule contaminants or dyes. Periodic arrays of nanoparticles are feasible with lithographic techniques [3], allowing the control of size, shape, and lattice parameter, those features determine the optical response, and hence, the application. We have determined by numerical simulations within the Discrete Dipole Approximation [4] the Surface Lattice Resonances (SLR) of spherical Ag nanoparticles (NPs) in a 2D honeycomb array. The effect of the coverage in the lattice has been studied by varying the lattice parameter and NP diameter. We have spanned the Ag NP diameter from 4 nm to 100 nm, identifying that small NPs (diameter less than10 nm) and big NPs (diameter larger than 10 nm) have different scattering and absorption contributions to the optical extinction efficiency. Also, the identification of the dipole SLR as the main resonance allows us to understand the shape-line of reflection, transmisión, and absorption of the 2D arrays. For possible SERS applications, near electric field in and out of resonance is presented.

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ELECTRONIC STRUCTURE FOR 2D GaAs DOPED WITH Si AMPHOTERIC IMPURITIES: A DFT STUDY

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Two-dimensional systems are a field with a lot of research interest in the last two decades, although these were theoretically reported by P.R. Wallace since 1947 [1] and there are many later works, it was in 2004 when Andre Geim and Konstantin Novoselov mechanically exfoliated a graphene sheet than gives then the Nobel Prize in 2010 "for groundbreaking experiments regarding the two-dimensional material graphene", that the 2D materials becomes a hight activity research topic. Without a doubt, the impact of the discovery of 2D systems such as graphene has led to both theoretical and experimental investigations of a large number of materials such as Silicene, Borene, Arsenene, Phosphorene, just to mention some of the most emblematic ones, but other materials and its heterostructures are also of interest. From this point of view, in this work we present the band structure, density of states as well as the imaginary part of the dielectric function of a 2D GaAs system by means of a density functional theory implementation. The aim of this study is to investigate the basic physical properties for a freestanding 2D GaAs sheet, as well as the effect of Si substitutional atoms, since it has an amphoteric nature in the GaAs, which means that depending on which atom is substituted, this can be an n- or p-type impurity atom. We report, as expected, that the levels do indeed appear near the conduction band (or valence) if the impurity is n-type (or p-type), respectively. Also the density of states due to the impurity is modified and as well as the imaginary part of the dielectric function.

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MOLECULAR SYMMETRY PROTECTED TOPOLOGICAL PHASES

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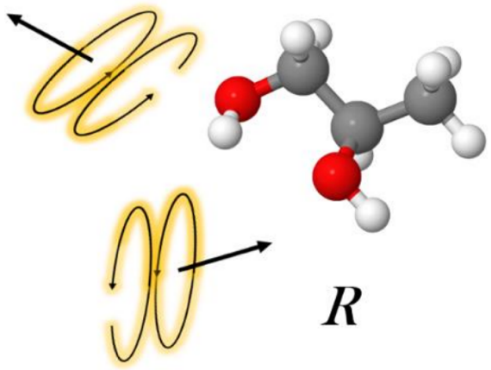
We will discuss interesting connections between topological phases of matter and chiroptical spectroscopy of molecules, describing a scheme to distinguish molecular enantiomers using the recently introduced ideas of topological frequency conversion [1,2].



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DYNAMICAL TUNING OF THE THERMAL CONDUCTIVITY VIA ELECTROPHONONIC, MAGNETOPHONONIC AND PHOTOPHONONIC EFFECTS

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The development of phononics, the discipline that investigates phonon transport and aims at engineering devices with the same functionalities as electronic or photonic ones, has been hindered by the inherently challenging nature of phonon manipulation. Here, we demonstrate theoretically a fully electric control of the phonon flux, which can be continuously modulated by an externally applied electric field in PbTiO3, a prototypical ferroelectric perovskite, revealing the mechanisms by which experimentally accessible fields can be used to tune the thermal conductivity by as much as 50% at room temperature. Additionally, we show how, by imposing epitaxial strain, it is possible to achieve a giant electrophononic response, i.e., the dependence of the lattice thermal conductivity on external electric fields. Specifically, we study the strain-induced manipulation of the lattice structure and analyze its interplay with the electrophononic response. We show that tensile biaxial strain can drive the system to a regime where the electrical polarization can be effortlessly rotated and thus yield giant electrophononic responses that are at least one order of magnitude larger than in the unstrained system. These results derive directly from the almost divergent behavior of the electrical susceptibility at those critical strains that drive the polarization on the verge of a spontaneous rotation. These ideas are then applied to magnetic materials, where the lattice structure, and thus the thermal conductivity, can be manipulated via external magnetic fields. In particular, we predict the existence of large magnetophononic effects in FeRh, a material that undergoes a metamagnetic phase transition near room temperature. These findings open the way to a fully-electromagnetic control of phonon transport that can be exploited for the design of thermal transistors and pave the way to signal processing with phonons.

Search and analysis of the most stable structures of small AgAu bimetallic clusters and their adsorption and reactivity properties.

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In this work we report the most stable structures of silver and gold atomic clusters that were obtained by means of a genetic algorithm technique. The number of structures that can be had for a cluster of fixed size increases exponentially with the number of atoms, even more so when there are two types of atoms. This type of system generates a complex potential energy hypersurface and requires the use of a global minimum search technique. The Mexican Enhanced Genetic Algorithm (MEGA), developed by one of the authors, makes use of the ideas of evolutionary theory to perform a selective search for the best (and most probable) structures by relaxing the candidates by means of a package based on density functional theory (DFT). In addition to analyzing the characteristics of the clusters thus obtained, vibrational spectra are generated for comparison with experimental results of far-infrared spectroscopy and their adsorption and reactivity properties.

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SYNTHESIS AND CHARACTERIZATION OF Fe NANOPARTICLES

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Fe nanoparticles (Fe-NPs) were synthesized by varying the reaction temperature of 5, 10, 15, 20 and 25 °C to study the changes in their optical and morphological properties. The results indicate that the reaction temperature plays an important role in synthesizing Fe-NPs. At low temperatures, Fe-NPs are not oxidized; however, as the synthesis temperature increases, the degree of oxidation increases. The oxidation process starts with the formation of FeOOH (10 °C) to form FeO and Fe_2O_3 (15-25 °C) [1-3].

Due to the magnetic character of Fe-NPs, the colloidal dispersion of Fe-NPs is unstable, and aggregates with a hydrodynamic diameter of about 1000 nm are formed. To avoid the increase in the size of the Fe-NPs, the NPs must be functionalized with carboxymethylcellulose.

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Theoretical approach to the optical properties and vibrational spectroscopies of semiconductor nanostructures

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Semiconductor nanostructures have attracted much attention of the solid-state physics community due to their exciting properties, in most cases different to that of their bulk counterparts. One example of such nanostructures is porous silicon that has fotoluminescense contrary to the bulk crystalline Silicon. On the other hand, computational calculations and simulations, have become an essential tool for the discovery of new materials and their characterization. Many properties can be estimated such as optical properties (absorption spectrum and refractive index), vibrational properties (phonon dispersion and DOS), vibrational spectroscopies (Raman and IR) amongst others. Therefore, these computational tools would be useful for the characterization of new nanostructures and predicting their new properties. In this work we study the optical properties and vibrational spectroscopies nanoporous semiconductors and nanowires, using the template of the first principles Density Functional Theory. The nanostructures were modelled using the supercell scheme [1,2]. For reference the properties of the bulk systems were also calculated, with the results showing and excellent agreement with respect to the experimental results. The nanoporous structures showed a heavy reliance of the optical properties with respect to their surface as the passivation scheme determined important optical characteristics such as the band gap energy. Also, the effects of phonon confinement that would impact their vibrational spectroscopies are diminished by the presence of passivating atoms. This effect is also present in the nanowires, however for both systems the quantum confinement effects paradoxically become more evident as the confinement decreases. These results could be important for the characterization of semiconductor nanostructures.

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Tight-binding calculation of band-gap energy in a four-channel model DNA and its dependence on temperature, length, hydration, and basis sequence

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In this work, we investigate the localization and delocalization of electronic states in a ladder model that mimics DNA molecules described within a four-channel tight-binding model as a function of sequence, system length and the presence of backbones, temperature, and hydration. Localization and delocalization can be characterized by the participation ratio (PR) that depends on the size of the system. PR corresponds to the inverse of the second moment and can be obtained from the electronic wave function defined for each site. The results show how the band-gap energy increases with increasing temperature, suggesting semiconductor behavior at room temperature. On the other hand, the hydration induces a semiconductor-to-insulator phase-like transition, which is independent of the temperature

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LOW-DIMENSIONAL THERMOELECTRICITY IN BILAYER GRAPHENE SUPERLATTICES

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Low-dimensional thermoelectricity is based on the redistribution-accumulation of the density of states of electrons in low-dimensional structures such as superlattices [1]. In this work we study the thermoelectric properties of superlattices based on graphene bilayer [2]. We present an analysis of the impact of mini-band formation and its interaction with the intrinsic Fano resonances of the graphene bilayer on the Seebeck coefficient, the power factor, and the figure of merit [3]. We show the calculation of the density of states to verify whether the redistribution-accumulation of electronic states is involved in the thermoelectric response of graphene bilayer superlattices [4]. For the calculation of the transport and thermoelectric properties we make use of the four-band effective Dirac Hamiltonian, the hybrid matrix method and the Landauer formalism [5].

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ELECTRONIC TRANSPORT IN PHOSPHORENE JUNCTIONS

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The band structure of phosphorene in the zigzag direction has been trivialized, regarding the charge carriers as Schrödinger electrons. However, phosphorene is a 2D material with a special pseudospin texture [1]. Here, we show that this special pseudospin texture gives rise to exotic phenomena in zigzag phosphorene junctions such as electronic cloaking of confined states, persistent electronic cloaking and Fano resonances. The characteristics of these phenomena on the transmission and transport properties are unveiled. As far as we know phosphorene beyond graphene is the only 2D materials in which these exotic phenomena are presented.

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ANALYSIS OF PERFORMANCE PARAMETERS OF A SPR OPTICAL SENSOR BASED IN 2D MATERIALS FOR CO_2 DETECTION

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Optical sensors based on surface plasmon resonance (SPR) have recently been used for real-time detection of a wide range of compounds, from ions, proteins, and viruses to small molecules; at the same time this allows them numerous fields of application such as environmental monitoring and food and water quality, as well as industrial safety, clinical diagnosis, among many others. In addition, some 2D materials or combinations of 2D materials, such as graphene, dichalcogenides of transition metals, black phosphorene, hexagonal boron nitride, metal elements, metal oxides, semiconductors, dielectrics, have been recently incorporated into these sensors, and which, given their extraordinary optical properties, have allowed a great advance over traditional sensors [1–3]. In this work, we want to focus on the study of the performance parameters such as sensitivity, detection accuracy, quality factor, and combined sensitivity of sensors, focused on the detection of CO_2. We propose an optical SPR sensor based on 2D materials, which is composed of a multilayer structure with metal (Au, Ag, Cu, etc), 2D material (graphene layers, or ZnO, or dichalcogenides of transition metals, among others) and dielectrics, to monitor different CO_2 concentrations. On this study the performances of the SPR sensors, was compute via the Attenuated Total Reflection spectra (ATR) using the transfer matrix method in the scheme of Pochi Yeh. The ATR spectra were obtained in the Kretschmann configuration, where the metal is embedded between prisma and 2D materials multilayers structures. The sensing media is collocated on graphene. We found that performance parameters factor was improved by combining the metals, the number of layers of the 2D materials and the chemical potential of graphene included in sensor, we take wavelength of the incident light in 633nm.

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Ballistic transport in gated phosphorene superlattices including disorder effects.

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Recently, the investigation of the nanostructuring process using gated superlattices in two-dimesional materials has increased notably. In fact, it has been reported that by employing superlattices of electrostatic and magnetic barriers applied to graphene-like materials[1-2], it is possible to manipulate the electron transport properties and therefore improve phenomena such as magnetorresistance, thermoelectric effect and spin-valley polarization [3-4], which are highly relevant for future applications in nanoelectronics. Phosphorene, another like-graphene material, is formed by phosphorus (P) atoms distributed in a puckered honeycomb layer and linked by covalent bonds in sp^3 hybridization. Phosphorene, exhibit moderate bandgap (~1.5 eV) in the gamma (Γ) point and high anisotropy in the band structure [5], which differentiates the propagation between zigzag (Γ-X) and armchair (Γ-Y) directions. The behavior of charge carriers (holes and electrons) can be explained by the low-energy effective Hamiltonian derived from the tight binding two-band model. Our work theoretically explores the effects of structural disorder in the ballistic transport properties of the gated phosphorene superlattices. Our results show high degradation of the miniband transmission structure depending on type of disorder and also on the charge carrier. Specifically, the disorder in the width interferes with the Fabry-Perot resonances and the tunneling effect. On the other hand, the disorder of the height affects mainly evanescent waves. Consequently, the conductance gradually loses its oscillatory behavior and the peaks are flattened. We conclude that structural disorder is an important factor to consider in the potential fabrication of phosphorene-based electronic devices.

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CHARGE TRANSFER IN TWISTED TiS_2-G HETEROSTRUCTURE

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In recent years, vertically stacked heterostructures by van der Waals interactions have become a hot topic for researcher groups because of their vast prospects of using different two-dimensional (2D) layers, increasing the possibility of modulating or combining the physical properties of constituents [1].

In this work and using first-principles calculations through SIESTA code [2], I studied the electronic properties of the TiS_2-G, a heterostructure constituted by one titanium disulfide monolayer in the 1T phase and graphene. Graphene is a semimetal with electronic bands exhibiting a linear disperson around the K point in its irreducible Brillouin zone [3]. In contrast, there are discrepancies about whether 1T-TiS_2 monolayer is a semimetal or a semiconductor with a small indirect energy bandgap [4-5]. Herein, four TiS_2-G heterostructures with different twisted angle were studied. Because graphene and TiS_2 layers have incommensurate lattice parameters, graphene is under tensile/compressive biaxial strain whereas the lattice parameter of TiS_2 is kept fixed.

Results show that interlayer interaction originated by vertical stacking induces an electric dipole that generates an electronic charge transfer from TiS_2 to graphene, which is observed by the position of the Dirac point localized in the TiS_2 conduction bands of the heterostructure. Hence, TiS_2-G heterostructure emerges as an ohmic contact [6], contrasting with other based-graphene heterostructures like MoS_2-G or WS_2-G. Finally, the influence of the twisted angle on the charge transfer and the intelayer-induced electric dipole is studied.

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Optical Properties of heterostructures based on twisted bilayer graphene

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With the purpose to determine future and multiple applications in modern photonics and because the twisted bilayer graphene (*TBG)* presents interesting optical properties [1–3], the transmission, reflection, and absorption of *TBG* heterostructure were studied when graphene chemical potential is zero [1] . In this research, we obtain the transmittance, reflectance, and absorption spectra for different number of *TBG* for several twisted bilayer angles, separation between bilayer, using a transfer matrix method. We found that the transmission and absorption spectra strongly depend on the twist angle between the layers; and by on the other hand, the absorption amplitude decreases as the twist angle between layers decreases in both, *TE* and *TM* polarizations. Furthermore, for *TE* polarization we obtain that, as the incidence angle of the electromagnetic wave increases, the transmission spectrum decreases its amplitude; and for *TM* polarization the transmission spectrum increases its amplitude. Finally, the amplitude of the absorption increases for TE and decreases for TM as incident angle increases.

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BOUND STATES IN THE CONTINUUM IN NANORIBBONS WITH WIDER SECTIONS: A DIVIDE-AND-CONQUER ALGORITHM BASED ON SCATTERING MATRICES

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Firstly, we propose a divide-and-conquer algorithm to find the Scattering matrix (S-matrix) of general tight-binding structures [1]. The S-matrix allows a direct calculation of transport properties in mesoscopic systems by using the Landauer formula. The algorithm is based on the recursive S-matrix method (RSMM) that allow us to find recursively the S-matrix of a system from the S-matrices of its subsystems [2,3]. The method is exact, and by analyzing the performance of the algorithm in square, triangular and honeycomb lattices, we show a significant improvement in comparison to other state-of-the-art recursive and non-recursive methods. We utilize this algorithm to analyze the conductance of a rotated graphene nanoribbon side-contact junction.

Next, we present a novel algorithm based on the RSMM to efficiently and accurately determine bound states in and out of the continuum in systems with semi-infinite leads [4]. This algorithm is used to explore the formation of bound-states in the continuum (BICs) in nanoribbons with wider sections, some of which are shown in Fig. 1.

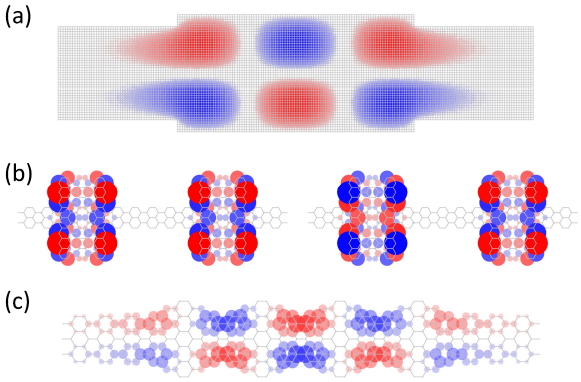

Fig. 1. BICs in (a) a square lattice nanoribbon, (b) a quantum-dot-like junction, and (c) a graphene nanoribbon with smooth wider sections

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Generalized Hamiltonian for Kekulé graphene and the emergence of valley-cooperative Klein tunneling

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We introduce a generalized Hamiltonian describing not only all topological phases observed experimentally in Kekulé graphene (KekGr) but predicting also new ones, as shown in Fig. 1. These phases show features like a quadratic band crossing point, valley splitting, or the crossing of conduction bands, typically induced by Rashba spin-orbit interactions or Zeeman fields. The electrons in KekGr behave as Dirac fermions and follow pseudorelativistic dispersion relations with Fermi velocities, rest masses, and valley-dependent self-gating. Transitions between the topological phases can be induced by tuning these parameters. The model is applied to study the current flow in KekGr pn junctions evidencing a cooperative transport phenomenon, where Klein tunneling goes along with a valley flip. These junctions act as perfect filters and polarizers of massive Dirac fermions, which are the essential devices for valleytronics. The plethora of different topological phases in KekGr may also help to establish phenomena from spintronics.

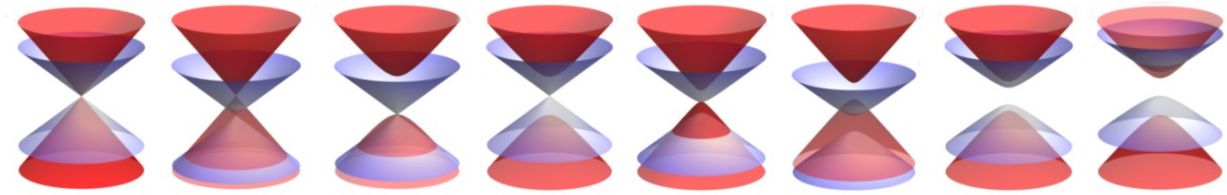

Figure 1: Topological phases of Kekulé graphene (KekGr) where reddish and blueish colors correspond to valleys K^+ ($\nu = 1$) and K^- ($\nu = -1$), respectively.

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Surface Li effects on the electronic properties of Ge nanowires: A first principles approach

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Si and Ge are the most relevant semiconductors for the development of anodic materials for rechargeable batteries, due to their high theoretical specific capacity (4000 mAh/g and 1600 mAh/g respectively) compared to graphite anodes (372 mAh/g) [1]. In this work, we present a theoretical study of the electronic properties and energy stability of H pasivated Ge nanowires grown along the [111] crystallographic direction, and considering four differente diameters. The model considers the replacement of H atoms by Li in different concentrations by unit cell. This study is developed by using the Density Functional Theory (DFT), in the Local Density Approximation (LDA) incorporated in the SIESTA code. The results indicate that the formation energy of the nanowires is a function of the concentration of Li atoms, revealing energetic stability for all studied systems. The Hirshfeld population analysis, reveals that the Li atoms give up charge to the surfce Ge ones, while the charge on H atoms remains almost constant. Likewise, the binding energy values are between 2.4 and 2.6 eV per Li atom, indicating the existence of Ge-Li bonds. On the other hand, the maximum theorical storage capacity (C_M) corresponds to the Ge nanowire with the minor diameter. Finally, the open circuit voltaje diminishes as a function of the concentration of Li atoms. These results help to understand the effect of Li on the electronic properties, energy stability, and charge capacity of Ge nanowires and open the possibility of incorporate them as anode materials.

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This work was partially supported by the multidisciplinary projects IPN-SIP, 2020-2091, -2093, -2106, and UNAM-PAPIIT IN109320. Computational resources were provided by the DGTIC-UNAM Miztli supercomputer (LANCAD-UNAMDGTIC-180 Project) and Laboratorio Nacional de Supercómputo del Sureste de México de la BUAP (# proyecto). RJS thank CONACYT and BEIFI-IPN for their financial support.

ADSORPTION OF SARIN NERVE AGENT SIMULANT BY METAL-DECORATED SILICENE: A DFT CALCULATION

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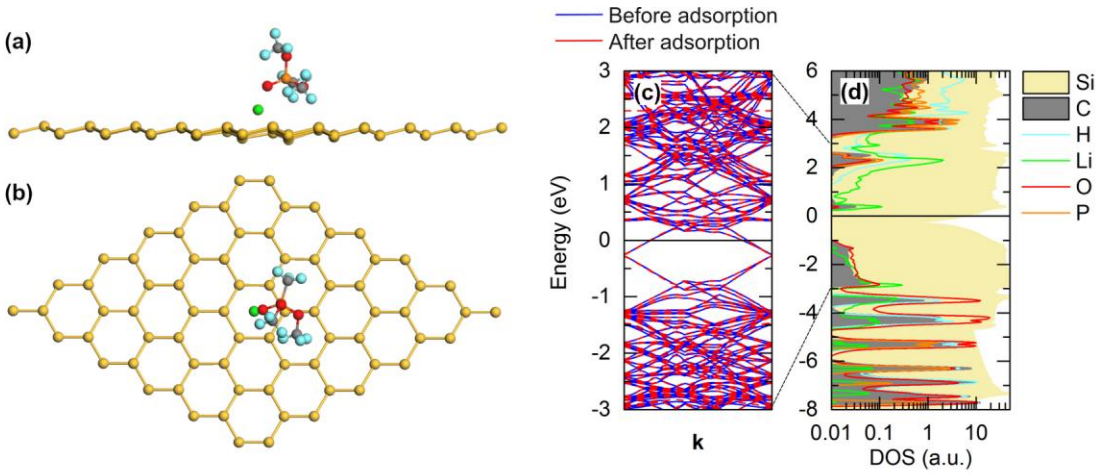
Sarin ($C_4H_{10}FO_2P$) is a highly volatile colourless liquid used as a nerve agent. It is banned by international treaties, but it has been used in terrorist attacks. Such clandestine use makes its detection and neutralization an important matter. Usually, the harmless dimethyl methylphosphonate ($CH_3PO(OCH_3)_2$, abbreviated DMMP, is used as a sarin simulator in experimental investigation, since both are organophosphorus compounds and have similar polarity and volatility. In this paper, the adsorption of DMMP on silicene is investigated using Density Functional Theory calculations, to aid in the development of devices capable of detecting or neutralizing sarin. Metal adatoms on silicene are used as adsorption sites. Results suggest that the DMMP molecule can be chemisorbed through its P=O group by Li-decorated silicene with an adsorption energy of 1.6 eV. However, since the electronic band structure of lithiated silicene is barely affected by the molecule adsorption, the electric sensing may be difficult.



(a) Side and (b) top views of the adsorption configuration of DMMP on Li-silicene. (c) Electronic band structure of Li-silicene before (blue) and after (red) DMMP adsorption. (d) Species-projected density of states.

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EFFECTS OF DOPING AND VACANCIES ON THE STRUCTURAL AND ELECTRONIC PROPERTIES OF THE SiC MONOLAYER

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Since the discovery of graphene, two-dimensional materials have attracted attention due to their unique properties, such as their high surface-to-volume ratio [1]. In addition, recent research shows that electronic properties can be modified by doping or vacancies [2]. In this work, we present a density functional theory study on the effects of doping, vacancies, and simultaneous doping and vacancies on silicon carbide monolayers' (SiC-ML) electronic and structural properties. B, Al, Ga, N, P, As, Si, and C were used as dopants, and substitutional doping on either Si or C lattice sites was studied. Single vacancies and double vacancies were made by removing one Si or C atom or both in SiC-ML. The results show that the most energetically favorable substitution is in the Si atom. The lattice parameter of the supercell increases based on the size of the dopant. N-type dopants exhibit a spin-polarized ground state. The most stable dopant species is B. The deformations suffered by the structures due to the vacancies are more significant with heavier dopant species. Through the modulation of the band gap by these defects, the SiC-ML may be helpful in applications like chemical sensing; at the same time, the local irregularities of the charge density may lead to adsorption sites useful for energy storage applications.

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Acknowledgements

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Some Strategies to Integrate 2D Materials into Functional Applications

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2D Materials are exciting platforms with a huge potential for the development of new advanced technologies. The unique combination of properties, such as high specific surface area, charge transport, chemical stability, mechanical strength, flexibility, high electrical and thermal conductivity, tunable band gap, and optical transparency make them the ideal substrates for the development of a number of applications including intelligent sensors, inks, reinforced composites, biomedical devices, and environmentally friendly materials. Unfortunately, for applicability, several problems arise, including quality, scalability, dispersibility and stability. Here, I will describe our recent efforts on the production of 2D materials and van der Waals heterostructures, their characterization, handling, and performance towards proof-of-concept devices. In particular, to address the production of nanohybrids for surface enhanced Raman spectroscopy (SERS) and sensors [1-5], and photocatalytic materials [6-7]. I will discuss our approach to the above-mentioned applications, the limitations found and the strategies followed to increase the knowledge on the production and applicability of 2D-based materials.

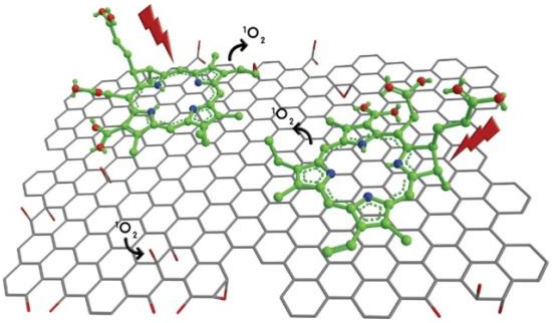

Fig. 1. Functional 2D Materials.

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EFFECTS OF F AND CL IN THE VIBRATIONAL PROPERTIES OF POROUS SILICON CARBIDE WITH SI AND C-TERMINATED PORE SURFACE.

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Silicon carbide has been studied in recent years due its attractive applications like quantum photonics [1] and Li-ion batteries [2] Most of the studies of this material focus on its electronic properties and seldom on the vibrational properties. In this work, we calculate the effects of passivation on the vibrational properties of porous silicon carbide (p-SiC). To model the nanopores, a 3C-SiC supercell with a lattice parameter of a=13.044 Å was modelled, then columns of atoms were removed in the [0 0 1] direction, creating 2 kinds of surfaces, one with only Si atoms and other with only C atoms, the dangling bonds were passivated with hydrogen. After optimizing the structures, one H atom from the wall of each pore was substituted with fluorine (F) or chlorine (Cl) atoms as seen in figure 1 where the red spheres represent F or Cl. The phonon dispersion and density of phonon states (Phonon DOS) were calculated using the DFPT approach and the linear response method. The results indicate a displacement of the optical modes to lower frequencies when the F and Cl atoms substitute and H. These results confirm which structures are viable to synthesize and support the research to use this material for different applications.

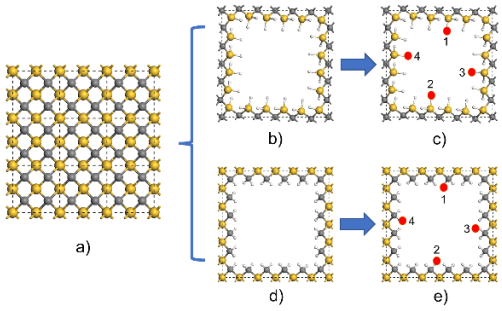

Figure 1. Graphical representation of a)a 3C-SiC supercell with 13.044 Å, and the porous structures with b) Only Si and d) Only C pore, finally c) and e) represent the sequence on substitution of H atoms with either F and Cl from the Only Si and Only C, respectively. The grey, yellow, white and red spheres represent C, Si, H atoms and H replacement sites respectively

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STUDY OF ELECTRONIC PROPRIETIES OF CSSNI3 NANOWIRES: A DFT APPROACH

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Recently, hybrid perovskites of NH3CH3Pb3 have attracted the attention of the scientific community due to the possibility of improving the photovoltaic cell efficiency. However, their low stability and high toxicity avoid their wide use on this sector. That's why inorganic perovskites like CsSnI3 [1] are being studied owing to their similar capacities but with a higher stability and lower toxicity compared to the Pb hybrid perovskites . The effect of quantum confinement in the proprieties of this kind perovskite have not yet been analyzed, this could be useful for doing engineering of the band gap energy and improve their capacities as solar absorbers. In this investigation through density functional theory, with generalized gradient approximation, electronic proprieties of CsSnI3 nanowires were analyzed. The nanowires were modeled removing atoms out from a circumference in the direction [0 0 1] from a pristine crystal of CsSnI3. Results show that, as anticipated, the energy gap of the perovskite increase compared with its counterpart in bulk and the band gap decrease with increasing diameter. Results show that it's possible perform a bandgap engineering through quantum confinement since the control of the wire size could be more controlable compared to other methods such as doping, this increases the possibility of application of this perovskite in photovoltaic applications

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New materials with spin crossover phenomena for the harvest of residual thermal energy

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This work aims to study new materials with high potentialities for creating a sustainable energy system where all available energy sources are used, including residual thermal energy that, for thermodynamic reasons, is continually being generated in all technological processes, more evident in internal combustion processes and of nature. A desirable option focuses on materials that convert the entropic component to electrical energy. This work is aimed at these materials and applications, such as The Internet of Things (**IoT**). Materials with spin crossover around room temperature are attractive for harvesting residual thermal energy and other environmental energy sources and converting them into electrical energy. This work describes the synthesis and characterization by infrared, Raman and squid magnetometry of ferrous nitroprusside with spin crossover phenomena.

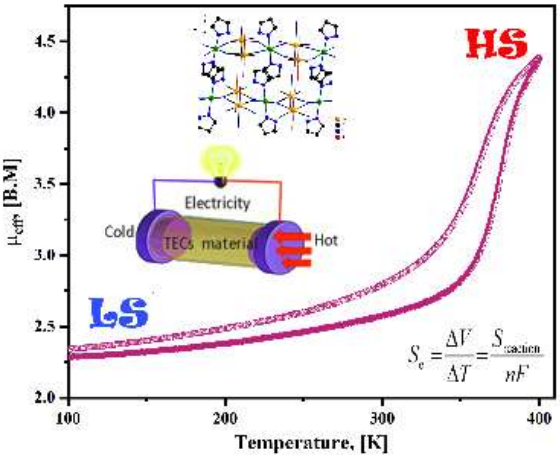

Figure 1 – Spin crossover phenomena in iron nitroprusside intercalated with organic molecule.

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MICROMAGNETIC SIMULATIONS OF MAGNETITE NANOPARTICLES

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Magnetite nanoparticles (NP's), with grain size of 10 nm ≤ *D* ≤ 128 nm, were investigated using micromagnetic simulations [1] and relaxation time calculations [2], where superparamagnetic (SPM), single domain (SD), and vortex (V) states were obtained. Smaller NP's (*D* < 58 nm) are in the thermally unstable SPM state, whereas SD_{111} states aligned in the easy direction [111] are stable only for sizes of 58 nm < *D* < 73 nm. Larger NP´s (*D* > 73 nm) adopt the magnetic vortex configuration where their magnetization decays fastly with the increase in size. Due to the subtle balance between exchange interaction and the small anisotropy energies the core of the V states rotates from the hard direction [100] towards the easy direction [111] at *D* ~ 100 nm. No multidomain (MD) particles were observed for the size range investigated. Relaxation time calculations indicate that SPM magnetite NP's are unsuitable as carriers of the geomagnetic field record; instead, they are very useful as a magnetic material for diverse biomedical applications.

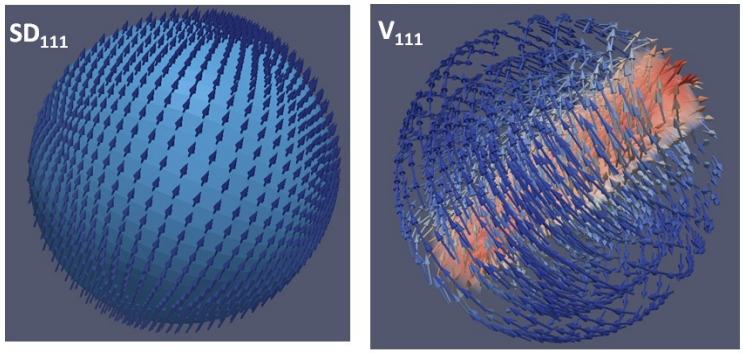

Figure 1 Magnetite NP's in single domain (SD_{111}) and easy axis vortex (V_{111}) states.

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MAGNETIC ANISOTROPY FIELD DETECTION IN COBALT FOIL BY MEANS OF A MAGNETOIMPEDANCE SENSOR

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The giant magnetoimpedance effect is widely used for the design of sensor devices [1, 2]. Moreover, amorphous Co-rich microwires are one of the most popular elements due to their soft magnetic properties and negative near-to-zero magnetostriction. In this work, a magnetoimpedance (MI) effect sensor was developed, with an amorphous microwire as its sensing element and it is based on a microstrip transmission line. A network analyzer is used to energize and detect changes in the magnetoimpedance of the microwire. Consequently, the sensor is energized with 1mW (0 dBm) in a frequency range from 1 to 10 MHz. The microwire magnetoimpedance is modified by the magnetization of the cobalt foil and left-wise and right-wise shifts in these curves can be quantified. The microwire sensitivity allows for the measurement of subtle modifications in the MI curves and these can be associated with the magnetic anisotropy in the Co foil. The measurements were carried out by the rotation of the sample over the microwire sensor. Therefore, we have found that the curve shift depends on the rotation angle of the foil, but it is independent of the excitation frequency.

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Acknowledgements

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An analysis of different magnetometry protocols to determine dipolar interactions in particle assemblies

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The use of magnetic particles as building blocks to construct complex 3D or hierarchical macrostructures is presently a very active and promising approach in different areas of nanomagnetism and spintronics. The combination of chemical and physical fabrication techniques have led to the production of a variety of well defined and tailor-made macrostructures that exhibit a wealth of novel and interesting properties. Dipolar interactions play a fundamental role in these systems as it results in an additional contribution to the energy of the individual particles. For this reason interactions have been shown to modify the magnetic properties of particle assemblies but also as a design parameter to tailor the properties of the assembly. A central problem regarding the interactions in particle assemblies is its quantification using magnetometry-based protocols. In this presentation an overview will be given of the different methods, qualitative and quantitative, available up to date that are used to study inter-particle interactions. These methods are based on standard magnetometry measurement protocols such as remanence curves, first order reversal curve diagrams or minor loops. Each with their own advantages and limitations, which will be discussed in the interest of showing that the best practice is to use different complementary protocols to gain a more reliable and robust measurement of the interaction field in particle assemblies.

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Spin wave localization in magnonic crystals with defects

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A broken translational symmetry in a magnonic crystal via the introduction of tailored defects can beneficially enhance or modify its properties leading to scenarios with outstanding capabilities to connect fundamental physics with applications at microwave frequencies. Their characteristics have inspired multiple studies where detailed results on the behavior of the frequency-amplitude characteristic as a function of different structural parameters have been demonstrated. However, up to now, all the scientific reports deal exclusively with the resulting spin wave spectrum for the complete structure and little has been said about the behavior of the spin wave inside the defects. Here, we present a detailed study of the propagation of surface spin waves (MSSW) through a MC with broken translational symmetry, the influence of the defect in the spin wave propagation, the evolution of frequency bandgaps inside the MC, and the spatial energy distribution as a function of frequency and position. A time and space resolved magneto inductive probing system has been used to map the spin wave propagation in a magnonic crystal with tailored defects. The results show that the spin wave modes get trapped by the defect and the energy is localized in the space for specific frequencies.

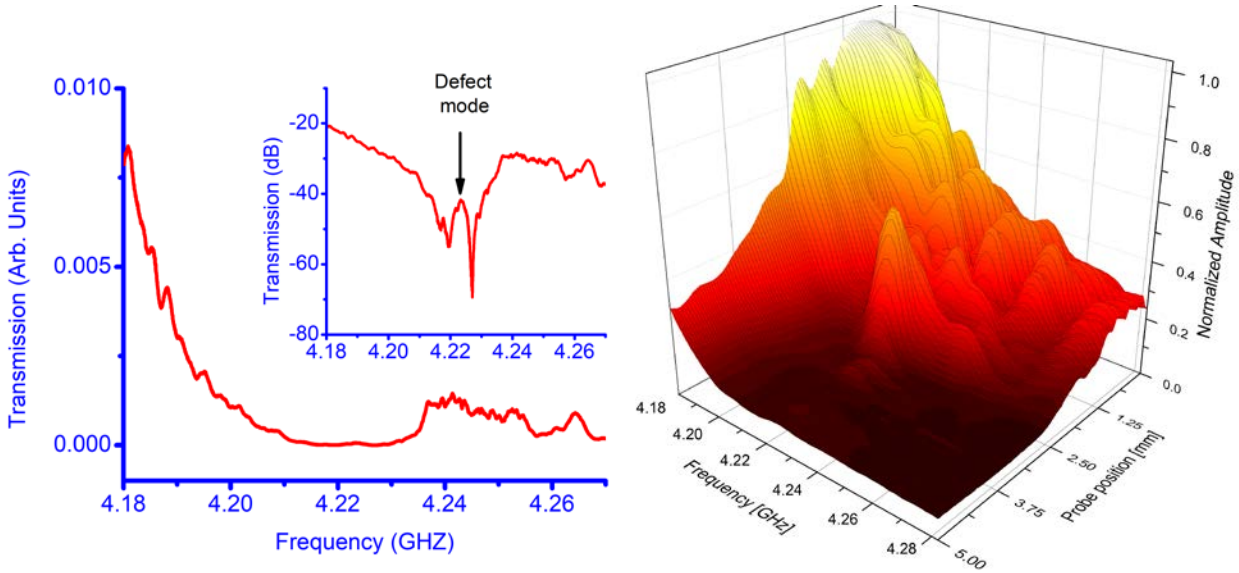

Figure 1. Left: Amplitude frequency characteristic for the magnonic structure in linear and logarithmic (inset) amplitude scales. Right: Normalized surface of the distribution of the spin wave energy as function of the frequency and the probe position inside the magnonic structure.

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STRAIN ENGINEERING ON THE IMPURITY-INDUCED MAGNETISM IN GRAPHENE NANOSTRUCTURES

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Magnetism in low-dimensional materials is an attractive research topic due to its potential application in emerging quantum technologies. To increase the applications of magnetic systems it is crucial to have strategies for controlling their properties, such as mechanical strain, which has been shown to be an effective modulation technique of the electronic structure and magnetism in different systems. In recent years, impurity-induced magnetism in graphene nanostructures has been an active field of study. In particular, it has been shown that different substitutional impurities from the p-block of the periodic table as phosphorus, arsenic, antimony, and bismuth give rise to a magnetic phase in graphene [1]. Furthermore, the biaxial strain induces a magnetic phase transition from a magnetic to a non-magnetic state in phosphorus-doped graphene [2]. In this work, we present a systematic study of the effect of uniaxial strain in the range from 0 to 10% of deformation on the phosphorus-induced magnetism in graphene and its nanoribbons, performed through first-principles calculations. To contrast the effect of the dimensionality, we studied the monolayer and nanoribbons of different widths and edges (armchair and zigzag). For the monolayer, the uniaxial strain slightly modulates the magnetic moment. For armchair graphene nanoribbons, the strain induces a magnetic phase transition, but the critical strain depends on the nanoribbon width. In the case of nanoribbons with zigzag edges, we found a magnetic transition between two different magnetic states via strain which also is dependent on the nanoribbon width.

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Towards high-performance permanent magnets with reduced-rare earth content: The effect of Zr and Nd substitution on $SmFe_{11}V$ alloy

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In the last decade there has been an increasing industrial demand for permanent magnets driven by the development of clean energy applications such as electric car motors and sustainable energy. The use of rare-earth (RE) metals classified as critical, such as Nd, Pr, Dy and Tb in permanent magnets continues to be a source of greater concern owing the supply, mining (58% in 2020) and purification (90%), as well as most permanent magnet production (90%), are concentrated in China [1]. In response to the increasing stress on the limited RE resources, a global effort is underway to explore permanet magnet materials that reduce the dependency of RE. Interest in compounds with $ThMn_{12}$-type structure has recently been reactivated [2-4], as they only contain 7.7 at.% of RE elements, compared to 11.8 at.% in $Nd_2Fe_{14}B$ and 10.5 at.% in Sm_2Co_{17}. In this direction, we have studied structural and magnetic behavior of polycrystalline alloys of $Sm_{1-x}Y_xFe_{11}V$ (Y=Nd, Zr). Substitution of Nd for Sm promoted the formation of 3:29 phase, which deteriorated the intrinsic magnetic properties. In the case of Zr-substitution, all the optimally heat-treated alloys crystallize into tetragonal $ThMn_{12}$-type structure 1:12 phase and bcc α-(Fe,V) phase. For high Zr content of x = 0.4 and 0.6, Laves phase $ZrFe_2$ was also detected with Curie temperature of 709 and 697 K, respectively. The substitution of Zr resulted in a contraction of 0.7% of the 1:12 cell volume. Oriented powder XRD patterns indicated that the easy magnetization direction was along (002) c-axis. As Zr content increased from x = 0 to 0.6, anisotropy field decreased from 11 to 8.8 T and Curie temperature from 625 to 583 K. On the other hand, the saturation magnetization increased from 114 to 138 Am^2kg^{-1}. The RE reduced alloy with Zr-substitution ($x \leq 0.4$) exhibit a suitable intrinsic magnetic properties for permanent magnet applications. Magnets based on 1:12 phase with x=0.4 of Zr may utilize up to 38% of less Sm-metal.

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MAGNETOELECTRIC EFFECT IN COMPOSITE OF PIEZOELECTRIC CERAMICS AND Ni-Mn-Ga FERROMAGNETIC SHAPE MEMORY ALLOY: DESIGN AND MEASUREMENT

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Magnetoelectric composites made of magnetostrictive and piezoelectric elements have a high technological interest because their potential applications in multifunctional devices such as transducers, actuators, and sensors [1,2]. The highest magnetostriction material known is Terfenol-D, which is a rare-earth iron alloy that requires magnetic fields larger than 1 T to achieve deformations around 2,000 ppm [3]. In this work we designed a set-up based on a double coil and an electromagnet to measure the magnetoelectric effect of a composite fabricated from piezoelectric PZT ceramics and a $Ni_{49.3}Mn_{29.6}Ga_{21.1}$ single crystal shape memory alloy (a kind of materials that can show several percent deformations under moderate fields [4,5], i.e. a quite superior response as compared to Terfenol-D). The single crystal showed the martensitic transformation at T_M = 298 K; as well as T_C = 368 K, and μ(302 K) = 2.87 μ_B/f.u. The maximum strain response at room temperature was of 4% for magnetic fields larger than 0.4 T. As for the magnetoelectric effect, the induced magnetoelectric voltages were very moderate, increasing linearly with the frequency. There was only a slight change in the response with the DC applied magnetic field. For low frequencies (f < 1 kHz) the magnetoelectric voltage were on the order of 10 mV and for higher frequencies about 50 mV. The best magnetoelectric response (~210 mV/cm Oe) was obtained under an AC field of 10 Oe and a static magnetic field of 0.7 T.

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Magnetic elastomers with reconfigurable properties controlled by temperature and external magnetic fields

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Magnetic elastomers in which the arrangement of the magnetic particles they contain can be reconfigured using a mild thermal treatment and an applied external magnetic field have been fabricated and studied. The goal was to have a material whose magnetic response is adaptable in order to provide a wider range of uses and applications. To this end, magnetic iron oxide particles, either micro or nano sized, are dispersed in a phase changing media, in particular paraffin or gelatin [1]. Controlled quantities of these materials are then placed in an silicone based elastomer which is then cured. This leads to a deformable elastomer with well defined and localized magnetic regions, which can respond to the stimuli of an applied magnetic field [2],[3]. To change the configuration of the magnetic particles, and thus the way the system responds, the samples are heated to 40-60ºC in order to melt the paraffin (gelatin) allowing the particles to reorder by applying an external magnetic field. The resulting configuration is set once the temperature is lowered. We provide examples to show that using different arrangements of the magnetic regions as well as different applied field configurations, it is possible to obtain a variety of magnetic responses from the system, thus making this an attractive reconfigurable soft composite.

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SINTERING EVALUATION OF CoCrMo POWDERS BY DILATOMETRY

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The objective of this work is to study the sintering behavior of CoCrMo powders that could be used as bone implants. For which, sintering at two different temperatures with four different heating rates between 2 and 15 °C/min was performed. The characterization of the samples was carried out by means of optical and electronic observation, as well as X-ray diffraction. The mechanicl properties were evaluated by microhardness test. The results indicated that the best temperature for sintering CoCrMo powders was 1350 °C, in addition to the fact that the faster heating rate generated the samples with higher density. It was also found that the porosity was reduced up to 5% for the sample sintered at 1350°C and at 15°C/min. The microstructure found was a mixture of the ε-Co and γ-Co phases characteristic of the alloy. The hardness was affected by the remaining porosity, finding that it increases with the reduction of the pores in the samples. It can be concluded that CoCrMo sintering is a viable alternative for the manufacture of materials with potential application in joint implants.

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MAGNETIC BIOCHAR FROM WATER LILY AS A ROUTE FOR THE VALORIZATION OF THIS INVADING SPECIES

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Currently there is a variety of environmental problems caused by the influence of invading plant species; among these, the great impact generated by the existence of the water hyacinth or water lily, in freshwater bodies stands out. Water hyacinth exists around the world causing negative impacts in wildlife native to the area due to changes in the pH, its high absorption of oxygen and a privation of sunlight inside water bodies[1]. In this sense, developing novel processes that allow the valorization of the water hyacinth, leading to the relief of environmental affections are a current topic of interest[2]. In the present work we develop magnetic biochar based on water lily with the incorporation of either nickel or magnetite particles, with which it is possible to modify the physicochemical properties of the final material and providing additional value to the material for new applications[3], [4]. The physicochemical properties were studied using environmental SEM to acquire information on the surface morphology of the sample. Infrared spectroscopy was used to analyze chemical interactions between the carbonized samples and the metallic particles, while the structural properties were obtained by means of x-ray diffraction. FInally, the magnetic properties were analyzed by the hysteresis loops measured at room temperature using a Physical Property Measurement System (PPMS)

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SYNTHESIS OF CuO NANOPARTICLES OF A COPPER ORE CUPRITE USING PAPAYA

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Mexico is a country with great sources of wealth, both in terms of biodiversity and raw material, the main resources are rare earths and precious metals, such as silver and copper, Mexico ranks first in silver and seventh place in copper production in the world[1]. Mining in Mexico is a very large industry, despite being of utmost importance for the country; few investigations are carried out focused on new areas of science such as nanotechnology. We report the synthesis of CuO nanoparticles[2] starting from the mine stone ore and through the use of green chemistry such as the papaya peel (*Carica papaya*)[3] which implies something novel and low cost. The structure and optical absorption analysis of these nanoparticles was studied using X-ray diffraction (XRD) and UV-Visible spectrophotometer. The XRD analysis indicated a monoclinic phase of bulk crystals of CuO nanoparticles and the size of the synthesized nanoparticle is about 20 nm and optical absorption analysis indicated a peak in the 264 nm range.

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Production and characterization of micrometer α-Al_2O_3 powder produced by sol-gel method

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Alumina (Al_2O_3) is an advanced ceramic material develop for different applications as refractories, precision tools, pacemaker, etc[1]. Solid state sintering of alumina starting from powders. In fact, there are three methods to be used in synthesis to produce alumina powders. The first method is the Bayer process wich starts from bauxite ore[2,3]. The resulting hydrated alumina contains elements such as clay, silica and iron oxide, this impurities can affect the manufacture of ceramic. Therefore, the production of Al_2O_3 by this method is mainly metallurgical grade for the production of aluminium metal[2]. A second method consists on the desulphation of commercial aluminum sulphate using ammonia. This case requires careful monitoring of the reactions in order to get crystalline pseudoboehmite[3]. The third method is the sol-gel technique[3,4]. Under moderate reaction conditions produced through a colloidal suspension is obtained a pseudo-crystallized aluminum hidroxide gel[3,5]. In this work, Al_2O_3 powder manufactured by precipitation of pseudoboehmite (PB) throught sol-gel process were studied. PB powders were characterized at each processing stage using infrared spectroscopy (IR), X-ray diffraction (XRD) and scanning electron microscopy (SEM) techniques. The results showed an uniform Al_2O_3 powder morphology of submicron size. Crushing and sifting are necessary prior the heating of PB. To obtain α-Al_2O_3 phase, calcination at temperatures above 1000°C is necessary. At lower heating, the transition phases γ, δ or θ of Al_2O_3 are obtained, which can affect subsequent processes.

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OXIDATION KINETICS OF Ti6Al4V ALLOY DEPOSITED BY WIRE ARC ADDITIVE MANUFACTURING USING ARGON GAS AS PROCESSING ATMOSPHERE

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Ti6Al4V alloy is currently the most common metal alloy of the α+β phase type, its application is increasing as it has excellent properties at elevated temperatures. The main users of Ti6Al4V alloy are industries like of aerospace, naval, and biomedical; therefore, Ti6Al4V alloyis one of the most studied material w worldwide [1,2]. One of the great advantages that Ti6Al4V alloy offers is the possibility of manufacturing components in situ by means of additive technologies [3]. The oxidation effect in electric arc additive manufacturing occurs in the solid state during multilayer deposition. Similar studies, in additive manufacturing, have found the formation of titanium oxide on the surface of the material, followed by an oxygen-enriched region called "alpha-case" [4,5]. By means of thermogravimetric analysis (TG), the oxidation effect on the surface of Ti6Al4V samples obtained by additive manufacturing as well as samples obtained from conventional manufacture process were studied. Argon gas, with oxygen as impurity, was used as the oxidation atmosphere within the range of 550°C to 950°C and dwell times of 1 and 3 hrs. For the oxidation reaction, the kinetic analyses led to calculate the activation energy as 250 kJ/mol and 166 kJ/mol for the Ti6Al4V alloy processed by conventinal and additive manufacturing, respectively. Following the oxidation model of Wagner and described by Khanna [6], the results of the TG experiments were fitted to a parabolic-type kinetic model. A mathematical model proposed by Dong E. et al. [7] was used based on the parabolic model. The experimental data fit the mathematical model in the range of 750 - 950°C. The high reactivity of titanium by oxygen produced a maximum oxidizing layer of approximately 62.2 microns(μm) as observed by scanning electron microscopy (SEM).

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Praseodymium-doped $BiYO_3$ for the photocatalytic degradation of oxytetracycline

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Praseodymium-doped $BiYO_3$ photocatalyst materials were synthesized by the Pechini method. Crystalline powders were obtained by calcination of precursor resin performed between 400 °C and 800 °C for 1h.The materials were characterized by X-ray difraction (XRD), Fourier-transformed infrared spectroscopy (FT-IR), UV-Visible diffuse reflectance spectroscopy, Scaning Electron Microscopy (SEM), and Transmition Electron Microscopy (TEM). From the XRD and IR results it was observed that there is coexistence between cubic and tetragonal phases for those samples calcined at 400°C. On the other hand, for materials heat treated at 600 °C and 800 °C only a cubic phase was observed. The synthesized powders are agglomerates of nanocrystals which can observed in the SEM and TEM images. The band gap of the Pr-doped samples decreased as the amount of praseodymium increased, and this confirms the absorption in the visible light region. The photocatalytic activity of the samples was evaluated from the degradation of oxytetracycline in water.

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SOLID STATE TRANSFORMATIONS IN HOLLOW Fe SPHERES

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Hollow spheres can be used for manufacturing Metal Hollow Sphere Structures, such as Metal Matrix Syntactic Foams [1]. Among these spheres, hollow Fe-spheres obtained through sintering excell [2]. In this work, solid state transformations for 3 mm in diameter and 130 μm in wall thickness hollow iron spheres were studied. These transformations included the sintering process for the spheres to obtain hollow structures, measuring characteristics such as neck width, penetration, porosity and packing. The microstructural transformations in the sphere walls were also analyzed, using Scanning Electron Microscopy (SEM) for this purpose. In order to study these transformations, the spheres were heated at temperatures ranging from 700 to 1200 °C, for times between 1 and 3 h. Results showed important differences depending on the process variables. Densities of the sintered spheres ranged from 0.6 g cm^{-3} to a maximum of 1.1 gcm^{-3} for spheres 100% packed, where it was observed a sphere-to-polyhedron shape transformation, with maxima values of penetration and sintering neck width. Using Design of Experiments, correlations were obtained between sintering variables and these characteristics of the final hollow structures. SEM studies also showed significant modifications of the Fe particles forming the sphere walls, with the development of grains which grew and were completely packed, presenting polyhedral structures. This led to decrease almost to zero the porosity in the sphere walls.

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Effect of Nb on the mechanical and corrosion properties of Ti-xNb alloy fabricated by powder metallurgy

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Abstract

The manufacture of compounds the use of protection elements and specialized techniques that favor obtaining specific properties requires according to the required application [1]. Currently, Titanium alloys are frequently used for the design and manufacture of medical implants due to their mechanical and corrosion properties [2]. In terms of adaptability, some Ti alloys lose long-term performance due to the toxicity of metal ions released that can be associated with different chronic diseases such as Alzheimer's [3]. But the addition of non-toxic elements such as Nb in Ti alloys has been of special interest to obtain low Young's moduli and increase corrosion resistance [4, 5]. The objective of this work focuses on characterizing Titanium (Ti) based compounds by adding Niobium (Nb), Ti-xNb compounds were manufactured from the powder metallurgy technique with different Nb contents. The microstructural characterization of the compounds was performed by scanning electron microscopy. The image analysis allowed to observe the distribution of the components of the material, as well as the diffusion of Nb in the Ti matrix. The mechanical properties were evaluated from compression tests where it's found that Young's modulus reduce its value due to the addition of Nb and the presence of the β-Ti phase, finding values between 10 and 42 GPa. These values being similar to the human bones moduli. Finally, corrosion tests were carried out, which revealed that the increase in the amount of Nb in the system favors corrosion resistance. It was concluded that the manufacturing methodology used and the addition of Nb in the compound allows reducing the Young's modulus of Ti to manufacture implants with specific characteristics.

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Sintering analysis of the Ti-12.5Ta-12.5Nb composite by in-situ dilatometry

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Abstract

Currently, the development of specialized materials that meet specific characteristics such as biocompatibility, mechanical properties and microstructure are of great interest in the field of bioengineering [1]. Composites and alloys are designed to mimic the mechanical properties of human bone [2]. The selection of materials in the manufacture of medical implants depends on the property to be obtained, such as: compatibility with biological tissues or the mechanics of the system, although combining both properties to ensure optimal performance of the system in the long term is an important challenge in optimizing these materials [3, 4]. This work analyzes the sintering kinetics of Ti matrix composites reinforced with Ta and Nb. The physical behavior of solid state sintering was evaluated by dilatometry tests, the microstructure obtained was observed by SEM and mechanical properties were evaluated by simple compression tests. The results indicate that activation energy is driven by the diffusion of Ta and Nb into the Ti crystalline structure. The densification is improved by slow heating rate because it favors the diffusion of Ta and Nb in solid state. As a result of such diffusion the stabilization of the β-Ti phase is obtained, with the formation of martensitic α'-Ti phase during cooling. The β-Ti stabilization leads to a reduction on the mechanical strength, which is important for bone implant applications. It can be concluded that by means of the sintering process is possible to control the final properties of Ti12.5Ta12.5Nb composite.

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PLASMONIC RESPONSE OF NANOPARTICLES ARRAYS AND ITS POTENTIAL APPLICATIONS

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By employing a spectral representation formalism,[1] recent results in the study of plasmonic response metal nanoparticles individually and forming arrays. The spectral representation allows us to analyze the optical response by separating the geometry contributions from the dielectric properties of each nanoparticle and its surroundings. Neither numerical nor analytical methods can do this separation. These insights into the physical origin of the optical response are very useful for designing systems with desired properties and potential applications, such as the near-field energy transfer between nanoparticles by considering the coupling between all the thermal electric fields. In this talk, I discuss our results of near-field energy transfer between nanoparticles,[2] the chiro-optical near-field response of achiral lattices,[3] the plasmonic response of nanoparticles in non-Bravais,[4] a honeycomb and vertical-stacked plasmonic lattices,[5] as well as its influence on shaping and enhancing halide perovskites quantum dots photoluminescence.[6]

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THERMAL EVOLUTION OF EQUIVALENT SITES IN A GOLD - COPPER CLUSTER FROM MOLECULAR DYNAMICS

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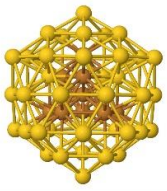
The precise atomistic structure of clusters affect their thermal behaviour. Predicting properties such as their melting point is fundamental when using metallic clusters as catalysts. Of particular interest are bimetallic particles, where the inclusion of two types of atoms produces a wider range of behaviors due to the additional degrees of freedom given by chemical composition and ordering. Gold-copper (AuCu) clusters tipify such bimetallic clusters [1], and it is our interest to analyze their thermal performance.

To study the atomistic configuration of the clusters, we use a method previously proposed to measure amorphousness [2], based on a set of parameters computed from molecular dynamics. Total energy, mean square deviation, Lindemann index and centrosymmetry parameter are averaged to classify atoms in groups of equivalent sites.

We apply this method to examine the evolution over a range of temperatures of 58-atom AuCu clusters spanning all their stoichiometric configurations to find trends and patterns in their parameters as a function of temperature. We identified critical points and thermal transitions of the structure and the evolution of each equivalent site is tracked to obtain its thermal performance. This approach could be used to design clusters where a particular behavior is attained for each of their sections at independent temperatures.



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Steering the current flow in twisted bilayer graphene

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A nanoelectronic device made of twisted bilayer graphene (TBLG) is proposed to steer the direction of the current flow. The ballistic electron current, injected at one edge of the bottom layer, can be guided predominantly to one of the lateral edges of the top layer. The current is steered to the opposite lateral edge, if either the twist angle is reversed or the electrons are injected in the valence band instead of the conduction band, making it possible to control the current flow by electric gates. When both graphene layers are aligned, the current passes straight through the system without changing its initial direction. The observed steering angle exceeds well the twist angle and emerges for a broad range of experimentally accessible parameters. It is explained by the twist angle and the trigonal shape of the energy bands beyond the van Hove singularity due to the Moiré interference pattern. As the shape of the energy bands depends on the valley degree of freedom, the steered current is partially valley polarized. Our findings show how to control and manipulate the current flow in TBLG. Technologically, they are of relevance for applications in twistronics and valleytronics.

Figure 1: Schematic representation of the studied TBLG device. It consists of two stacked graphene nanoribbons, where the upper layer is twisted by the angle θ with respect to the lower one that remains fixed. Electrons are injected through the source contact at the left edge of the bottom layer. They pass through the twisted bilayer region and are detected by three drain contacts at the edges of the top layer (blue, red, and green bars).

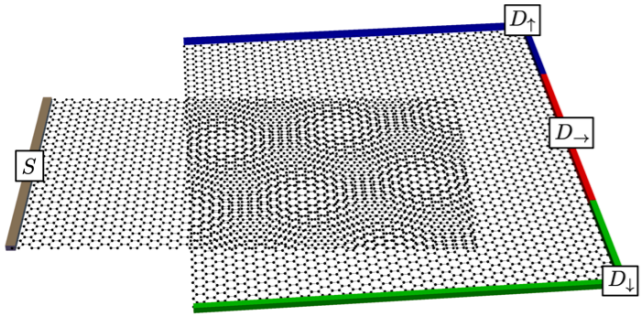
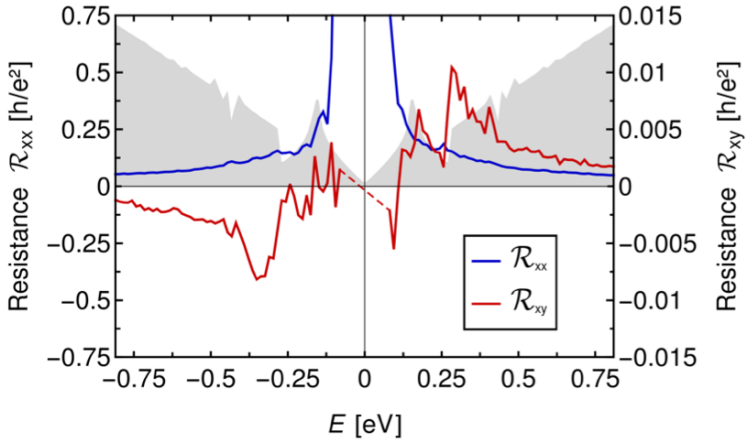


Figure 2: Longitudinal resistance Rxx (blue curve) and Hall resistance Rxy (red curve) as a function of energy for the TBLG device at a twist angle of θ=2.9 degree. The steering of the current flow to one of the lateral edges generates a non-local Hall resistance. The DOS (in arbitrary units) is indicated by the gray color shading.



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Role of geometry in hinge-states in second-order topological phases

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The search for materials with new electronic phases characterized by unusual properties is a crucial goal for developing new technology. Among the materials with usual properties, the second-order topological materials are exampled. One-dimensional conducting hinge-states characterize these three-dimensional materials [1]. In this work, we explore the possibility of tailoring the appearance of more hinge-states and the case of unconfined hinge-states to one dimension. First, we explore the formation of more hinge-states in a four-orbital tight-binding Hamiltonian in a cubic lattice, making holes in a finite sample [1]. Second, using a three-orbital tight-binding Hamiltonian in a hexagonal lattice [2-3], we unconfined hinge-states to one dimension, changing the base of a finite prism sample (triangular, hexagonal, and parallelogram base). Finally, we calculate the topological invariant using the non-abelian Berry phase [4].

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Nanostructures made by sputtering for applications in magnetism, medicine, energy and aerospace industry

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In this talk I will discuss different kinds of nanostructures made by sputtering. On the one hand, nanostructures prepared with the help of lithographic techniques: patterned antidots with focused ion beam [1], suitable for magnetic separation, and T-shaped magnetic nanostructures with electron beam lithography [2], which are able to store two bits of information. On the other hand, large-area nanocolumnar films (NCs) fabricated by glancing angle deposition. I will show several NCs with interest for new devices in magnetism, medicine and energy:
-Fe-based NCs with different morphologies and consequently different magnetic properties [3];
-Pt NCs with improved properties as bioelectrodes for an electric stimulation platform in vitro [4];
-TiO_2 NCs that can be used as electron transport layers for advanced perovskite solar cells [5] and as nanostructured surfaces with photo-induced self-cleaning activity [6].
Finally, I will discuss noble metal NCs as anti-multipactor coatings for the aerospace industry [7] and I will present our CSIC spin-off Nanostine (https://nanostine.com/).

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MAGNESIUM MATRIX COMPOSITES PRODUCED BY PRESSURELESS INFILTRATION

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The magnesium and its alloys have recently become one of the most important structural materials for weight reduction solutions [1]. Magnesium is considered lowest density structural material with the higest specific strenght, high specific young´s modulus, high specific stiffnes, good damping properties and high velocity projectil resistance. Nevertheless, magnesium have low mechanical properties, low elastic modulus and a great difficulty of machinability to compite with aluminum and steels used in automotive and aeroepace industries [2]. Magnesium matrix composites (MgMC) have a several adventajes over magnesium alloys and its competitors, such as high elastic modulus, high corrosion resistance, excelent wear behavior and good thermal properties [3]. The manufacturing processes of MgMC are limited for liquid magnesium surface tension among magnesium alloys and several advances ceramic materials, such as pressureless infiltration, one of the best cost-efficient processes [4]. In this work a surface treatment of silicon nitride (Si_3N_4) was studied in order to increase the wettabillity between Mg alloy AZ91E and Si_3N_4. A succesfull fabrication of MgMC produced by pressureless infiltration was achieved.

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Nonreciprocal Linear Transmission of Sound in a Viscous Environment with Broken P Symmetry

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Reciprocity is a fundamental property of the wave equation in a linear medium that originates from time reversal symmetry, or T symmetry. For electromagnetic waves, reciprocity can be violated by an external magnetic field. It is much harder to realice nonreciprocity for acoustic waves. Here we report the experimental observation of linear nonreciprocal transmission of ultrasound through a water-submerged phononic crystal consisting of asymmetric rods[1]. Viscosity of water is the factor that breaks the T symmetry. Asymmetry, or broken P symmetry along the direction of sound propagation, is the second necessary factor for nonreciprocity. Experimental results are in agreement with numerical simulations based on the Navier-Stokes equation. Our study demonstrates that a medium with broken PT symmetry is acoustically nonreciprocal. The proposed passive nonreciprocal device is cheap, robust, and does not require an energy source.

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DISORDER EFFECT ON TRANSPORT AND MAGNETORESISTANCE PROPERTIES IN A FERROMAGNETIC SUPERLATTICES BASED ON PHOSPHORENE

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The inevitable structural disorder associated with fluctuation of barrier and well widths, as well as barrier heights in superlattices of 2D materials, can greatly affect electron transport and related phenomena. In this work, we study the impact of structural disorder on electron transport and Tunneling Magnetoresistance (TMR) properties of Gated Ferromagnetic Phosphorene Superlattices (GFPSs). An effective low-energy Hamiltonian has been used to describe the electrons in phosphorene. To obtain the transport and TMR properties, the transfer matrix approach and the Landauer-Büttiker formalism, have been implemented. The results show that the disorder related to the width and height of the barriers and to the applied magnetic field are not equivalent and have a destructive effect on transmission and conductance. On the contrary, the structural disorder benefits more the properties of the TMR. Therefore, our results indicate that in the design and manufacture of GFPSs, a precise control of the height of the barriers is required to have and preserve good electrical and TMR properties.

Size effects on the physical properties of superconductors and semiconductors

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In small particles, the spacing between the energy levels increases when the particle size decreases and when this parameter is larger than the superconducting gap, it is predicted that superconductivity disappears [1]. In contrast, the presence of shell structure and the accompanying high level degeneracy leads to a strengthening of the pairing interaction in some metallic nanoclusters [2]. Here, the effects of quantum confinement on the superconducting ground state are studied within the Bogoliubov-de Gennes formalism [3] and an attractive Hubbard model. We consider a periodic arrangement of two-dimensional superconducting grains surrounded by insulating, metallic or superconducting stripes. The results show a clear enhancement of the superconducting gap and critical temperature induced by the electron confinement in the grain, being larger for the insulating boundary case [4].
On the other hand, two-dimensional materials have been intensively investigated mainly due to their potential applications in catalysis, transistors, batteries and chemical sensing. In particular, the detection or trapping of toxic gas molecules, such as nitrogen oxides, is important to fight atmospheric pollution and their adsorption can be improved with metal adatoms and vacancies. Although the synthesis of bulk tin carbide has not been achived since the elements precipitate out during growth, it has been theoretically predicted that graphene-like tin carbide monolayer is a stable, indirectgap semiconductor [5]. In this work we also examine the adsorptive and catalytic properties of this novel material which is only stable in nanostructured form [6-9].

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Coatings to improve magnesium alloys as orthopedic biomaterials

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Biodegradable magnesium alloys are promising candidates for temporary fracture fixation devices in orthopedics; nevertheless, its fast degradation rate at the initial stage after implantation remains as one of the main challenges to be resolved.
Three main strategies have been explored to improve the biological performance of magnesium: alloying elements, microstructure, and coatings. An overview of both biological and mechanical demands, later developments and remaining challenges is presented. Finally, the main results of our investigation concerning the production of a Zn and Ca containing alloy, produced by a twin roll method and annealing treatments to get a fine structure are presented. Moreover, different thin coatings were tested to reduce the initial degradation rate of the Mg-0.7Zn-0.6Ca (ZX11) alloy.
The results include the mechanical integrity, corrosive behavior, biocompatibility-osteoinduction, and bacterial adhesion of the bare and coated alloys as a function of the annealing temperature, 350 and 450 ° C. Short-term degradation coated and uncoated samples was assessed considering electrochemical techniques and H_2 evolution (gas chromatography). Additionally, long term degradation was assessed by mass-loss measurements. The results showed that a 380 nm ZrO_2 coating reduces the degradation rate and H_2 evolution of the alloy during the initial 3 days after immersion but allows the degradation of the bare alloy for the long-term. The ZrO_2 coating does not compromise the biocompatibility of the alloy and permits better cell adhesion and proliferation of mesenchymal stem cells directly on its surface, in comparison to the bare alloy.

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Specific energy and power measures of an electric battery configuration based on the graphene oxide electrodes

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Due to the increased consumption of electronics and the energetic transition that has occurred in the last decades, the development of new solid-state batteries that replace liquid-state batteries, which are still available in the market, it is crucial [1]. In this work, we present the measure of the specific energy and power in an electric battery configuration from a solid-state, based on graphene oxide electrodes. The electrolyte was prepared by dissolving sodium chloride into a polyvinyl alcohol mold with a 5%wt, as a fixed concentration. The measure of the specific energy and power was made using the current-voltage curve method, in battery configurations elaborated by an electrode-electrolyte and packaged in epoxy resin [2, 3], as shown in Figure 1. The electrodes were elaborated by employing multilayer graphene oxide films, from the bamboo Guadua as a material source, using the double thermal decomposition method at 973K, as the carbonization temperature and a controlled nitrogen atmosphere. The specific energy measure exhibits maximum values of 0.008Wh/Kg, a 15W/Kg specific power, with battery voltage close to 100mV, displaying a power-specific value, that was expected in batteries, as presented in the Ragone diagram of Figure 2. These results suggest that graphene oxide can be an excellent element for the development of solid-state batteries.

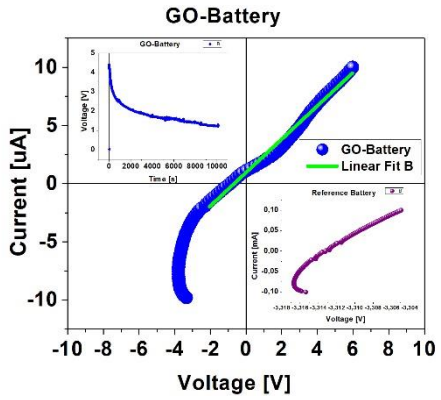

Figure 2. Current voltage curves in graphene oxide battery and reference commercial battery.

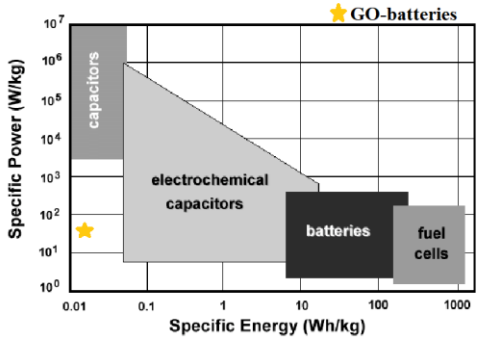

Figure 1. Ragone diagram of Conductive Polymers and Hybrid Materials as Insertion Electrodes for Energy Storage Applications - Scientific Figure on ResearchGate. Available from: https://www.researchgate.net/figure/Schematic-Ragone-plot-for-various-energy-storage-a

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EXCITONIC AND STRUCTURAL PROPERTIES OF EPITAXIAL SUBNANOMETRIC QUANTUM DOTS AND QUANTUM WELLS OF II-VI SEMICONDUCTORS

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Utrathin semiconductor nanostructures present many interesting phenomena, their elaboration with high structural quality represents an important challenge, and their direct structural characterization requires sophisticated and precise experimental techniques, however, the appropriate interpretation of their excitonic emission properties offers a great amount of information about their optical and structural properties. Here, we will present the results of detailed studies of subnanometric quantum wells (QWs) of CdSe/ZnSe in heterostructures containing single, double, and triple ultra-thin quantum wells (UTQWs). The excitonic properties are studied by means of low temperature photoluminescence (PL) spectroscopy. In some cases, the structural properties are also studied by scanning transmission electron spectroscopy (STEM). CdSe quantum wells of 1, 2, and 3 monolayers (ML) thickness are grown by atomic layer epitaxy (ALE) between ZnSe separating barriers grown by molecular beam epitaxy (MBE). In the case of the double and triple quantum wells the ZnSe barriers are grown with thicknesses in the 5 -100 nm range to study QW coupling as a function of barrier thickness [1, 2]. The results of the growth and excitonic characterization of a very thin heterostructure containing a 1 ML CdSe UTQW (the thinnest possible QW) within very thin ZnSe barriers, which represents an epitaxial growth challenge, will be presented with a detailed discussion concerning the interpretation of its excitonic properties.

CdSe fractional monolayer quantum dots (FMQDs) are produced by epitaxially depositing submonlayer coverages of CdSe on ZnSe; then 1 ML thick islands with reduced lateral dimensions are produced. They present very interesting properties such as their r narrow photoluminescence (PL) linewidth which can be taken as indicative of a narrow distribution in composition, size, and shape [3]. These FMQDs are suitable device applications in the active region of optically pumped lasers and laser diodes in the blue spectral range. We present the results of the elaboration and characterization of FMQDs with submonolayer coverages of 0.5 and 0.25 ML [3]. We elucidate with detail the origin of the typical excitonic doublet which has been an imporant subject of discussion, and obtain the lateral dimensions of these FMQDs from calculations based on the factorized-envelope approximation.

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Incorporation of Mn into w-AlN nanostructures by MBE

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Diluted magnetic semiconductors (DMSs) have attracted significant attention due to their attractive applications for spintronic devices. These materials are semiconductors incorporated with transition metals as magnetic dopants, which can induce the spin degree of freedom to create a ferromagnetic material. Progress has been made in the effort to fabricate DMSs, especially in the III-V semiconductor systems. More studies have focused on GaMnN, with Curie temperatures ranging from 10 to 300 K [1]. Given the success with GaMnN, research is currently underway on other III-N based DMSs including alloys based upon AlN. The predicted Curie temperature of AlMnN is higher than that of Mn-doped GaN [2].

In this work AlN nanostructures were grown by molecular beam epitaxy (MBE). All the structures were grown on (111) oriented silicon substrates employing a buffer layer of AlN with 200 nm of thickness. Samples were prepared with different levels of Mn during growth to study the characteristics and parameters of its incorporation into AlN. The growth substrate was varied from 790 to 830 ºC; for each sample three layers of 60 nm in thickness were grown with Mn temperatures of 800, 820, and 840 ºC, respectively.

Different characterization technics were used to estimate Mn incorporation in AlN, as well as the structural, electronic, and magnetic properties of the system. Employing secondary ion mass spectrometry (SIMS), we observed the Mn concentration variation as a function of depth and confirm the Mn incorporation in the layers. Structural properties have been studied with atomic force microscopy (AFM) and scanning electron microscopy (SEM). High resolution x-ray diffraction (HRXRD) indicated that the sample with the lowest growth temperature presented oscillations around the AlN peak, which we assign to Pendellösung interference indicating the formation of a coherent AlMnN layer.

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EVOLUTION OF PHOTOLUMINESCENCE OF POROUS SILICON WITH THERMAL OXIDATION CONDITIONS.

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Many studies have been reported about the remarkable photoluminescence (PL) properties of porous silicon (PSi) and its degradation effect. Some reports describe that thermal annealing and oxidation improve the PL of PSi and others state that they are PL quenchers. One important application of PSi is to be used as a host matrix for organic and inorganic materials [1]; thus, it is necessary to functionalize the PSi surface terminating it with oxygen groups by thermal oxidation to improve its chemical linkage with other molecules [2]. However, specific oxidation conditions are not very well specified.

In the present work we report the effect of thermal oxidation at different temperatures and processing times on the PL of PSi. Mesoporous layers were synthesized by electrochemical etching of single side polished silicon p-type (100) wafers with resistivity of 0.01- 0.02 Ω·cm. The etchant contained Ethanol:HF:Glycerol (60:30:10 v/v/v) and 20 mA/cm^2 of anodizing current density was used. The porosity and thickness of PSi layers were determined by gravimetric measurements and index of refraction was measured by ellipsometry. PSi layers were oxidized at temperatures ranging from 800 to 1100 °C for short and prolonged times (5-120 min) under oxygen flux. Oxidizing at 800 °C for short times effectively quenches the PL of PSi. This occurs because thermal oxide passivates the PSi surface dangling bonds that present radiative transitions. In contrast and unexpectedly, oxidation for prolonged times or at higher temperatures re-activates PL with different characteristics, whose intensity even increases with etching time. This PL band could be ascribed to thermal oxide matrix.

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Proyecto VIEP-BUAP-224-2022

THERMAL OXIDATION CONDITIONS EFFECT ON THE PHOTOLUMINESCENCE OF POROUS SILICON

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In the present work we report the effect of thermal oxidation at different temperatures and processing times on the PL of PSi. Mesoporous layers were synthesized by electrochemical etching of single side polished silicon p-type (100) wafers with resistivity of 0.01- 0.02 Ω·cm. The etchant contained Ethanol:HF:Glycerol (60:30:10 v/v/v) and 20 mA/cm^2 of anodizing current density was used . The porosity and thickness of PSi layers were determined by gravimetric measurements and index of refraction was measured by ellipsometry. PSi layers were oxidized at temperatures ranging from 800 to 1100 °C for short and prolonged times (5-120 min) under oxygen flux. Oxidizing at 800 °C for short times effectively quenches the PL of PSi. This occurs because thermal oxide passivates the PSi surface dangling bonds that present radiative transitions. In contrast and unexpectedly, oxidizing for prolonged times or at higher temperatures re-activates PL with different characteristics, whose intensity even increases with etching time. This PL band could be ascribed to thermal oxide matrix.

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Proyecto VIEP-BUAP-224-2022

Growth of zinc-blende and wurtzite III-N heterostructures and nanostructures by molecular beam epitaxy

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III-N semiconductors (GaN, AlN and InN) are of great scientific and technological interest due to their relevant applications in micro and optoelectronics. Alloys of these materials enable the development of novel devices that can operate at wavelengths from infrared to ultraviolet, as well as high-power, high-mobility transistors. For most of device applications the wurtzite cristal structure is employed because it is the stable phase of III-N materials [1]. On the other hand, the zinc-blende structure of III-N materiales is a meta-stable phase with important advantages over the wurtzite counterpart. For example, spontaneous and piezoelectric polarization are not present along the cubic (100) orientation, in addition due to its high symmetry holes mobility should be larger than that obtained for the wurtzite phase [2]. The optical and transport properties of III-N semiconductors strongly depend on the conditions under which these materials are grown. In this talk we will present the synthesis of III-N semiconductor materials by Molecular Beam Epitaxy (MBE). MBE is a growth technique that allows a very precise control of the amount of material deposited on a substrate at the level of atomic layers. This characteristic makes MBE an ideal technique for the fabrication of heterostructures and nanostructures. In the first part of this talk, I will present the results of the growth of wurtzite III-N structures on Si(111) substrates by MBE employing a radio-frequency (RF) plasma source to produce reactive atomic nitrogen [3]. In the second part of this talk, I will present details of the growth of III-N semiconductors on GaAs (100) substrates to induce the formation of the zinc-blende phase. In particular I will show the method that we used to control the very early stages of heteroepitaxy to obtain GaN with a high cubic phase content. The optical, electrical and structural properties of nanostructures and heterostructures of III-N semiconductors with wurtizte and zinc-blende phase will be discussed.

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Optical and Structural Characterization of High Crystalline Quality InGaAsSb Semiconductor Layers Grown by LPE for Near and Mid-Infrared Applications

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Antimonide-based quaternary semiconductor alloys such as $In_xGa_{1-x}As_ySb_{1-y}$ have been currently investigated for their potential application for the development of optoelectronic devices emitting and detecting in the mid-infrared optical spectrum. In the last years, we have developed expertise in the growth of these types of semiconductor alloys using the liquid phase epitaxy technique (LPE) under supercooling conditions. In this work we present our latest results on the growth of high quality p-type Si-doped InGaAsSb alloys; using XPS spectra we show that Si atoms behave as acceptors. Using Raman spectroscopy analyze the phonon-plasmon L_ in the surface depletion region. Low temperature photoluminescence (PL) spectra showed a bound exciton emission peak associated to neutral Sb acceptors with an activation energy of 10 meV. We also present results on the effect of varying the As content on the alloy on the layer crystalline quality due to the effect on the nearly lattice-matched epitaxial growth to the GaSb substrate, and also on the bandgap energy which can be engineered in the near infrared range; we show HRXRD, XPS, Raman and PL spectra for the layers grown with different As contents. From XPS spectra and Raman we identified the stable atomic arrangements to be Ga-Sb and In-As.

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Study and evaluation of thin films synthetized by chemical deposition for the design of a window buffer layer.

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Semiconductor materials used for the build-up of thin films are one of the topics studied globally, due to the various uses that these materials can provide. The production of photovoltaic cells from metallic sulfides has taken a great boom since 2011[1]due to the present abundance of the compounds and their low toxicity. The noticeable advantage related to the use of these materials comes from the diverse methods of elaboration of a thin film [2]. In the following work, the S.I.L.A.R method is used to obtain thin films of tin oxide, cadmium sulfide, and zinc sulfide. Where it is intended to deposit said materials in a single thin film for the formation of a semitransparent window buffer layer. It is worth mentioning that the chemical deposit technique used in this project handles different cycle times that are important to establish: draining, and submerging time varies between each material to be deposited and favors the absorption reaction in the substrate and the growth of the semitransparent film. A reaction mechanism is proposed for the first layer between glass and SnCl2 to explain the reaction that takes place in it. The X-ray Diffraction (XRD) and Raman spectroscopy studies showed that all the multilayer films exhibited polycrystalline nature. The absorbance data obtained from the analysis of the films in a visible light spectrophotometer gives a wide panorama of information about the deposit that was made on the substrate. In both methods, the characteristic absorbance values of the deposited materials are found (glass = 320 nm, SnO2 = 350 nm, ZnS = 333.33 and CdS = 500 nm). These films were analyzed by the four-point Kelvin method in various regions of the film to specify the electrical resistance for the two methods established the values are 25 Ω and 0.1 Ω respectively. Said characterizations in principle give a positive idea of the deposit made on the substrate and give rise to new characterization methods that will be carried out later.

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(2) Nicolau, Y. F. SOLUTION DEPOSITION OF THIN SOLID COMPOUND FILMS BY A SUCCESSIVE IONIC-LAYER ADSORPTION AND REACTION PROCESS. 14

Inverse band gap versus polarization relation in ferroelectric materials from first principles

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New pathways to design functional ferroelectrics, materials with a spontaneous and switchable polarization under an electric field, are desired for electro-optic and solar energy conversion devices [1,2]. Previous work has focussed on searching ferroelectrics with small band gaps in the visible solar spectrum. In this work, we take an alternative route, and use first principles methods and the modern theory of polarization [3] to perform a high-throughput search of ferroelectrics that display an inverse relation between electronic band gap and polarization, such that the band gap decreases as the polarization increases with an external parameter. To our knowledge, such material property has not been reported before, and we propose it as a new way to design small band gap ferroelectrics. We start by studying the list of 200 materials previously reported in the ferroelectrics database [4], and later generalize our search to identify new ferroelectrics with inverse band gap versus polarization relation within the Materials Project database [5]. We have found 21 ferroelectrics with the proposed property among different families of ferroelectric materials (Table 1) and use hydrostatic strain as an external parameter to explore their band gap and polarization relation.

Table 1: Ferroelectric materials with non zero polarization and decreasing band gap. We show polarization value and the difference of energy formation and band gap between non polar and polar structures.

Material	Polarization ($\mu C/cm^2$)	Energy ΔE (meV)	band gap ΔE_g (eV)
$Al(HO)_3$	8.1	359	0.40
Ag_3SI	1.1	671	0.31
H_2SO_4	51.0	393	0.33
$InHO_2$	13.2	60	0.12
K_4CO_4	16.7	160	0.87
$KP(HO_2)_2$	5.2	80	0.15
Li_4CO_4	49.0	483	1.01
$Mg_3B_7ClO_{13}$	0.3	469	0.23
Na_4CO_4	39.2	295	1.01
Rb_4CO_4	42.8	156	0.07
$YBiO_3$	9.7	638	0.30
$YScO_3$	6.6	265	0.07
$Zn(NO_3)_2$	1.1	190	0.17
$CsAs(HO_2)_2$	9.01	137	0.23
$AlHO_2$	21.4	78.03	0.22
$YCoO_3$	16.7	786.4	0.52
$DyErO_3$	7.68	144.23	0.15
$Cd(NO_3)_2$	1.01	466.2	0.49
$RbP(HO_2)_2$	7.32	95.5	0.17
$Mg(NO_3)_2$	12.4	612.22	0.20
$YNiO_3$	5.43	914	0.10

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FLAT-BANDS AND SUPERCONDUCTIVITY IN MAGIC ANGLE TWISTED GRAPHENE MULTILAYERS

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An introduction is made on the relevant aspects of flad-bands and its relationship with superconductivity in magic angle twisted graphene bilayers and trilayers. Then we present a chiral Hamiltonian able to reproduce such flat-band. Next such Hamiltonian is renormalized into a 2x2 matrix Hamiltonian [1]. This allows to produce the most simple Hamiltonian available. The action of the proposed renormalization maps zero-modes flat-bands into ground states. On each graphene layer, modes near zero energy have an antibonding nature in a triangular lattice. This leads to a phase-frustration effect associated with massive degeneration. At magic angles, the intralayer frustration is zero while for other angles is proportional to the Fermi velocity [1]. The methods brings the main physical actors of twisted systems: kinetic energy, confinement potential and an interlayer interaction operator which is divided in two parts: a non-Abelian interlayer operator and an operator which contains an interaction energy between layers. Each of these components is analyzed as a function of the angle of rotation, as well as in terms of the wave-function localization properties. In particular, it is proved that the non-Abelian operator represents interlayer currents between each layer triangular sublattices, i.e., a second-neighbor interlayer current between bipartite sublattices. A perturbative analysis performed around the first magic angle allows to explore analytically the details of such energy balance between each contribution: interlayer currents, kinetic energy and confinement energy [2].

Finally, a discussion is made about the possible pairing mechanisms behind superconductivity, specially the Kohn-Luttinger one in which the Columb potential is screened by particle-hole excitations. This effect can be calculated from the dynamical polarizability in the Random Phase Approximation (RPA).

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STRUCTURAL, MAGNETIC AND ELECTRICAL MAGNETO-TRANSPORT PROPERTIES OF NANOWIRE NETWORKS

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Electrodeposited nanowire arrays are flat systems with a large surface area and composed of millions of one-dimensional metallic nanostructures with a high aspect ratio of diameter over length [1]. Their electrochemical fabrication in nanoporous membranes allows the combination of a wide range of materials to form both homogeneous networks and alloys with specific composition. This fabrication technique also allows the control of geometrical characteristics to obtain nanotube networks and multilayered nanowires. The magnetic properties of the nanowires can be modified by controlling the diameter, packing density or spatial arrangement characteristics. On the other hand, one type of systems that has attracted great interest are networks of interconnected one-dimensional nanostructures, which can be used to precisely tune their magnetic and electrical magneto-transport properties [2]. Specifically, interconnected multilayered nanowire networks with a succession of ferromagnetic and non-magnetic layers have also been successfully fabricated, resulting in giant magnetoresistance (GMR) responses measured in the current-perpendicular-to-plane configuration. In summary, nanowire arrays have high potential as integrated, reliable and stable magnetic field sensors; magnetic devices for memory and logic operations; neuromorphic computing; as well as for microwave signal absorption applications.

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SURFACE-ENHANCED RAMAN SCATTERING (SERS) SUBSTRATES BASED ON Ag-NANOPARTICLES AND Ag-NANOPARTICLES/POLY (METHYL METHACRYLATE) COMPOSITES

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In recent years, Surface-Enhanced Raman Spectroscopy (SERS) has become a very useful molecular identification technique in many areas of scientific and technological research since, it provides information on molecular compounds present in the sample under study in concentrations considerably low [1]. In this sense, we describe the synthesis method to obtain SERS substrates based on Ag-nanoparticles (Ag-NPs) using three different concentrations: 0.94, 1.41 and 1.88 mM. Similarly, Ag/PMMA composites were prepared in the form of films on Si wafers by the co-deposition technique, from a mixture of Ag-NPs (0.94, 1.41 and 1.88 mM) and PMMA solutions, in which the solvent was removed by evaporation. SEM micrographs show that the Ag-NPs have a quasi-spherical shape with 15 $\pm$ 3.7 nm average diameter and PMMA microspheres with a diameter of 298 ± 8 nm average diameter.

The sensitivity of these SERS substrates was evaluated using Methylene Blue as a molecular probe at different concentrations (0.5-2.5 μM). The results show that SERS substrates based on Ag-NPs present an Enhanced Factor (EF) of 5.18 ± 0.09×10^6 which is one order of magnitude greater than that of the Ag/PMMA composites (3.69 ± 0.11×10^5). However, in both the Ag-NPs substrates and the SERS composites substrates, the EF values increase as the concentration of the Ag-NPs increases. It should be noted that SERS substrates with higher concentrations of Ag-NPs have higher EF due to the formation of metallic clusters (hot-spots) adsorbed on the film surface which enhance the local electromagnetic field [2].

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SURFACE-ENHANCED MICRO-RAMAN SCATTERING SUBSTRATES BASED ON Ag-NANOPARTICLES AND Ag-NANOPARTICLES/POLY (METHYL METHACRYLATE) COMPOSITES

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In recent years, Surface-Enhanced Raman Spectroscopy (SERS) has become a very useful molecular identification technique in many areas of scientific and technological research since, it provides information on molecular compounds present in the sample under study in concentrations considerably low [1]. In this sense, we describe the synthesis method to obtain SERS substrates based on Ag-nanoparticles (Ag-NPs) using three different concentrations: 0.94, 1.41 and 1.88 mM. Similarly, Ag/PMMA composites were prepared in the form of films on Si wafers by the co-deposition technique, from a mixture of Ag-NPs (0.94, 1.41 and 1.88 mM) and PMMA solutions, in which the solvent was removed by evaporation. SEM micrographs show that the Ag-NPs have a quasi-spherical shape with 15 $\pm$ 3.7 nm average diameter and PMMA microspheres with a diameter of 298 ± 8 nm average diameter.

The sensitivity of these SERS substrates was evaluated using Methylene Blue as a molecular probe at different concentrations (0.5-2.5 μM) and the correspondent micro-Raman spectra. The results show that SERS substrates based on Ag-NPs present an Enhanced Factor (EF) of 5.18 ± 0.09×10^6 which is one order of magnitude greater than that of the Ag/PMMA composites (3.69 ± 0.11×10^5). However, in both the Ag-NPs substrates and the SERS composites substrates, the EF values increase as the concentration of the Ag-NPs increases. It should be noted that SERS substrates with higher concentrations of Ag-NPs have higher EF due to the formation of metallic clusters (hot-spots) adsorbed on the film surface which enhance the local electromagnetic field [2].

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THYROXINE QUANTIFICATION BY MEANS SURFACE-ENHANCED RAMAN SPECTROSCOPY SUBSTRATES BASED ON Au AND Ag NANOPARTICLES

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Thyroxine (T4) is a hormone responsible for regulating cellular metabolism and growth hormone, so its detection during fetal development is of utmost importance since a deficit in thyroxine leads to lower development of the reproductive organs and a lack of physical development. T4 is detected in blood plasma by chemiluminescence.

Au and Ag nanoparticles can be used as SERS substrates for T4 detection and be an alternative, at the laboratory level, for quantifying the organic compound up to 1 nanomolar concentration with good reliability.

SERS substrates of Au nanoparticles (Au-NPs) and Ag-NPs were prepared to use as amplifiers of the Raman bands of thyroxine. Au-NPs and Ag-NPs were synthesized by the seed-mediated growth method. The metallic nanoparticles present a spherical morphology and sizes of 50 nm in diameter. The metal NPs are stable and have a negative charge on the surface due to ascorbic acid and tannic acid for Au NPs and Ag NPs, respectively. The UV-Vis spectroscopy results showed bands located at 537 nm and 421 nm correspond to the surface plasmons of Au NPs and Ag NPs, respectively.

The application of metal NPs as SERS substrates were carried out using T4 as the test molecule. The effect of the analyte concentration (0.01, 0.03, 0.10, 0.30, and 1.00 mM) on the SERS response of the materials was studied. T4 Raman spectrum, at the different concentrations and without metal NPs, did not show any Raman bands characteristic of the organic compound. The Raman spectra of T4, at different concentrations and deposited on the metallic NPs, presented an increase in the intensity of the Raman bands of the organic compound as the concentration of T4 increased. Considering the Raman band of T4 located at 1042 cm^{-1}, in the absence and presence of the metal NPs and the number of thyroxine molecules excited by the laser beam, SERS enhancement factor (SERS-EF) was determined. The results showed that as the concentration of thyroxine increases, the SERS-EF increases. For the case of Au NPs, the SERS-EF was $1.2x10^2$ and $2.2x10^6$ for concentrations of 0.01 and 1.00 mM T4, respectively. On the other hand, the SERS-EF with Ag-NPs were $3.8x10^3$ to $4.5x10^6$ for concentrations of 0.01 to 1.00 mM thyroxine, respectively. These results show that Ag NPs are more efficient in detecting thyroxine at low concentrations than Au NPs.

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C-V model of CdS/CdTe thin films solar cells with the dependence of the applied voltage frequency

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In CdS/CdTe solar cells, the dependence on the frequency of the applied voltage is essential to improve theoretical results. Our model is based on the conservation of energy, and charge, plus adding a ternary and the existence of plasmons in the interface, the description and analisys has been considering the previous theoretical methodology [1]. In this work, the capacitance dependence as a function of the frequency of the induced field in the heterojunction is observed. Furthermore, a plasmon was formed in the interface in the Surface semiconductor.

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Perovskites, and chalcogenides for energy storage/conversion systems

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The growing number of electronic devices, and their demanding applications are linked to the increasing demand for energy conversion, as well as for better energy storage devices. More safety and an increasing number of charge/discharge cycles are expected from batteries; for the fuel cells, the search is for better efficiencies, without environmental contamination, less noise and no electrodes' poisoning; also, better mass' densities might be allowed for hydrogen storage at low pressures. Then, on the way to contribute to satisfy what is expected from those energy storage/conversion systems, we explored some compounds by means of modeling and calculations in the Density Functional Theory scheme. Among those materials we studied the structural, electronic, and magnetic properties, as well as the thermodynamic stability, of the perovskites $LaTiO_3$, $Li_xLa_{1-x}TiO_3$, (LTO and LLTO, respectively) [1]. Also, TiO_2-, LaO- and LiO-terminated LTO and LLTO (001) surfaces were studied to model functional oxide electrolytes. Looking for better materials, the electronic and mechanical properties of the bulk $TiSe_2$ were studied, and the effects of the confinement on the compound (into mono-, bi-, and tri-layered systems) on the electronic and mechanical properties; for the same reasons, Li atoms were placed at different adsorption sites of the $TiSe_2$ monolayer, to identify the most favorable adsorption site for Li in the $TiSe_2$ systems [2].

It was found a transition from semiconductor to insulator for the LLTO, and the thermodynamic stability would diminish with the Li concentration in the LLTO. For the thin films, it was found that the TiO_2- termination is the most likely for the LTO at the (001) free surface, but it is the most unstable for the LLTO. Taking account of the good thermodynamic stability, the LTO and the LLTO slabs (TiO_2- and LiO-terminated, respectively) could be compatible with different electrodes, to form highly cohesive chemical bonds at the electrode/electrolyte interface. The $TiSe_2$ systems are metallic: the bulk, the pristine monolayers and the monolayers with Li atoms at the surface.

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Enhancement of parameters performance of an SPR optical biosensor based on bimetal - 2D materials structures

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Abstract. In the last decades, the study of optical biosensors based on surface plasmon resonance (SPR), has gained great relevance due to its wide variety of applications in various fields. In the biomedical field, biosensors can detect cancer cells, DNA hybridization, and even the recent detection of SARS CoV-2 [1-3]. In the field of biosensing, biosensors are used to detect biomolecules, because this type of biosensors have high sensitivity and facilitate the study and analysis of the analyte in real time [1]. One of the main problems with this type of biosensor is that, by improving some specific performance parameter, another parameter is affected. In this work, we carry out a theoretical study of an SPR optical sensor based on structures of different 2D material bimetal combinations. The metals used were gold and silver, and graphene was used as the 2D material. We find that the value of the performance parameters is greatly increased for when we use a gold-silver structure as bimetal and graphene as 2D material. This is due to the fact that gold as a metal provides us with high sensitivity due to the large spectrum shift that occurs when detecting the analyte, while in the case of silver we obtain high detection accuracy and a high-quality factor. because silver has a sharp resonance spectrum; while graphene contributes to improve sensitivity, because it has a large surface area and large absorption capacity. The combination of other metals and 2D materials allows us to modulate the behavior of the different performance parameters of the biosensor and also to show different line shapes in them.

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FIRST-PRINCIPLES CALCULATIONS OF MOLECULAR ADSORPTION ON GRAPHENE

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Graphene (G) is a two-dimensional honeycomb atomic lattice composed of carbon atoms with an atomic thickness. It presents high electronic conductivity because its charge carriers behave like Dirac fermions according to the band structure, characterized by its linear behavior at the Fermi energy. Besides, G does not present a forbidden gap between valence and conduction bands that is desirable for optoelectronic applications. Within this context, G has been functionalized by adsorbing atoms and molecules [1], which allows the modification of its electronic structure, increasing its charge density when G is in the presence of an external potential.

Here, we present our study of the adsorption of ten different molecules on a G monolayer based on the density functional theory (DFT) performed on the SIESTA code [2]. This methodology described G in its isolated state and for molecules, where atomic bases are built by a *simplex* algorithm [3]. These bases reproduce electric dipole moments and geometric structures of G and molecules considered here. First, we study the binding energies of the adsorbed molecules on G, which are found in the physisorption range [4]. After that, the band modification was studied employing an unfolding band approach for electronic bands of the Graphene-molecule systems. From this, it is concluded that molecules with a larger dipolar moment distort the G band structure significantly. Finally, a linear relationship is obtained between the adsorption energy and the HOMO level of the molecules. Such that when the HOMO level is below and far from the Fermi level, the molecule shows smaller adsorption energy.

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NH_3 adsorption on functionalized thin carbide monolayer: A DFT study

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Ammonia (NH_3) is a chemical that occurs naturally in humans, animals, and plants. It is a colourless gas with a very penetrating and characteristic odour. This substance is also produced industrially, mainly for producing fertilizers and to a lesser extent for applications in textiles, plastics, coolants, cleaning products, etc. Exposure to high levels of NH_3 in the air can irritate the skin, eyes, throat, and lungs, and can cause coughing and burns. Exposure to very high levels of NH_3 over a long period can cause lung damage and even death. The US Occupational Safety and Health Administration (OSHA) has set a limit of 25 parts of NH_3 per million parts of air (25 ppb) at work for 8 hours per day and a limit of short exposure (15 minutes) of 35 ppm [1]. Two-dimensional (2D) nanostructures are nanomaterials that have been extensively investigated as sensors for gases and molecules. It has been reported that the functionalization of 2D nanomaterials can improve their ability to interact with different molecules [2, 3]. In this work, the effects of functionalization with different metal atoms (alkali, alkaline earth and transition) on the adsorption and detection of NH_3 in monolayers of tin carbide (2DSnC) are studied using first-principles calculations based on DFT theory. Electronic properties, adsorption energies, charge transfers, recovery times and conductivity were studied to analyze the feasibility of the application of this nanomaterial for the detection and adsorption of NH_3. The results show strong adsorption of the metallic atoms in the monolayer, it is also observed that the adsorption of NH_3 in the monolayer is of the order of physisorption. On the other hand, the interaction between NH_3 and 2DSnC is remarkably enhanced due to the functionalization of the monolayer with metal atoms. The changes in the electronic properties, the charge transfer of NH_3 towards the monolayer, the changes in conductivity, as well as the recovery times, suggest that the functionalized monolayer could detect and trap the NH_3 molecule.

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Theoretical study of various noncovalent interactions in larger molecules

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The development of the density functional theory (DFT) was of paramount importance for the description of the physical properties of solid-state materials, however one of its mayor setbacks was its inability to properly describe non-covalent interactions. Multiple schemes have arisen to describe these interactions, specially the semiempirical one developed by Grimme[1] which has been used successfully to describe Van der Waals forces in multiple systems. However, in these schemes the effects of these interactions are not described specifically, rather is incorporated to the overall results. An analysis of these forces becomes more important, as the development of new nanoscale systems leads to many monolayers of so-called Van der Waals structures, such as graphene or the transition metal dichalcogenides. Non-covalent forces become even more relevant, since there are many studies on the adsorption of many chemical species on these monolayers, where their effects are expected to be prevalent. Also, the development of hybrid organic perovskites has shown that by using an organic molecule as one of the cations, its efficiency in solar cell development increase drastically. These organic molecules are contained in the perovskite structure, therefore weak interactions are expected to have a mayor contribution to their relative stability. In this work, using data obtained from DFT calculations, the weak non-covalent interactions are described in two test systems: a semiconductor monolayer with adsorbed DNA nucleobases and the Halogen hybrid perovskite $CH_3NH_3CaBr_3$. Both systems were chosen due to their significance for DNA sensing and for solar cell materials, and the importance of the non-covalent forces in both. The results show that the main mechanism for the DNA adsorption in the semiconductor monolayers is a non-covalent one. While for the perovskite these interactions provide an explanation of the most stable positions of the $CH_3NH_3CaBr_3$. Therefore, it can be concluded that for many of the most attractive systems for the development of solid-state physics, the proper description of non-covalent forces is of great importance.

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Atomic scale modelling of aperiodic heterostructures

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Celebrating the first centenary of Quantum Mechanics, one of current research challenges is the use of this atomic-scale theory to improve the design and innovation of electronic and optical devices, as ocurred 75 years ago with the first working transistor invention guided by the single-electron band theory. Such devices contain a macroscopic number of heterogenous atoms with non-periodically placed interfaces, which prevents the use of reciprocal space, while directly solving 10^{23} coupled Schrödinger equations in the real space would require unavailable yottabytes (YB) of memory just for recording the spatial positions of this huge number of atoms.

A presently viable alternative is the real-space renormalization method, which explicitly keeps only exterior sites of each region, while the interior sites are absorbed by the effective interactions between exterior ones; in analogy with solving a set of algebraic equations using the substitution method to eliminate the coordinates of interior sites and preserving only the exterior ones [1]. This method is exact and can be repeated to reach a macroscopic number of sites in several tens of steps. When it is combined with the convolution technique [2] or independent channel transformation [3], macroscopic three-dimensional heterostructures with aperiodically located interfaces can be properly addressed. In this talk, we will review possible applications of this approach to devices, such as thermoelectric and photovoltaic ones.

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Two particle wavefunctions and electron pairs in periodic and aperiodic systems.

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Superconductivity theory needs a paring mechanism to explain the charge carriers by electron pairs. Usually this is explained supposing a attractive force due phonons. Nowadays, Winkler [1] have experimentally proved that repulsively bound pairs can be formed in a optical lattice with remarkable stability, a phonomenon that can be explained using the Hubbard model for two particles [2], nevertheless these electron pairs have a energy almost equal to the repulsive energy U of the Hubbard model.
In this talk, we present a method to find two particle states for periodic systems in the Hubbard model. Using this method we have found that repulsively bound pairs are formed in the SSH model with energies below zero no matter the value of the repulsive energy U. We also describe a numerical way to find two-particle bound states in complex systems like superlattices and quasicristals. Density of states of two-particle wavefunctions in the Fibonacci chain and Penrose quasycristal are presented.

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NONLOCAL OPTICAL RESPONSE OF METAMATERIALS AND METASTRUCTURES

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The physics of metamaterials is rather interesting because of the striking phenomena and extraordinary properties, which have been discovered in such artificial periodic structures. Photonic metamaterials may exhibit negative refractive index, which makes possible the fabrication of superlenses breaking the diffraction limit, as well as invisibility cloak devices. The observed physical phenomena can be explained by considering the periodic structure as a homogeneous medium with effective (or average) parameters, which depend not only on the shape and properties of the materials inside the unit cell, but also on the type of periodic arrange (Bravais lattice). Besides, the effective parameters may be tuned by several physical mechanisms, broadening the range of applications of metamaterials. Despite the fact that photonic metamaterials include a great variety of systems, their optical response can be described by using nonlocal effective parameters. Here, we demonstrate that layered systems such as metal-dielectric nanostructures, periodic structures of semiconductor quantum wells, and even nanostructured systems with superconductors can be homogenized even beyond the long wavelength limit in a unified form by employing a nonlocal homogenization approach [1]. In addition, we will discuss the Berreman effect in the optical response of bimetallic metamaterials, as well as the diffraction spectra for periodic arrays of bimetallic-metamaterial bars. Also, we shall show that metamaterials with semiconductor quantum wells exhibit strong resonances in their optical spectra as a result of the interaction between the confined excitons (or even magnetoexcitons) and the electromagnetic eigenmodes in the photonic nanostructure. In the case of nonlocal metamaterials with layered superconductors, the optical spectra provide information about the excitation of additional electromagnetic modes, called Josephson plasma waves. Finally, novel designs of layered photonic metamaterials and metastructures are here presented and analyzed.

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STUDY OF ELECTRONIC CORRELATION IN A LOW DIMENSIONAL SYSTEM

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Electronic correlation in superconducting materials has been subjected to multiple interpretations as new materials with different dimensionality are reported. The recent discovery of superconducting Twisted Bilayer Graphene (TBG) and Quasicrystals (QC) opens a new outlook in the study of electronic correlation. In this work, the object of study are two coupled periodic chains, that can alse be viewed as a ladder. We solve the one and two electron problem using the tight-binding Hamiltonian and the Hubbard model for the bulk, in a periodic and a quasiperiodic system. To solve the two interacting electrons, we use a real-space mapping method, which accounts the dynamics of the particle density in the neighborhood. The energy dispertion of the bound states is obtained and their wavefunction is studied.

References

Acknowledgements

2D SiGe as anchoring material for Li – S batteries: a DFT study

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Having an estimated energy density larger than 2600 WhKg -1 , which is 3 to 6 times larger than the energy densities offered by current batteries, Li – S batteries have attracted the interest of the scientific community. However, these batteries rapidly loss their efficiency due to the so-called *polysulfide suttle effect*, which leads to the unwanted Li_2S, Li_2S_2, Li_2S_4, Li_2S_6, Li_2S_8 and S_8 compounds.These polysulfides considerably reduce the number of charge/discharge battery cycles and then, the search for new nanostructures that could serve as anchoring material for these polysulfides has been intensified. On the other hand, the study of two-dimensional materials with honeycomb structures like graphene has increased due to the physical properties offered by these materials. In particular, their large surfaces allows for an enhanced interaction with different atoms or molecules. In this work, the interactions between polysulfides and a siligene monolayer (2D SiGe) were studied by using first principles calculations based on the Density Functional Theory. The calculated adsorption energies of the polysulfides on the 2D SiGe have values between 1.5 eV and 2.2 eV, indicating that there is a strong adsorption between them and suggest that 2D SiGe could be used to anchor these compounds.

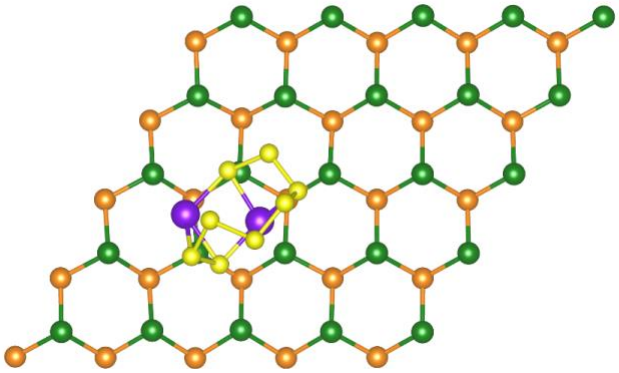

Figure 1. Adsorption of Li_2S_8 on 2D SiGe (orange, green, yellow and purple spheres represent Si, Ge, S and Li atoms respectively).

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This work was partially supported by the multidisciplinary projects IPN-SIP 2020-2093, 2022-0600 and UNAM-PAPIIT IN109320. Computational resources were provided by the DGTIC-UNAM Miztli supercomputer (LANCAD-UNAMDGTIC-180 Project). BJC thank CONACYT and BEIFI-IPN for their financial support.

Doped silicon nanowires for the adsorption of urea: an *ab-initio* study

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An important indicator in medical, environmental, and industrial fields is urea. Particularly, the anormal levels in the human body (8-20 mg/dl is normal) of this molecule are the main indicator for the diagnosis of renal failure, gastrointestinal bleeding, dehydration, hepatic failure, etc. Common urea sensors are based on the catalytic conversion of urea to hydrogen bicarbonate and ammonium. In this way, the development and study of new devices and materials capable to adsorb and detect this molecule in its pure form are important tasks for the scientific community [1, 2]. In this work, we propose a hydrogenated silicon nanowire (SiNW), grown along the [001] direction with (110) exposed surfaces, undoped and doped with different elements of groups III, IV and V for adsorbing the urea molecule and its possible electronic detection. After the creation of a Si dangling bond, doping consisted of replacing that silicon atom from the surface for one element of the dopants, and this atom is used as the adsorption site of the urea molecule. The results show that the doped SiNWs are capable to adsorb the urea molecule, having the highest adsorption energy for the Al-doped SiNW, followed by the boron case. The adsorption of urea on the doped SiNWs modifies the electronic states inside the valence and conduction bands, this hybridization confirms that the urea molecule is adsorbed by doped SiNW. Also, changes in the work function of the systems, provoked by the urea adsorption, could allow the detection of the molecule. These nanostructures could be used for urea capture and detection, which could lead to potential nanosensors for the diagnosis of uremia.

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SEARCH FOR ATOMIC STRUCTURES BY AB INITIO METHODS AND EVOLUTIONARY ALGORITHMS FOR MONATOMIC SYSTEMS UNDER HYDROSTATIC PRESSURE

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Fluorine has not been as extensively studied compared to other single-element diatomic molecules (H2, N2, O2, Cl2, Br2, I2). In fact, the space group of solid fluorine at ambient pressure has been a source of controversy for many years. Despite multiple spectroscopy studies and theoretical calculations, the discussion regarding the most stable phase of this system at high pressures was still maintained. For this reason, and using computational techniques, only a few years ago, a study established the most stable phase at low pressures and its subsequent transformation to Cmca at 8 gigapascals (GPa) [1]. However, recent studies show profound differences between the phases found and their respective transition pressures for much higher pressures [2,3].

In this work, structural search calculations were carried out using evolutionary algorithms for pressure ranges in the order of terapascals to establish enthalpy relationships with those post-Cmca phases proposed through less impartial methods.

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Preliminary Design and Assessment of an 83 kW Electric Motorbike.

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The transportation electrification and the use of renewable energies have been exploited recently to produce and use clean and green electricity. Electromobility may be one of the keys to aid progress towards sustainable transport, [1]. Different type of electric systems for electric and hybrid vehicles have been studied, however, new improvements are requested. Electric bikes are considered an accessible alternative in the field of mobility.

This paper presents a preliminary overview of a first prototype of an 83 kW electric motorbike since, nowadays, electric motorbikes have advanced drastically in their technology in such a way that lately there is a boom in the field of competition. The field of electric vehicle racing mainly pursues the aim of obtaining an optimal performance of all the motorbike components in order to obtain a safe racing vehicle fast enough while looking for stability of all the systems onboard, [2]. A general description of the project is given up to the date, detailing the systems parts, integration, numerical estimations and a rearrangement proposal of the actual prototype with the aim to mechanically, [3] and thermally, [4] improve the vehicle.

Fig. 1. First prototype E-Bike from IPN LINC^{2}E^2 2022.

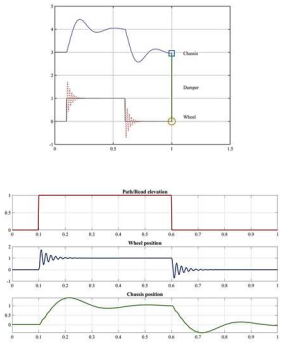

Fig. 2. MATLAB damping system simulation in actual prototype

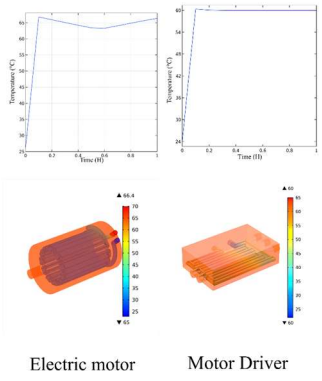

Fig. 3. Electric motor and Motor driver temperature´s cooling whit anti freezing liquid, 1 Hr. COMSOL simulation.

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	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
9.00 - 9.30	Opening	Plenary Lecture 4 Sandra Rodil	Plenary Lecture 8 Mildred Quintana	Plenary Lecture 12 Gerardo García	S9, S10, S11, S12
9.30 - 10.00	Plenary Lecture 1 Cecilia Noguez				
10.00 - 10.30		Plenary Lecture 5 Julio Mendoza	Plenary Lecture 9 Luis E.F. Foa	Plenary Lecture 13 Armando Encinas	S13, S14
10.30 - 11.00	Invited Talk Joel Yuen-Zhou				Invited Talk 8 Bertha Aguilar
11.00 - 11.30	Invited Talk 1 Eduardo Barrios	Invited Talk 4 Luis Pérez	S3 , S4	Invited Talk 5 Thomas Stegman	Invited Talk 9 Eliel Carvajal
11.30 - 12.00	**Coffee Break**				
12.00 - 12.30	Plenary Lecture 2 Riccardo Rurali	Plenary Lecture 6 José Miguel	Plenary Lecture 10 Alfredo Raya	Plenary Lecture 14 Felipe Pérez	Invited Talk 10 Joaquín de la Torre
12.30 - 13.00					**Closing**
13.00 - 13.30	Plenary Lecture 3 Máximo López	Plenary Lecture 7 Isaac Hernández	Plenary Lecture 11 Chumin Wang	S5, S6, S7, S8	
13.30 - 14.00					
14.00 - 16.00	**LUNCH**		**Excursion**	**LUNCH**	
16.00 - 16.30	**Coffee Break**			**Coffee Break**	
16.30 - 17.00	Invited Talk 2 Isaac Rodríguez	**POSTERS**		Invited Talk 6 Alejandro Trejo	
17.00 - 17.30	S1, S2			Invited Talk 7 Sara E. Pérez	
17.30 - 18.00	Invited Talk 3 Outmane Oubram			**Conference meeting**	
19.30 - 21.00			**Cocktail Centro Cultural UNAM**		