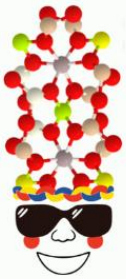

XXV Latin American Symposium on

Solid State Physics

Barranquilla, October 23 to 26, 2024

Book of Abstracts

MEMORIAS DEL EVENTO

ISSN: 3028-7073

SUE CARIBE
DOCTORADO EN CIENCIAS FÍSICAS

Universidad del Atlántico

Universidad de Cartagena
Fundada en 1827

ICTP 1964–2024

UNIVERSIDAD DEL MAGDALENA 1962

ACADEMIA COLOMBIANA DE CIENCIAS EXACTAS, FÍSICAS Y NATURALES

REVISTA MEXICANA DE FÍSICA

Book of Abstracts from the XXV Latin American Symposium on Solid State Physics (SLAFES), Barranquilla October 23 to 26, 2024.

Edited by:

Javier A. Montoya and Beatriz H. Cogollo-Olivo

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https://slafesxxv.sue-caribe.org/

CONTENT

Welcome Message

Dear Solid-State Community,

It is a great pleasure to welcome you to the XXV Latin American Symposium on Solid State Physics (SLAFES) hosted this year by the SUE-Caribe network of universities, represented in this occasion by the Universidad del Atlántico in the vibrant city of Barranquilla, from October 23 to 26, 2024. This symposium marks a significant milestone as we celebrate the 25th edition of SLAFES, a testament to decades of dedicated research, collaboration, and scientific advancement in the field of solid-state physics.

Since its inception in 1969, SLAFES has grown into one of the most prestigious and enduring conferences in Latin America, fostering connections between researchers, academicians, and industry experts. This year, we are proud to host over 180 participants, including esteemed plenary and invited speakers, students, and scholars from ten countries across Latin America, as well as contributors from Europe and the United States. They represent almost sixty distinguished academic and research institutions, which underscores the global nature of scientific inquiry and the shared commitment to pushing the frontiers of knowledge.

The program for SLAFES 2024 contains an exciting array of plenary talks, invited presentations, oral contributions, and poster sessions, adding up to over a hundred thirty contributions that cover cutting-edge topics, from electronic structure and magnetism to nanomaterials and novel technologies. We trust that these sessions will inspire rich discussions, spark new ideas, and promote collaborations that extend well beyond the conclusion of this event.

Barranquilla, known for its lively culture and warm hospitality, offers the perfect backdrop for both rigorous academic exchange and personal connection. We hope that your experience here will be enriching, both scientifically and culturally.

Thank you for being a part of this special edition of SLAFES. Your participation and enthusiasm are what make this symposium a thriving hub for innovation and progress. We look forward to an engaging and fruitful event.

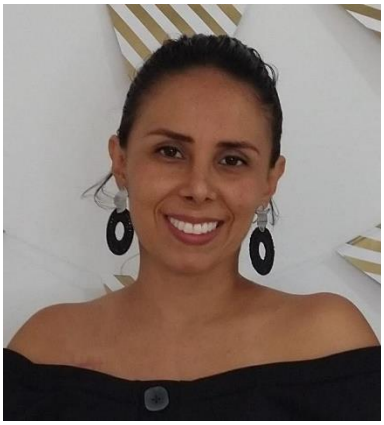
Welcome to SLAFES 2024!

With warm regards,

Javier A. Montoya M.
General Chair, XXV SLAFES

Organizing Committee

Javier A. Montoya
General and Financial Chair
Universidad de Cartagena, Colombia



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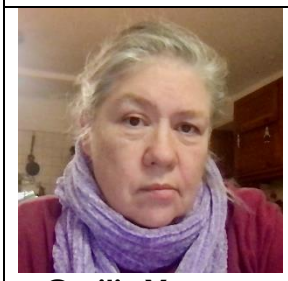
NANOMATERIALS, LOW-DIMENSIONAL SYSTEMS, AND NOVEL MATERIALS		THERMAL, OPTICAL, AND TRANSPORT PROPERTIES	
			
Luis E. F. Foa Torres *International Coordinator* Universidad de Chile, Chile	**Edgar E. Gonzalez** *National Coordinator* Pontificia Universidad Javeriana, Colombia	**Judit Lisoni** *International Coordinator* Universidad Austral de Chile, Chile	**Diogenes Campos** *National Coordinator* Universidad Nacional de Colombia, Colombia

CRYSTAL AND ELECTRONIC STRUCTURE		MAGNETISM, STRONGLY CORRELATED SYSTEMS, COLLECTIVE PHENOMENA, LOW-TEMPERATURE PHYSICS	
			
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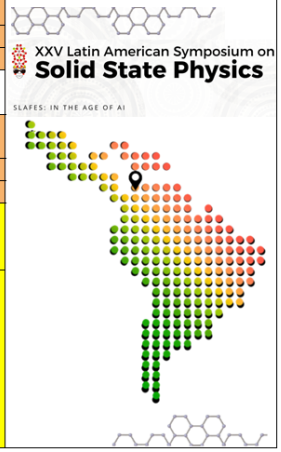
Programme Overview

Start	End	23-oct-24	24-oct-24		25-oct-24		26-oct-24
8:30	8:45	ARRIVAL IN BARRANQUILLA					
8:45	9:00		TOPIC PLENARY Caio LEWENKOPF		SPECIAL TOPIC PLENARY José Luis MORÁN LÓPEZ		
9:00	9:15						SPECIAL TOPIC PLENARY Luis E. F. FOA TORRES
9:15	9:30				TOPIC PLENARY Boris Alfredo MAIOROV		
9:30	9:45		Topic Talk 1.1 Paula GIRALDO-GALLO	Topic Talk 2.1 José Eduardo BARRIOS VARGAS			
9:45	10:00						
10:00	10:15	REGISTRATION FORMALITIES	COFFEE BREAK		COFFEE BREAK		COFFEE BREAK
10:15	10:30						
10:30	10:45		THURSDAY POSTERS SET-UP		Topic Talk 3.3 Ricardo FACCIO	Topic Talk 4.3 Rafael GONZALEZ-HERNANDEZ	SPECIAL TOPIC PANEL
10:45	11:00						
11:00	11:15		Topic Talk 1.2 Eric SUÁREZ MORELL	Topic Talk 2.2 Outmane OUBRAM	Topic Talk 3.4 Ana Cecilia NOGUEZ GARRIDO	Topic Talk 4.4 José Carlos EGUES	
11:15	11:30						
11:30	11:45		Oral Contribution 1.1	Oral Contribution 2.1	Oral Contribution 3.5	Oral Contribution 4.4	SLAFES XXVI VENUE REVEAL Javier MONTOYA
11:45	12:00		Oral Contribution 1.2	Oral Contribution 2.2	Oral Contribution 3.6	Oral Contribution 4.5	
12:00	12:15		Oral Contribution 1.3	Oral Contribution 2.3	Oral Contribution 3.7	Oral Contribution 4.7	CLOSING REMARKS
12:15	12:30		Oral Contribution 1.4	Oral Contribution 2.4	Oral Contribution 3.8	Oral Contribution 4.8	
12:30	12:45		LUNCH		LUNCH		
12:45	13:00						
13:00	13:15						
13:15	13:30						
13:30	13:45	OPENING SESSION					
13:45	14:00						
14:00	14:15		TOPIC PLENARY Andrés SANTANDER SYRO		TOPIC PLENARY Julio MENDOZA ALVAREZ		
14:15	14:30						
14:30	14:45	OPENING PLENARY Ana María LLOIS					
14:45	15:00		Topic Talk 3.1 César ORTEGA	Topic Talk 4.1 Cecila VENTURA	Topic Talk 1.3 Yonatan BETANCUR OCAMPO	Topic Talk 2.2 Ever ORTIZ MUÑOZ	
15:00	15:15						
15:15	15:30	OPENING PLENARY Andrea MARINI	Oral Contribution 3.1	Oral Contribution 4.1	Oral Contribution 1.5	Oral Contribution 2.5	
15:30	15:45		Oral Contribution 3.2	Oral Contribution 4.2	Oral Contribution 1.6	Oral Contribution 2.6	
15:45	16:00		COFFEE BREAK		COFFEE BREAK		
16:00	16:15	COFFEE BREAK					
16:15	16:30		Topic Talk 3.2 Verónica VILDOSOLA	Topic Talk 4.2 Juan Manuel FLOREZ URIBE	Topic Talk 1.4 Diana DULIC	Topic Talk 2.2 Caetano MIRANDA	
16:30	16:45	OPENING PLENARY Yenny HERNÁNDEZ					
16:45	17:00		Oral Contribution 3.3	Oral Contribution 4.3	Oral Contribution 1.7	Oral Contribution 2.7	
17:00	17:15		Oral Contribution 3.4	Oral Contribution 4.4	Oral Contribution 1.8	Oral Contribution 2.8	
17:15	17:30	OPENING PLENARY Bruno CUCCO	POSTER PRESENTATION		POSTER PRESENTATION		
17:30	17:45						
17:45	18:00						
18:00	18:15				SOCIAL ACTIVITY		
18:15	18:30						
18:30	18:45						
18:45	19:00						
19:00	19:15	Topic 1: Nanomaterials, Low-Dimensional Systems, and Novel Materials					
19:15	19:30	Topic 2: Thermal, Optical, and Transport Properties					
19:30	19:45	Topic 3: Crystal and Electronic Structure					
19:45	20:00	Topic 4: Magnetism, Strongly Correlated Systems, Collective Phenomena, Low-Temperature Physics					



Programme

Wednesday, 23 October 2024 — 10:00 – 18:00

10:00 **Registration formalities** *3h30'*

13:30 **Opening Session** *1h*

14:30 **Opening Plenary: Calculating Electronic and Magnetic Properties: A 30-Year retrospective on research in Low Dimensional and Complex Systems** *45'*

Speaker: Ana María LLOIS (Instituto de Nanociencia y Nanotecnología, CNEA-CONICET, Argentina)

15:15 **Opening Plenary: Ab–Initio simulations of equilibrium and out–of–equilibrium phenomena in complex materials: combining High–Performance computational tools with advanced theoretical approaches** *45'*

Speaker: Andrea MARINI (Istituto di Struttura della Materia, National Research Council, Italy)

16:00 **Coffee Break** *30'*

16:30 **Opening Plenary: On the Physical Response of Layered Materials Exfoliated in Liquid Phase: Evidence of Functional Groups and Size-Dependent Features** *45'*

Speaker: Yenny HERNÁNDEZ (Universidad de los Andes, Colombia)

17:15 **Opening Plenary: Materials design and ab initio modeling of novel materials for optoelectronics** *45'*

Speaker: Bruno CUCCO (Center for Quantum Materials Engineering, The University of Texas at Austin, United States)

Thursday, 24 October 2024 — 08:45 – 18:30

08:45 **Topic Plenary: Quantum phase transitions in strongly disordered topological insulators: A coordinate-space analysis** *45'*

Speaker: Caio LEWENKOPF (Universidade Federal Fluminense, Brazil)

	ROOM 1	ROOM 2
09:30	**Topic Talk 1.1: Room temperature multiferroicity in solid solutions of transition metal dichalcogenides** *30'* Speaker: Paula GIRALDO-GALLO (Universidad de Los Andes, Colombia)	**Topic Talk 2.1: Engineering adiabatic pumping in nanostructures** *30'* Speaker: José Eduardo BARRIOS VARGAS (UNAM, Mexico)

10:00 **Coffee Break** *30'*

10:30 **Thursday Poster Set-Up** *30'*

	ROOM 1	ROOM 2
11:00	**Topic Talk 1.2: Electronic localization and its fragility in rotated graphene layers** *30'* Speaker: Eric SUÁREZ MORELL (Universidad Técnica Federico Santa María, Chile)	**Topic Talk 2.2: Transport and magnetoresistance in disordered ferromagnetic superlattices on two-dimensional materials** *30'* Speaker: Outmane OUBRAM (Universidad Autónoma Del Estado de Morelos, Mexico)
11:30	**Contributed Talk 1.1: Hydrogen production using Co-Ni based electrodes obtained from wasted NiMH batteries** *15'* Speaker: Karina PULIDO DE LA CRUZ (Instituto Politécnico Nacional, Mexico)	**Contributed Talk 2.1: Enhancing exciton localization in two-dimensional semiconductors through dielectric environment modification** *15'* Speaker: Kelly Yohana MUÑOZ GOMEZ (Universidad Pedagógica y Tecnológica de Colombia, Colombia)
11:45	**Contributed Talk 1.2: Strong spin-lattice coupling and high-temperature magnetic ordering in monolayer chromium dichalcogenides** *15'* Speaker: Álvaro GONZÁLEZ GARCÍA (Universidad del Norte, Colombia)	**Contributed Talk 2.2: CuNbS3: A First-Principles Exploration of a Potential Photovoltaic Material** *15'* Speaker: Catalina RUIZ VERGARA (Universidad Andrés Bello, Chile)
12:00	**Contributed Talk 1.3: Non-spherical atomic effective pseudopotentials applied to the study of the electronic structure of Si nanowires** *15'* Speaker: Jairo Ricardo CARDENAS (Universidad del Atlántico, Colombia)	**Contributed Talk 2.3: Novel Kagome KMn3Sb5 metal: Chiral magnetism, lattice dynamics, and anomalous Hall conductivity** *15'* Speaker: Andrés Camilo GARCIA CASTRO (Universidad Industrial de Santander, Colombia)
12:15	**Contributed Talk 1.4: Long-Term Analysis of Electromechanical Properties in Cementitious Composites with Copper Nanoparticles** *15'* Speaker: Jorge H. QUINTERO-OROZCO (Universidad Industrial de Santander, Colombia)	**Contributed Talk 2.4: Control of the spin-polarized conductance in a bilayered 2D magnetic CrI3-based device** *15'* Speaker: Carlos Eduardo ARDILA GUTIERREZ (Universidad Industrial de Santander, Colombia)

12:30 **Lunch** *1h30'*

14:00 **Topic Plenary: Imaging the itinerant-to-localised transmutation of electrons across the metal-to-insulator transition** *45'*

Speaker: Andrés SANTANDER SYRO (ISMO, Université Paris-Saclay, Orsay, France)

	ROOM 1	**ROOM 2**
14:45	**Topic Talk 3.1: Strategic co-substitutions to increase magnetization in pristine AlN monolayer** *30'* Speaker: César ORTEGA (Universidad de Córdoba, Colombia)	**Topic Talk 4.1: Modeling Bi-based layered superconductors: electronic properties** *30'* Speaker: Cecilia VENTURA (Centro Atómico Bariloche (CONICET) & UNRN, Argentina)
15:15	**Contributed Talk 3.1: Catalytic activity and sensing properties of the M-MOF74 (M=Mn, Fe, Co) Metal-Organic Frameworks** *15'* Speaker: Victor HOYOS SINCHI (Universidad Andrés Bello, Chile)	**Contributed Talk 4.1: Discontinuous, compensation and hysteresis phenomena in a high-spin Ising-type ferrimagnet: S=3/ Q=7/2** *15'* Speaker: Nicolás DE LA ESPRIELLA VÉLEZ (Universidad de Córdoba, Colombia)
15:30	**Contributed Talk 3.2: Efficacy of vanadium oxide nanoparticles doped with reduced graphene oxide in the photocatalytic degradation of methylene blue** *15'* Speaker: Leydi Julieta CÁRDENAS FLECHAS (Universidad de América, Colombia)	**Contributed Talk 4.2: Formation, generation and stability of magnetic vortex in individual Co85Ni15 nanowires with transversal magnetic anisotropy** *15'* Speaker: Nicolás BARRIOS PIZO (Universidad del Valle, Colombia)

15:45 **Coffee Break** *30'*

	ROOM 1	**ROOM 2**
16:15	**Topic Talk 3.2: Lithium isotopic separation via electrochemical techniques: the role of electronic structure** *30'* Speaker: Verónica VILDOSOLA (CONICET-CNEA (CAC) Buenos Aires, Argentina)	**Topic Talk 4.2: Accelerating the discovery of 2D multiferroics** *30'* Speaker: Juan Manuel FLOREZ URIBE (Universidad Técnica Federico Santa María, Chile)
16:45	**Contributed Talk 3.3: Adsorption and diffusion of lithium, sodium, gallium, and sulfur atoms on the GaS monolayer** *15'* Speaker: Raúl MELÉNDEZ (Universidad de Córdoba, Colombia)	**Contributed Talk 4.3: Pairs and stripes phases in an antiferromagnet within the extended Hubbard model** *15'* Speaker: Uriel Alberto DIAZ REYNOSO (UNAM. Mexico)
17:00	**Contributed Talk 3.4: Effect of defects on the energetics and electronic properties of the (4×4) AlN/(5×5) graphene heterobilayer** *15'* Speaker: Ronald LARA (Universidad de Córdoba, Colombia)	**Contributed Talk 4.4: Study of effect of inclusion of multiwalled carbon nanotubes (MWCNTs) in structural and electrical properties of samples of $YBa_2Cu_3O_{7-\delta}$ (YBCO)** *15'* Speaker: Carlos PIÑEIRO (Universidad del Valle, Colombia)

17:15 **Poster Presentation** *1h15'*

Friday, 25 October 2024 08:45 – 20:00

08:45 **Special Topic Plenary: Understanding the magnetic behavior of Manganese** *30'*

Speaker: José Luis MORÁN LÓPEZ (Instituto Potosino de Investigación Científica y Tecnológica, Mexico)

09:30 **Topic Plenary: To (boldly) measure where no one has measured before: Possibilities for Condensed Matter in Pulsed Magnetic Fields** *45'*

Speaker: Boris Alfredo MAIOROV (Los Alamos National Laboratory, United States)

10:00 **Coffee Break** *30'*

	ROOM 1	ROOM 2
10:30	**Topic Talk 3.3: Nanostructured Titanates: unveiling their unique functional properties** *30'* Speaker: Ricardo FACCIO (Universidad de la República, Uruguay)	**Topic Talk 4.3: Altermagnetism: A novel magnetic phase** *30'* Speaker: Rafael GONZALEZ-HERNANDEZ (Universidad del Norte, Colombia)
11:00	**Topic Talk 3.4: Electronic Interactions on Moiré 2D van der Waals Heterostructures** *30'* Speaker: Cecilia NOGUEZ GARRIDO (UNAM, Mexico)	**Topic Talk 4.4: Quantum oscillations** *30'* Speaker: José Carlos EGUES (Instituto de Física de São Carlos, Brazil)
11:30	**Contributed Talk 3.5: Electronic flat-bands on twisted bilayer Penrose quasicrystals** *15'* Speaker: Ernesto HUIPE DOMRATCHEVA (UNAM, Mexico)	**Contributed Talk 4.5: Magnetic properties of Sr2-xCexFe1+x/2Mo1-x/2O6 double perovskite system** *15'* Speaker: Diana Litzajaya GARCÍA-RUIZ (UNAM, Mexico)
11:45	**Contributed Talk 3.6: MOF-5 Organometallic Structure as a Sensor for Pollutant Gas Detection** *15'* Speaker: Pedro SOUZA (Universidad Andres Bello, Chile)	**Contributed Talk 4.6: Order-disorder dynamic phase transition in a magnetite nanoparticle and its relationship with magnetic hyperthermia: A micromagnetic approach** *15'* Speaker: Johans RESTREPO (Universidad de Antioquia, Colombia)
12:00	**Contributed Talk 3.7: Ab-initio study of topological properties of A3BO Antiperovskites** *15'* Speaker: Joan Sebastián IBAÑEZ SOTELO (Universidad Nacional de Colombia, Colombia)	**Contributed Talk 4.7: Ge-NW/LaTiO3 nanostructured materials** *15'* Speaker: Eliel CARVAJAL (Instituto Politécnico Nacional, ESIME-Cul., Mexico)
12:15	**Contributed Talk 3.8: High field magnetotransport measurements of the topological semi-metal and charge density wave compound TaTe4** *15'* Speaker: Diego Felipe SILVERA VEGA (Universidad de Los Andes, Colombia)	**Contributed Talk 4.8: Local symmetry of Co, in Co-Doped ZnO Nanocrystals** *15'* Speaker: Ovidio ALMANZA (Universidad Nacional de Colombia, Colombia)

12:30 **Lunch** *1h30'*

14:00 **Topic Plenary: GaSb-based Semiconductors for Optoelectronic Device Applications in the Mid-Infrared Spectral Region** *45'*

Speaker: Julio MENDOZA ALVAREZ (CINVESTAV-IPN, Mexico)

	ROOM 1	**ROOM 2**
14:45	**Topic Talk 1.3: Atomically thin current pathways in graphene through Kekulé-O engineering** *30'* Speaker: Yonatan BETANCUR OCAMPO (UNAM, Mexico)	**Topic Talk 2.3: On the high-temperature phase transition of Rb3H(SeO4)2: A polymorphic-superprotonic phase transition?** *30'* Speaker: Ever ORTIZ MUÑOZ (Universidad del Atlántico, Colombia)
15:15	**Contributed Talk 1.5: Optimization of photovoltaic cell properties and efficiency by incorporating functional groups into π-conjugated triphenylamine molecules** *15'* Speaker: Jonathan ROMERO ATENCIO (Universidad del Atlántico, Colombia)	**Contributed Talk 2.5: Electrical analysis of Caseinate-Borax biofilms** *15'* Speaker: Nayda Patricia ARIAS DUQUE (Universidad de Sucre, Colombia)
15:30	**Contributed Talk 1.6: Decoherence effects on quantum transport through topological domain walls** *15'* Speaker: Ricardo Yael DÍAZ BONIFAZ (UNAM, Mexico)	**Contributed Talk 2.6: Solid-state mechanisms enhancing fire resistance in niobium and boron alloyed structural steels** *15'* Speaker: Edwan Anderson ARIZA ECHEVERRI (Universidad del Magdalena, Colombia)

15:45 **Coffee Break** *30'*

	ROOM 1	**ROOM 2**
16:15	**Topic Talk 1.4: Designing a "perfect" porphyrin molecule for the Mechanically Controllable Break Junction Experiments** *30'* Speaker: Diana DULIC (Universidad de Chile, Chile)	**Topic Talk 2.4: Virtual Worlds, Real Solutions: Multiscale Materials Design for Global Challenges** *30'* Speaker: Caetano MIRANDA (Instituto de Física, USP, Brazil)
16:45	**Contributed Talk 1.7: Study and optimization of electronic and structural properties of two-dimensional materials (MXenes) for energy generation and storage through first-principles calculations** *15'* Speaker: Nicolás FORERO (Universidad de la Frontera, Chile)	**Contributed Talk 2.7: Propagation of electromagnetic waves throngs a bi-periodic 1D dielectric-graphene photonic crystal** *15'* Speaker: Jesús MADRIGAL-MELCHOR (Universidad Autónoma de Zacatecas, Mexico)
17:00	**Contributed Talk 1.8: Ferroelectric switching in monolayer WSe2 via concurrent antisite and vacancy defects. A DFT study.** *15'* Speaker: Camilo ESPEJO (Universidad del Norte, Colombia)	**Contributed Talk 2.8: Enantiospecific electron transport in chiral-modified molecular junctions** *15'* Speaker: Omar HERNÁNDEZ MONTES (UNAM, Mexico)

17:15 **Poster Presentation** *45'*

18:00 **Social Activity** *2h*

Saturday, 26 October 2024 09:00 – 12:30

09:00 **Navigating Peer Review: Critical Tips for Authors** *1h*

Speaker: Luis E. F. FOA TORRES (Universidad de Chile, Chile)

10:00 **Coffee Break** *30'*

10:30 **Promoting science exchange through networks** *1h*

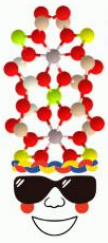
Panelists: Nayda Patricia ARIAS DUQUE (Universidad de Sucre, Colombia), Oracio NAVARRO (UNAM, Mexico), Javier MONTOYA (Universidad de Cartagena, Colombia), Eric SUÁREZ MORELL (Universidad Técnica Federico Santa María, Chile)

11:30 **SLAFES XXVI venue reveal** *30'*

Chair: Javier MONTOYA (Universidad de Cartagena, Colombia)

12:00 **Closing remarks** *30'*

KEYNOTE LECTURES



XXV Latin American Symposium on

Solid State Physics

Barranquilla, October 23 to 26, 2024

Special Plenaries

CALCULATING ELECTRONIC AND MAGNETIC PROPERTIES: A 30-YEAR RETROSPECTIVE ON RESEARCH IN LOW DIMENSIONAL AND COMPLEX SYSTEMS

Ana María Llois

Instituto de Nanociencia y Nanotecnología, CNEA-CONICET, Argentina

Inaugural Lecture

AB–INITIO SIMULATIONS OF EQUILIBRIUM AND OUT–OF–EQUILIBRIUM PHENOMENA IN COMPLEX MATERIALS: COMBINING HIGH–PERFORMANCE COMPUTATIONAL TOOLS WITH ADVANCED THEORETICAL APPROACHES

A. Marini[1]

[1]*Istituto di Struttura della Materia and Division of Ultrafast Processes in Materials (FLASHit) of the National Research Council, via Salaria Km 29.3, I-00016 Monterotondo Stazione, Italy*

FLASH (Free Electron Laser in Hamburg) and Lumi (Large Unified Modern Infrastructure) my appear as the opposite sides of the moon. They are both key actors in the world of tools used by material science researchers but they couldn't appear to be more further away.

Lumi is a petascale supercomputer located at the CSC data center in Kajaani, Finland. As of January 2023, the computer is the fastest supercomputer in Europe. Similarly FLASH is the world's first Free Electronc Laser (FEL). It is part of the Desy Synchrotron and has provided extremely bright, coherent and ultra-short XUV pulses for a broad science programme conducted by scientists from all over the world since 2005.

In this talk I will discuss how the physics investigated in ultra–fast Pump&Probe experiments can connect Lumi and FLASH providing an unprecedent insight in the elemental processes occurring at the microscopic atomic scale on a ultra–short time–scale. I will briefly review the Ab Initio Many–Body Perturbation Theory (Ai–MBPT) [5] and Ab Initio Non Equilibrium Green's Function Theory (Ai–NEGF) [4]. I will then discuss how High–Performance Centers (HPC) resources can help in investigating regimes of matter and of theory, almost impossible to access using paper and pencil or a standard, even if large, Beowulf cluster.

I will describe the actual implementation of the Ai–MBPT and Ai–NEGF in the Yambo [1;8] code discussing some recent numerical and methodological developments that have been implemented towards to exploitation of next generation HPC supercomputers.

I will also illustrate some recent results [2;3;6;7;9] obtained with yambo highlighting some challenges and open problems that are the focus of my theoretical and numerical reserach.

References

[1] M. G. D. V. Andrea Marini, Conor Hogan. yambo: An ab initio tool for excited state calculations. Computer Physics Communications, 180:1392–1403, 2009.

[2] A. Marini. Equilibrium and out-of-equilibrium realistic phonon self-energy free from overscreening. Phys. Rev. B, 107, 2023.

[3] A. Marini. Nonadiabatic effects lead to the breakdown of the semiclassical phonon picture. Phys. Rev. B, 110, 2024.

[4] A. Marini, E. Perfetto, and G. Stefanucci. Coherence and de-coherence in the time-resolved arpes of realistic materials: An ab-initio perspective. Journal of Electron Spectroscopy and Related Phenomena, 257:147189, 2022.

[5] G. Onida, L. Reining, and A. Rubio. Electronic excitations: density-functional versus many-body green's-function approaches. Rev. Mod. Phys., 74(2):601–659, Jun 2002.

[6] F. Paleari and A. Marini. Exciton-phonon interaction calls for a revision of the "exciton" concept. Phys. Rev. B, 106:125403, Sep 2022.

[7] F. Pressacco, D. Sangalli, V. Uhlír, D. Kutnyakhov, J. A. Arregi, S. Y. Agustsson, G. Brenner, H. Redlin, M. Heber, D. Vasilyev, J. Demsar, G. Schönhense, M. Gatti, A. Marini, W. Wurth, and F. Sirotti. Subpi-cosecond metamagnetic phase transition in ferh driven by non-equilibrium electron dynamics. Nat Commun, 12:69, 2021.

[8] D. Sangalli, A. Ferretti, H. Miranda, C. Attaccalite, I. Marri, E. Cannuccia, P. M. Melo, M. Marsili, F. Paleari, A. Marrazzo, G. Prandini, P. Bonfà, M. O. Atambo, F. Affinito, M. Palummo, A. M. Sanchez, C. Hogan, M. Grüning, D. Varsano, and A. Marini. Many-body perturbation theory calculations using the yambo code. Journal of Physics: Condensed Matter, 31:325902, 2019.

[9] V. Smejkal, F. Libisch, A. Molina-Sanchez, C. Trovatello, L. Wirtz, and A. Marini. Time-dependent screening explains the ultrafast excitonic signal rise in 2d semiconductors. ACS Nano, 15:1179–1185, 2021.

ON THE PHYSICAL RESPONSE OF LAYERED MATERIALS EXFOLIATED IN LIQUID PHASE: EVIDENCE OF FUNCTIONAL GROUPS AND SIZE-DEPENDENT FEATURES

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Liquid phase exfoliation of layered materials has shown great potential for various applications [1]. However, challenges remain, such as the need for a wide range of organic solvents and the broad distribution of flake thicknesses [2]. These challenges can be mitigated by incorporating intercalation steps, like electrochemical or solvothermal expansion, which result in thinner crystals within the dispersion [2, 3]. In this talk, I will discuss the impact of electrochemical exfoliation on the basal functionalization of graphene and propose a more accurate method for determining the optical extinction coefficient based on oxidation levels, aimed at standardization [4]. Additionally, I will present examples of MoS2 and WS2 exfoliated through ultrasonication, highlighting their non-linear optical effects in fluorescence spectroscopy [5]. Finally, I will explore how crystal-size selection influences the piezoresistive and photoconductive responses of MoS2 and WS2 exfoliated via lithium intercalation.

References:

[1] Yenny Hernandez, et al, Nature Nanotechnology, 3, 563–568 (2008)

[2] Jonathan N. Coleman et al. Science 331, 568-571 (2011)

[3] Zhongfen Ding, et al, J. Mater. Chem., 2009, 19, 2588-2592 (2009)

[4] Khaled Parvez, et al, ACS Nano 2013, 7, 4, 3598–3606 (2013)

[5] J Rico, et al, J. Phys.: Condens. Matter 34 105701 (2022)

[6] Gabriel Cardenas-Chirivi, et al, Optical Materials, 133,112890 (2022)

Keywords: *graphene, 2D materials, TMDs*

MATERIALS DESIGN AND AB INITIO MODELING OF NOVEL MATERIALS FOR OPTOELECTRONICS

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Halide perovskites (HP) arose as formidable building blocks for optoelectronic applications setting record-breaking solar cell performances. The combination of 3D HP with their layered (2D) counterparts allowed for harvesting the high efficiency of the 3D materials while maintaining the high stability of layered compounds. However, it is well-known that layered HP exhibits considerably poorer carrier transport than 3D HP, and to date, the mechanisms underlying these lower mobilities remain unknown. In this work, we employ a combination of state-of-the-art many-body approaches and symmetry analysis to investigate the electron-phonon coupling (EPC) origin in layered halide perovskites. By modeling layered and 3D perovskites, we demonstrate that the origin of low carrier mobilities in layered systems primarily originates from differences in the carrier's lifetimes. The vibrational modes contributing to carrier scattering are identified via EPC symmetry analysis. Finally, we show that the carrier mobilities are mostly limited by an abrupt increase in the electronic density of states near the band edges. These findings provide a fundamental understanding of the EPC mechanisms intrinsically limiting the charge carrier transport of layered HP, providing pathways for device improvement.

Keywords: *DFT, semiconductor, Perovskites, Optoelectronics, electron-phonon*

UNDERSTANDING THE MAGNETIC BEHAVIOR OF MANGANESE

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The applications of manganese to current technological devices have grown appreciably in recent years. The multifarious magnetic behavior makes this chemical element one of the most studied. Due to the competing effects, the maximization of the spin magnetic moment imposed by the Hund rule, and of the bond distance, make Mn systems extremely sensitive to the atomic environment. In this contribution I make a short review of the particular magnetic behavior of manganese and the efforts to understand the physical basis.

Keywords: *magnetic materials, nanomaterials, magnetic alloys*

NAVIGATING PEER REVIEW: CRITICAL TIPS FOR AUTHORS

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In today's competitive scientific landscape, successfully navigating the peer review process is crucial for researchers aiming to publish their work in different journals. This talk will offer insights drawn from both sides of the editorial desk. From crafting compelling abstracts and responding effectively to reviewer comments, to understanding what editors look for in submissions, this presentation will provide practical, actionable advice. Whether you're an early-career researcher or an established scientist, these tips will help you navigate the complexities of peer review and hopefully increase the visibility of your research.

Keywords: *Peer review.*

Nanomaterials, Low-Dimensional Systems, and Novel Materials

QUANTUM PHASE TRANSITIONS IN STRONGLY DISORDERED TOPOLOGICAL INSULATORS: A COORDINATE-SPACE ANALYSIS

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Topological materials are characterized by topological invariants whose evaluation usually relies on translational symmetry. As a consequence, the natural question that arises is: Can strongly disordered, non-crystalline, and amorphous display topological properties? Substantial theoretical work show that this is indeed the case. After a brief review on the tools to characterize topological phases, I will discuss the most important recent advances in the research of strongly disordered and/or amorphous topological insulators, with focus on our ab initio studies that aim at proposing physical realizations of amorphous topological insulators. Next, I will show how topological phase transitions can be understood in terms of insights obtained from a real-space analysis using simple lattice models, both for Anderson disorder [1] and amorphous systems [2]. Finally, I will introduce a new mathematically rigorous real-space topological indicator that allows one to characterize topological phases of strongly disordered, amorphous, and/or alloy systems.

References:

[1] B. D. Assunção, G. J. Ferreira, C. H. Lewenkopf, Phase transitions and scale invariance in topological Anderson insulators, Physical Review B 109, L201102 (2024).

[2] V. Regis, V. Velasco, M. B. Silva Neto, C. Lewenkopf, Structure-driven phase transitions in paracrystalline topological insulators, Physical Review B 110, L161105 (2024).

[3] C. S. Setescak, C. Lewenkopf, M. Ludewig, Coarse geometric approach to topological phases: Invariants from real-space representations, arXiv:2407.16494 (2024).

Keywords: *topological systems, topological phase transitions.*

Thermal, Optical, and Transport Properties

GASB-BASED SEMICONDUCTORS FOR OPTOELECTRONIC DEVICE APPLICATIONS IN THE MID-INFRARED SPECTRAL REGION

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InxGa1-xAsySb1-y quaternary epitaxial layers have been grown by the liquid phase epitaxy technique (LPE) in which the bandgap energy of the semiconductor layers can be tuned, by changing the layer stoichiometry of the growth melt, between 1.71 and 4.2 μm under lattice-matched conditions. These InGaAsSb layers have been used for fabricating optoelectronic devices such as semiconductor lasers and infrared photodetectors. For these purposes, a precise control on the layer doping to obtain n- and p-type quaternary layers, and in the growth conditions to get high crystalline quality layers are essential for device applications. We present results on InGaAsSb high quality lattice-matched layers to GaSb substrates, studied by High-Resolution X-ray Diffraction, Atomic Force Microscopy, Low Temperature Photoluminescence, and Raman Spectroscopy; we have studied lateral strain effects as the As content in the layers is changed. Also, we present results on the controlled doping of these InGaAsSb layers with Te and Si to get high quality n-and p-type quaternary semiconductors, and we show results on the fabrication of a p-n photodetector with peak spectral responsivity around 2.03 μm.

Crystal and Electronic Structure

IMAGING THE ITINERANT-TO-LOCALISED TRANSMUTATION OF ELECTRONS ACROSS THE METAL-TO-INSULATOR TRANSITION IN V2O3

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According to the "Standard Model of Condensed-Matter Physics", the Bloch theory, metal or insulator are mutually exclusive states of matter. In insulators the highest occupied quantum-mechanical energy band is totally filled with electrons, while in metals it is partially filled. Thus, as temperature cannot change the number of electrons in a solid, it should not change either its intrinsic nature, i.e. metallic or insulating. However, V_2O_3 , a metal at room temperature, shows a first-order metal-to-insulator transition (MIT) when cooling below , with an abrupt resistivity change of over six orders of magnitude. The very existence of a metal-to-insulator transition shakes the foundations of the well-tested Bloch model!

In fact in V_2O_3 , as in many other transition-metal oxides, the last partially filled band is formed out of d-orbitals, which are rather localized in space. Thus, electrons in these bands can hardly avoid each other, and are subject to their strong mutual repulsion –the electron correlations, neglected in Bloch theory. The strong repulsion between electrons can inhibit their movement and result in a "Mott" metal-to-insulator transition (MIT), a fundamental phenomenon whose understanding has remained a challenge for over 50 years. A key issue is how the wave-like itinerant electrons in the metallic state change into a localized-like state in the insulator due to increased interactions. However, observing the MIT in terms of the energy- and momentum-resolved electronic structure of the system, the only direct way to probe both itinerant and localized states, has been elusive.

In this talk, I will discuss our recent experimental studies of the MIT in V_2O_3 [1] using angle-resolved photoemission spectroscopy. We found that in this material the temperature-induced MIT is characterized by the progressive disappearance of the conduction band of itinerant electrons, without any change in its energy-momentum dispersion, and the simultaneous shift to larger binding energies of a quasi-localized state initially located near the Fermi level. Only when the state of itinerant electrons crossing the Fermi level has vanished, a complete gap of about 700 meV is observed, associated to the final energy position of the quasi-localized state. Furthermore, the spectral weights of the itinerant and quasi-localized states show a clear thermal hysteresis that tracks the one observed in resistivity data across the MIT.

References

[1] M. Thees et al., Science Advances 7, eabj1164 (2021).

Keywords: *Correlated electron systems, metal-insulator transition, photoemission spectroscopy.*

Magnetism, Strongly Correlated Systems, Collective Phenomena, Low-Temperature Physics

TO (BOLDLY) MEASURE WHERE NO ONE HAS MEASURED BEFORE: POSSIBILITIES FOR CONDENSED MATTER IN PULSED MAGNETIC FIELDS

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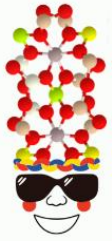
Magnetic field is one of the principal variables we can change to study condensed matter. The generation of strong magnetic fields is also key for a large number of applications such as MRIs, Maglebs, rails gun, material growth, and isotope separation.

However, accessing repeatedly and non-destructively magnetics fields above 40T requires pulsed magnetic fields, which bring problem with fast changing magnetic fields, high-vibration environment, large electrical noise and short amount of time for measurements. These conditions require developing unique techniques to solve such exceptional challenges. In this talk I will show several examples of techniques and systems where pulsed fields can access.

In particular, the promise of fusion technology enabled by high magnetic fields produced by high temperature superconductors flexible tapes and recent records in all-superconducting magnets reinforce the need to study critical current density (J_c) in magnetic fields above 30T. Achieving J_c measurements in pulsed magnetic fields provides a tool for this. Using Fast Programmable Gate Array electronics, we measured reproducible current–voltage curves (I-V) in different superconductor thin films on single crystals and metal substrates grown by different methods. We show it is possible to measure J_c in high pinning coated conductors up to 65T. We compare measurements in two of the magnet systems available at Los Alamos Pulsed Field Facility of the National High Magnetic Field Laboratory and show that we are now able to measure J_c continuously as a function of field (H) in our newly commissioned mid-pulse magnet. We explore extending J_c determination to higher dH/dt and compare the J c performance of standard samples and those with nanoparticle additions, and irradiated samples that are key to predict the performance and lifespan of compact fusion reactors.

Keywords: *pulsed high Magnetic Fields, superconductors, critical currents*

TOPIC TALKS



XXV Latin American Symposium on

Solid State Physics

Barranquilla, October 23 to 26, 2024

Nanomaterials, Low-Dimensional Systems, and Novel Materials

ROOM TEMPERATURE MULTIFERROICITY IN SOLID SOLUTIONS OF TRANSITION METAL DICHALCOGENIDES

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The coexistence of multiple ferroic orders, i.e. multiferroicity, is a scarce property to be found in materials. Historically, this state has been found mainly in 3-dimensional complex oxides, but so far this state has still been elusive for the most widely studied and characterized family of 2-dimensional compounds, the transition metal dichalcogenides (TMDs). In this talk we will introduce the strategy of alloying compounds that are solely ferromagnetic and ferroelectric in order to achieve multiferroicity in 2-dimensional van der Waals materials. This strategy has resulted in the first experimental realization of multiferroic states in the family of the TMDs, at room temperature, in bulk single crystals of the solid solution of WSe 2 and WTe 2 . We observe the coexistence of ferromagnetism and ferroelectricity through the presence of magnetization and piezoresponse force microscopy hysteresis loops. We will also present our recent results in the search for other multiferroic solid solutions among these van der Waals materials. Our findings open the possibility of widening the use and study of van der Waals-based multifunctional devices for new nanoelectronics and spintronics applications.

References:

[1] G. Cardenas-Chirivi, K. Vega-Bustos, H. Rojas-Páez, D. Silvera-Vega, J. Pazos, O. Herrera, M.A. Macías, C. Espejo, W. López-Pérez, J. A. Galvis, and P. Giraldo-Gallo. "Room temperature multiferroicity in a transition metal dichalcogenide". npj 2D Mat. and Appl. 7 (2023) 54.

Keywords: *Multiferroicity, van der Waals materials, transition metal dichalcogenides, ferromagnetism, ferroelectricity, solid solutions*

ELECTRONIC LOCALIZATION AND ITS FRAGILITY IN ROTATED GRAPHENE LAYERS

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In this presentation, I explore the electronic localization and its fragility in rotated graphene layers, specifically the superconductivity in multiple graphene layers, by analyzing the behavior of various structures, such as twisted bilayer, trilayer, and double twisted bilayer graphene. We show the relationship between the rotation angles of these layers and the presence or absence of superconductivity, finding that only certain specific structures lead to superconductivity states. The presentation further discusses the role of edge states in moiré structures and the impact of electric fields on these systems.

Keywords: *Superconductors, twisted bilayer graphene, Multilayer graphene.*

ATOMICALLY THIN CURRENT PATHWAYS IN GRAPHENE THROUGH KEKULÉ-O ENGINEERING

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We demonstrate that the current flow in graphene can be guided on atomically thin current pathways by the engineering of Kekulé-O distortions. A grain boundary in these distortions separates the system into topologically distinct regions and induces a ballistic domain-wall state. The state is independent of the orientation of the grain boundary with respect to the graphene sublattice and permits guiding the current on arbitrary paths. As the state is gapped, the current flow can be switched by electrostatic gates. Our findings are explained by a generalization of the Jackiw–Rebbi model, where the electrons behave in one region of the system as Fermions with an effective complex mass, making the device not only promising for technological applications but also a test-ground for concepts from high-energy physics. An atomic model supported by DFT calculations demonstrates that the system can be realized by decorating graphene with Ti atoms.

Keywords: *Quantum transport, Graphene, Kekulé distortions, Solitons, Jackiw-Rebbi model.*

DESIGNING A "PERFECT" PORPHYRIN MOLECULE FOR THE MECHANICALLY CONTROLLABLE BREAK JUNCTION EXPERIMENTS

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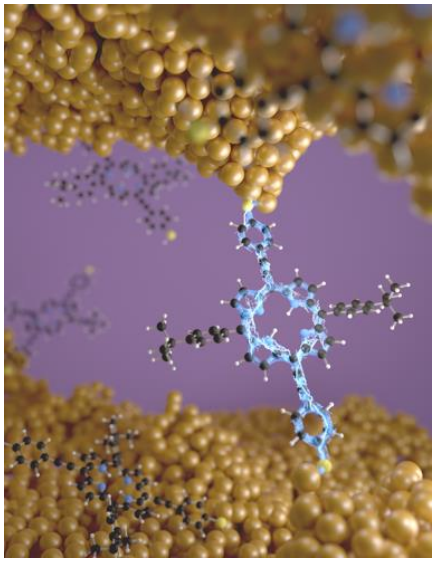
The biggest challenge of molecular electronics is to condense the functionality of an electronic device into a single molecule and to exploit the functional versatility offered by the chemical diversity of molecules for electronic device purposes.

Porphyrins and their related macrocycles are promising building blocks for the construction of bio-inspired molecular devices. Nature itself offers magnificent examples of porphyrin usefulness, such as activating and transporting molecular oxygen in mammals and harnessing sunlight in plant photosynthetic systems.

In spite of their potential, obtaining well defined single-molecule conductance features is a difficult task. Due to π-stacking porphyrins can form a variety of junction configuration, leading to a large spread in conductance values using the mechanically controllable break junctions (MCBJ) technique. This limits the further progress in investigating the molecular functionalities on a single molecule level in porphyrin molecules.

In this presentation, I will show that by close interaction between synthetic chemists and physicists a "perfect" porphyrin molecular design for mechanically controllable break junctions can be achieved, leading to well defined, highly conducting molecular junctions. This opens further prospects for studying mechano-sensitive porphyrin based molecular junctions.



Thermal, Optical, and Transport Properties

ENGINEERING ADIABATIC PUMPING IN NANOSTRUCTURES

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The bulk-boundary correspondence links the topological properties of a material's bulk to its edge states. Edge states can be adjusted by modifying the boundary. Using a higher-order topological Hamiltonian, we set up a one-corner state that can move between corners with a periodic parameter, acting as a pumping mechanism. We characterized this state by the inverse participation ratio and associated it with a topological invariant, proving it has a topological origin. Our results are published in Phys. Rev. B 109, 085402 (2024).

Acknowledgments: We gratefully acknowledge funding from CONAHCYT Proyecto Frontera 428214.

Keywords: *Geometric & topological phases, Kagome lattice, Su-Schrieffer-Heeger model.*

TRANSPORT AND MAGNETORESISTANCE IN DISORDERED FERROMAGNETIC SUPERLATTICES ON TWO-DIMENSIONAL MATERIALS

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Ballistic transport and tunneling magnetoresistance (TMR) in disordered ferromagnetic superlattices on two-dimensional materials, such as silicene and phosphorene, have been investigated [1-3]. It is fundamental to consider the effects of both voluntary and involuntary disorder on transport and magnetoresistance properties in large-scale manufacturing devices on 2D materials. The studies focus on the effects of structural disorder on the width and height of the electrostatic barrier potential and the magnetic field. A low-energy Hamiltonian derived from the tight-binding model was employed. The electronic transport properties, including transmission, conductance, polarization, and magnetoresistance, are calculated using the transfer matrix technique, the Landauer-Büttiker formalism, and the MRT relation. It is found that both the type and intensity of structural disorder can either suppress or enhance transport and TMR properties[1-3]. Moreover, achieving precise transport and tunneling magnetoresistance requires rigorous control over fluctuations in externally applied fields.

References:

[1] Oubram, O. "Gap engineering effects on transport and tunneling magnetoresistance properties in phosphorene ferromagnetic/normal/ferromagnetic junction." Journal of Physics: Condensed Matter 36.22 (2024): 225302.

[2] Guzmán, E. J., et al. "Disorder effects on the ballistic transport of gated phosphorene superlattices." Physical Rseview B 107.4 (2023): 045407.

[3] Oubram, O., et al. "Improvement of tunneling magnetoresistance and spin-valley polarization in magnetic silicene superlattices induced by structural disorder." Physical Review B 105.11 (2022): 115408.

Keywords: *Structural disorder, Transport, Transmission, conductance, Magnetoresistance.*

ON THE HIGH-TEMPERATURE PHASE TRANSITION OF RB3H(SEO4)2: A POLYMORPHIC-SUPERPROTONIC PHASE TRANSITION?

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A comprehensive study was conducted to investigate the phase transition of trirubidium hydrogen biselenate [$Rb_3H(SeO_4)_2$] from a low-symmetric monoclinic phase, which exhibits low proton conductivity, to a high-symmetric triclinic phase, known for its superprotonic conductivity [1, 2]. This transition occurs within the temperature range of 173 to 183 °C. Using impedance spectroscopy, modulated differential scanning calorimetry, simultaneous thermogravimetric and differential thermal analysis, and temperature-dependent X-ray diffraction, we analyzed the nature of this transformation. Our findings indicate that the enthalpy change observed at this temperature, previously attributed to a bulk triclinic superprotonic conducting phase transition, is instead due to chemical-surface thermal decomposition. Consequently, we propose that the reported triclinic superprotonic conducting phase in $Rb_3H(SeO_4)_2$ does not actually occur. Instead, the surface of the sample undergoes decomposition, resulting in the formation of solid crystalline Rb_2SeO_4, a liquid phase, and a gas phase. To our knowledge, this is the first study questioning the existence of the triclinic superprotonic conducting phase in this solid acid.

References:

[1] Baranov AI, Makarova IP, Muradyan LA, Tregubchenko AV, Shuvalov LA, Simonov VI. Phase transitions and proton conductivity in Rb3H(SeO4)2 crystals. So. Phys Crystallogr. 1987;32:400-7.

[2] Goñi-Urtiaga A, Presvytes D, Scott K. Solid acids as electrolyte materials for proton exchange membrane (PEM) electrolysis: Review. Int J Hydrog Energy. 2012;37:3358–72.

Keywords: *$Rb_3H(SeO_4)_2$, superprotonic conducting phase transition, thermal surface decomposition.*

VIRTUAL WORLDS, REAL SOLUTIONS: MULTISCALE MATERIALS DESIGN FOR GLOBAL CHALLENGES

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This work explores advancements in multiscale materials design to address global challenges in sustainable energy and environmental applications. By integrating atomistic and macroscale simulations, techniques like molecular dynamics, density functional theory, and computational screening guide material selection and experimental designs. Focus areas involve carbon capture and lithium/boron separation from produced water using innovative materials such as graphene-based membranes and metal-organic frameworks. Advanced characterization methods, including X-ray diffraction at synchrotron Sirius facility in Brazil and pilot-scale testing, ensure scalability and industrial applicability, bridging computational insights with practical solutions. We also introduce The RCGI Digital Lab, which leverages virtual and augmented reality to foster an immersive understanding of nanoscale phenomena. Interactive molecular dynamics and machine learning accelerate material discovery, particularly for energy and CO_2 utilization applications. This interdisciplinary approach, combining computational tools, experimental validation, and risk analysis, highlights the potential of sustainable technologies to mitigate climate change impacts while addressing economic and technological challenges. Acknowledgments: This project has the support of Fapesp, CNPq, and Petronas Petróleo Brasil Ltda (PPBL) within the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R& D levy regulation.

Keywords: *Materials Design, Multiscale molecular Simulations, Virtual Reality.*

Crystal Structure Prediction

STRATEGIC CO-SUBSTITUTIONS TO INCREASE MAGNETIZATION IN PRISTINE ALN MONOLAYER

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This study examines the co-substitutions of aluminum (Al) and nitrogen (N) with manganese (Mn) and oxygen (O), respectively, in the hexagonal planar AlN monolayer in the 4x4 hexagonal geometry (h-AlN (0001)4x4). The calculations are performed using density functional theory (DFT) along with atomic pseudopotentials and a plane wave basis set. The monolayer is modeled using the periodic slab approach. First, the substitutions of Al and N atoms with Mn and O, respectively, are carried out separately. Second, two separate co-substitutions of Al and N atoms with Mn and O, respectively, are performed. In the first case, the Al and N atoms are co-substituted with Mn and O atoms at a sufficiently large distance (≈14.54 Å) so that the Mn and O impurities do not interact. In the second case, the co-substitutions are placed at a sufficiently small distance so that the Mn and O impurities do interact. In all cases, the thermodynamic stability of the h-AlN monolayer with and without Mn and/or O impurities is established through formation energies.

The electronic properties of the h-AlN monolayer with and without Mn and/or O impurities are analyzed through DOS and Löwdin charge. When a N atom is substituted with O, the monolayer does not exhibit magnetic properties, while substituting an Al atom with Mn results in magnetic properties with a total magnetization of 4.0 μ 0/cell.

In both cases, involving interacting and non-interacting (Mn-O) atomic pairs, the monolayer exhibits magnetic properties, with a total magnetization of 5.0 μ 0/cell and 4.9 μ 0/cell, respectively. From these results, it is inferred that when Mn and O impurities interact, the magnetization in the codoped AlN monolayer increases compared to the case where the impurities do not interact.

Keywords: *h-AlN (0001) 4x4 monolayer, thermodynamic stability, DOS, Bader charge, Löwdin charge, DFT (GGA).*

LITHIUM ISOTOPIC SEPARATION VIA ELECTROCHEMICAL TECHNIQUES: THE ROLE OF ELECTRONIC STRUCTURE

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Natural lithium comprises two stable isotopes, ^{7}Li and ^{6}Li; materials enriched in each become crucial in various nuclear technologies due to their distinct neutron capture cross-sections. In recent years, electrochemical techniques have been revisited as efficient, environmentally friendly methods for lithium isotope separation. However, the role played by physicochemical variables—such as applied overpotential, electrolyte composition, or electrode materials—in the separation factor is still not well understood. In this talk, we demonstrate that electronic structure analysis through Density Functional Theory (DFT) simulations is essential for understanding how the electrode material and morphology of deposited lithium affect isotopic separation. We consider the isotopic equilibrium exchange reaction between two phases present in an electrochemical cell: strongly solvated lithium in solution on one side and adsorbed or inserted lithium on metallic substrates or layered carbon materials used as the cathode on the other. The results suggest a strong correlation between the strength of lithium bonds (deposited or inserted) and the resulting fractionation. We will describe different experimetal and theoretical results, considering metallic planar cathodes as nickel and gold, and hard carbons. We will show that providing a realistic description of the chemical bonds through DFT calculations can guide the development of improved electrochemical processes for lithium isotope separation, clarifying the roles of lithium morphology and its relationship with the cathode material.

Keywords: *DFT, lithium isotopic separation, electrochemical techniques*

NANOSTRUCTURED TITANATES: UNVEILING THEIR UNIQUE FUNCTIONAL PROPERTIES

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Dye-sensitized solar cells (DSSCs) exemplify how nanotechnology has contributed to developing renewable energies. The commonly used semiconductors need a good specific surface area and suitable optical properties. This positions TiO_2 and its derived titanates favorably for use in different nanostructures and aspect ratios [1]. Additionally, titanates can be used as electrolytes in lithium-ion and sodium-ion batteries, where their response to electrical and ionic transport is studied. This work presents results integrating simulation and experimentation for synthesizing and characterizing titanate nanotubes (NTs). Their structural characterization [2] and the assembly and electrical characterization of DSSC prototypes will also be shown, using the synthesis reactant and product as photoelectrodes and a potential electrolyte in batteries [3-5]. Structural characterization uses conventional X-ray diffraction and small-angle X-ray scattering (SAXS), TEM, atomic force microscopy (AFM), and Raman confocal microscopy. This information is combined with that obtained from computational simulation [6-9], which provides insights into the NTs' superstructure, morphology, and critical electronic properties [3, 10, 11]. DSSC prototypes are evaluated through I-V curves to determine photovoltaic conversion efficiency and impedance spectroscopy studies are conducted to analyze charge transfer phenomena. The NT-based prototypes performed better than anatase-based standards, with 8% and 6% efficiency rates, respectively [5, 10, 12]. The synthesized nanotubes were electronically characterized to assess their performance as electrolytes in lithium-ion and sodium-ion batteries [3, 5, 10, 11]. This presentation summarizes the most important characteristics of titanate nanotubes for energy applications, highlighting the role of computational simulation in understanding their relevant physical and structural properties at the nanoscale.

References:

[1] R. Faccio, L. Fernandez-Werner, et al., Recent Pat Nanotechnol, 5 (2011) 46-61.

[2] L. Fernández-Werner, F. Pignanelli, et al., Journal of Energy Storage, 12 (2017) 66-77.

[3] L. Amy, S. Favre, et al., Materials Today Communications, 33 (2022) 104908.

[4] J. Juan, L. Fernández-Werner, et al., Appl. Surf. Sci., 566 (2021) 150679.

[5] M. Esteves, L. Fernández-Werner, et al., Ceram. Int., 46 (2020) 2877-2886.

[6] E. German, R. Faccio, et al., Appl. Surf. Sci., 428 (2018) 118-123.

[7] L. Fernández-Werner, E.A. González, et al., The Journal of Physical Chemistry C, 122 (2018) 3363-3370.

[8] E. German, R. Faccio, et al., Journal of Physics Communications, 1 (2017) 055006.

[9] E. German, R. Faccio, et al., Appl. Surf. Sci., 426 (2017) 1182-1189.

[10] M. Esteves, L. Fernández-Werner, et al., Appl. Surf. Sci., 552 (2021) 149534.

[11] L. Amy, S. Favre, et al., Appl. Surf. Sci., 555 (2021) 149610.

[12] M. Esteves, D. Mombrú, et al., Appl. Surf. Sci., 535 (2021) 147733.

ELECTRONIC INTERACTIONS ON MOIRÉ 2D VAN DER WAALS HETEROSTRUCTURES

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Atomic layered materials have emerged as alternative systems to induce structural chirality, specific handedness, and electronic alterations of the pristine components. By applying a general unfolding method within density functional theory (DFT), we study typical mini gaps reported in heterostructures and other electronic deviations from pristine structures that are impossible to distinguish without an unfolding method. The combination of graphene (G), transition metal dichalcogenides (TMDCs), and other two-dimensional materials has attracted increasing interest as promising building blocks for future electronics, photonics, and optoelectronic devices. Our research not only identifies electronic minigaps, band hybridization, and splitting in different van der Waals structures but also underscores the immense potential of these two-dimensional materials in shaping the future of electronics. Electronic alterations are mainly caused by the interlayer interactions identified as electronic repulsions or avoided crossings and replicas due to the Moiré potential, depending on the interlayer angle. The results indicate that out-of-plane orbital interactions from different layers, depending on energy and k-region, induce the avoided crossings, band hybridization, and splitting. At the same time, Moiré replicas emerge because of the superperiodic potential associated with patterns. The minigaps energy position is intrinsically related to the interlayer angle and the commensurate conditions. Finally, we also show how these minigaps are related to the adsorption of chiral molecules, which distinguishes between left-handed and right-handed enantiomers, allowing us to study the enantiomeric recognition properties of TBG in the molecular adsorption of alanine.

Magnetism, Strongly Correlated Systems, Collective Phenomena, Low-Temperature Physics

MODELING BI-BASED LAYERED SUPERCONDUCTORS: ELECTRONIC PROPERTIES

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Superconductivity in layered BiS_2-based compounds was discovered in 2012. Though the crystal structure of the BiS_2 layers is similar to that of: CuO_2 planes in cuprate superconductors; Fe_2An_2 (An: Se, Te, S) layers in Fe chalcogenide superconductors; or FeAs planes in iron pnictides, other properties are different. There are experimental indications that electron-phonon coupling is weak, pointing to an unconventional pairing mechanism, but the origin and nature of the superconductivity is not yet clear in layered bismuth sulphides, with many different proposals still being investigated. Electron correlations are generally believed to be moderate in the Bi-based compounds.

We focus on the normal state properties of Bi-based superconductors and analize the effect of electron correlations: having started with the spectral properties, and the topology of the Fermi surface. Through an analytical treatment for a minimal model consisting of two correlated effective bands proposed to describe bismuth sulphides, related to our previous approach for Fe-based supercondctors [1], we determined the temperature-dependent electron Green's functions, from which we obtained the spectral density function [2], improving the description of ARPES results by including moderate electron correlations. We studied the dependence on doping and temperature, predicting also the k-dependence of the spectral density. We described the Fermi-surface topological transition at a critical doping value in bismuth sulphides.

To complete our study of the normal state properties, more recently (in yet unpublished results) we determined the normal-state electrical conductivity (resistivity) and the Hall coefficient, using the Kubo formalism, comparing our results with experimental data available for bismuthates, again obtaining improved descriptions of the experimental transport data with the inclusion of moderate electron correlations. We also evaluated thermal transport properties: the Seebeck factor as a function of doping and temperature, electronic thermal conductivity, the power factor, and the ZT figure of merit.

References:

[1] J. Querales, C.I. Ventura, R. Citro & J.J. Rodríguez Núñez, Phys. Lett. A 380, 1648-1657 (2016); J. Querales, M.L. Amigó, G.Nieva, & C.I. Ventura, EPL 113, 17005: 1 - 6 (2016)

[2] J.Querales C. I.Ventura, R. Citro & J.J. Rodríguez Núñez, Physica B 488, 32-42 (2016)

Keywords: *Modelization, Layered Superconductors, Electronic Properties*

ACCELERATING THE DISCOVERY OF 2D MULTIFERROICS

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Recently, the "A-Lab" has demonstrated that autonomous research agents can markedly accelerate the pace of materials research; 58 target materials were successfully realized at a rate of >2 new materials per day with minimal human interaction. Advances in ab initio computation, simulations, ML and robotics have intersected to enable "expert systems" that demonstrate autonomy as an emerging quality through the sum of its automated components. Such A-Lab demonstrates this by combining modern theory-driven and data-driven ML techniques with a modular workflow that can discover new materials with small human inputs. [1] Moreover, over the decades, experimental approaches have cataloged 20,000 computationally stable structures in the Inorganic Crystal Structure Database (ICSD). However, this strategy is impractical for scale due to costs, throughput, and synthesis complications. Instead, the computational approaches proposed by the new so called "materials informatics" [2-4] offer new scopes to access large configurational spaces with ab-initio calculations such a DFT. Combining DFT with simple substitutions allowed researchers to improve to 48,000 computable stable materials. [5] Such rapid discovery points to a wide landscape of opportunities in materials synthesis and development, particularly materials in two dimensions (2D), which call attention now; these materials have revolutionized the world of condensed matter and materials engineering, and today they are a reference in the nanoworld. [6,7] A variety of emerging phenomena and unprecedented applications have been found by confining atomic crystals into 2D, e.g., superconductivity, topological insulators, and beyond-CMOS devices. [6] In this work, we show the results of accelerating the discovery of new materials in two cutting-edge areas of the 2D nanoworld, i.e., slidetronics of hexagonal-like van Der Waals (hvdW) materials and freestanding-like layered perovskites (IP). [8-11] The combination of these two seemingly different groups of systems is expected to give rise to new high-performance electronic devices. [6] Motivated by recent developments in multiferroic materials' research, we focus on the "ferroic-observables" scope [6,7,10] and on the question: is it possible to automate simulations in 2D systems in search of systems conducive to the existence of ferroic order parameters that are reversibly tuned by interlayer sliding, straining of mixed layers and/or migration of topologically-ordered defects?, such effects represent very large configurational spaces, which are non-trivial to study with ab-initio methods. Here, we present results for the ferroelectric, magnetic, electronic and mechanical properties of mono/bilayers of AB1-xB'xO3- δ , with A = (Sr, Ba) and B, B' = (Ti, V, Cr, Mn, Fe, Co, Ni). We studied stoichiometric and oxygen deficient IP while paying attention to the multiple topologies given by the oxygen vacancies respect to the cation's distributions. Oxygen migration between different vacancies is also considered. We also studied the ferroelectric, electronic and mechanical properties of the BN and GaN nitrides within a sliding framework and considering anti-sides defects while paying attention to the topologies given by the distributions of such anti-sides onto the different layers. The migration of the anti-sides between out-of-plane metastable locations is considered as well.

References:

[1] Szymanski, N.J., Rendy, B., Fei, Y. et al. An autonomous laboratory for the accelerated synthesis of novel materials. Nature 624, 86–91 (2023). https://doi.org/10.1038/s41586-023-06734-w

[2] Jones, R. O. (2015). Density functional theory: Its origins, rise to prominence, and future. Reviews of Modern Physics, 87(3), 897-923. https://doi.org/10.1103/RevModPhys.87.897

[3] Rasmussen, F. A., & Thygesen, K. S. (2015). Computational 2D Materials Database: Electronic Structure of Transition-Metal Dichalcogenides and Oxides. The Journal of Physical Chemistry C, 119(23), 13169-13183. https://doi.org/10.1021/acs.jpcc.5b02950

[4] Jain, A., Ong, S. P., Hautier, G., Chen, W., Richards, W. D., Dacek, S., Cholia, S., Gunter,D., Skinner, D., Ceder, G., & Persson, K. A. (2013). Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. APL Materials, 1(1), 011002. https://doi.org/10.1063/1.4812323

[5] Merchant, A., Batzner, S., Schoenholz, S.S. et al. Scaling deep learning for materials discovery. Nature 624, 80–85 (2023). https://doi.org/10.1038/s41586-023-06735-9

[6] Yang, A. J.; Wang, S.-X.; Xu, J.; Loh, X. J.; Zhu, Q.; Wang, X. R. Two-Dimensional Layered Materials Meet Perovskite Oxides: A Combination for High-Performance Electronic Devices. ACS Nano 2023, 17 (11), 9748–9762. https://doi.org/10.1021/acsnano.3c00429.

[7] Shen, X.; Wang, F.; Lu, X.; Zhang, J. Two-Dimensional Multiferroics with Intrinsic Magnetoelectric Coupling in A-Site Ordered Perovskite Monolayers. Nano Letters 2023, 23 (2), 735–741. https://doi.org/10.1021/acs.nanolett.2c03457.

[8] Ye, W., Chen, C., Dwaraknath, S., Jain, A., Ong, S. P., & Persson, K. A. (2018). Harnessing the Materials Project for machine-learning and accelerated discovery. MRS Bulletin, 43(9), 664-669. https://doi.org/10.1557/mrs.2018.202

[9] Cho, E.; Kumar, A.; Ning, S.; LeBeau, J. M.; Ross, C. A. Perovskite-Derived Layered Crystal Structure in SrCo \textsubscript0.26 Fe \textsubscript0.74 O \textsubscript3- δ Thin Films. Advanced Materials Interfaces 2024, 11 (7), 2300807. https://doi.org/10.1002/admi.202300807.

[10] Chiabrera, F. M.; Yun, S.; Li, Y.; Dahm, R. T.; Zhang, H.; Kirchert, C. K. R.; Christensen, D. V.; Trier, F.; Jespersen, T. S.; Pryds, N. Freestanding Perovskite Oxide Films: Synthesis, Challenges, and Properties. Annalen der Physik 2022, 534 (9), 2200084. https://doi.org/10.1002/andp.202200084.

[11] Yang, L.; Wu, M. Across-Layer Sliding Ferroelectricity in 2D Heterolayers. Advanced Functional Materials 2023, 33 (29), 2301105. https://doi.org/10.1002/adfm.202301105.

Keywords: *two dimensional materials, multiferroics, hexagonal van Der Waals materials, freestanding perovskites, materials informatics*

ALTERMAGNETISM: A NOVEL MAGNETIC PHASE

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For nearly a century, the classification of magnetic phases has been confined to ferromagnetism and antiferromagnetism, defined by the alignment of atomic magnetic moments. This presentation will introduce altermagnetism, a newly identified magnetic phase that challenges traditional classifications [1]. Altermagnets are characterized by an alternating spin arrangement in momentum space, which breaks time-reversal symmetry while maintaining zero net magnetization. This emerging phase exhibits intriguing similarities to ferromagnets, such as giant magnetoresistance [2], but also unique properties, including the generation of spin currents with polarization that varies as a function of material rotation [3]. We will present experimental evidence supporting altermagnetism, including observations of the anomalous Hall effect in candidate materials like RuO_2, MnTe and Fe_2O_3. Although altermagnetism is still in its nascent stage of exploration, it holds significant promise for advancing spintronics, information storage technologies, and quantum electronics.

References:

[1] Emerging Research Landscape of Altermagnetism. Libor Šmejkal, Jairo Sinova, and Tomas Jungwirth. Phys. Rev. X 12, 040501 (2022)

[2] Giant and Tunneling Magnetoresistance in Unconventional Collinear Antiferromagnets with Nonrelativistic Spin-Momentum Coupling. Libor Šmejkal, Anna Birk Hellenes, Rafael González-Hernández, Jairo Sinova, and Tomas Jungwirth. Phys. Rev. X 12, 011028 (2022)

[3] Efficient Electrical Spin Splitter Based on Nonrelativistic Collinear Antiferromagnetism. Rafael González-Hernández, Libor Šmejkal, Karel Výborný, Yuta Yahagi, Jairo Sinova, Tomáš Jungwirth, and Jakub Železný. Phys. Rev. Lett. 126, 127701 (2021)

Keywords: *Magnetism, altermagnetism, spintronics, spin current*

QUANTUM OSCILLATIONS

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In this talk I will overview some of our recent works on quantum oscillations in topological and non-topological systems. More specifically, I will discuss: (i) the nonlocality of local Andreev conductances as a probe for Majorana wires in novel three-terminal superconducting 1D setups, asymmetrically coupled to normal leads [1]; (ii) phase driving hole spin qubits in double quantum dots under simultaneous transverse (Rabi) and longitudinal (phase) drives [2], which enables tunable additional side bands and (some) immunity against noise; (iii) probing 2D topological insulators via bulk resistitivity measurements of electrons and holes [3], and (iv) beating-free magnetoresistitivity in 2D electron gases with strong spin-orbit and Zeeman interactions, in which a new condition for the vanishing of beatings is derived [4,5]. These works have been partially supported by FAPESP and CNPq; see funding acknowledgement in the references below.

Refereces:

[1] Dourado, Penteado, and Egues, Phys. Rev. B 110, 014504 (2024).

[2] Bosco, Geyer, Camenzind, Eggli, Fuhrer, Warburton, Zumbühl, Egues, Kuhlmann, and Loss, Phys. Rev. Lett. 131, 197001 (2023), Editors' suggestion.

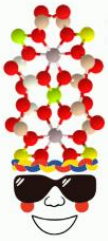
[3] Candido, Erlingsson, Costa and Egues, arXiv: 2406.08977.

[4] Candido, Erlingsson, Gramizadeh, Costa, Weigele, Zumbühl, and Egues, Phys. Rev. Research 5, 043297 (2023).

[5] Gramizadeh, Candido, Manolescu, Egues, and Erlingsson, Phys. Rev. B 109, 115303 (2024).

Keywords: *Majorana fermions, topological insulators, Rabi driving hole qubits, SdH oscillaYons.*

ORAL CONTRIBUTIONS



XXV Latin American Symposium on

Solid State Physics

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Nanomaterials, Low-Dimensional Systems, and Novel Materials

HYDROGEN PRODUCTION USING CO-NI BASED ELECTRODES OBTAINED FROM WASTED NIMH BATTERIES

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We are currently facing multiple challenges, one of the most urgent being the need to develop strategies to satisfy energy demands sustainably, using clean energy alternatives (free from greenhouse gases). One of the most promising options is hydrogen, a fuel with a high energy density of 33 KWh/Kg [1] and, produces only water and energy by products. Water electrolysis standing out as a key method for obtaining high-purity hydrogen. In this process, non-noble Co-Ni based catalysts emerge as an attractive option due to their excellent catalytic activity, stability in alkaline environments, and low overpotential. Notably, these catalysts can be derived from wasted NiMH batteries, which become a pollutant when their useful life ends. This study focused on obtaining Co-Ni-based electrodes from leachates of discarded NiMH batteries, which were then used to catalyze the hydrogen evolution reaction (HER). The leaching liquors from the batteries were recovered, and deposits were generated on carbon steel substrates using the pulsed current technique (PP). The electrodes were characterized using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) to analyze their morphology and elemental composition. The electrochemical performance of the electrodes was evaluated using techniques such as linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS), with KOH as the electrolyte. The results of electrochemical tests confirm the generation of hydrogen from water electrolysis using Co-Ni based catalysts obtained by varying parameters such as: pulse time (0.3 and 0.1 s), current density (-55 and -100 $mAcm^{-2}$) and charge (11 and 6 C).

References:

[1] A. Kazemi, F. Manteghi, and Z. Tehrani, ACS Omega 9, 7310 (2024).

Keywords: *Hydrogen, HER, NiMH batteries.*

STRONG SPIN-LATTICE COUPLING AND HIGH-TEMPERATURE MAGNETIC ORDERING IN MONOLAYER CHROMIUM DICHALCOGENIDES

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We detail the magnetic properties of monolayer CrX2 and its Janus counterparts CrXY (X,Y = S, Se, Te, with X ≠ Y) using ab initio methods and Landau-Lifshitz-Gilbert magnetization dynamics, and uncover the pronouncedly strong interplay between their structure symmetry and the magnetic order. The relaxation of nonmagnetic chalcogen atoms, that carry large spin-orbit coupling, changes the energetically preferential magnetic order between in-plane antiferromagnetic and tilted ferromagnetic one. The considered Janus monolayers exhibit sizable Dzyaloshinskii-Moriya interaction, in some cases above 20% of the isotropic exchange, and critical temperature of the long-range magnetic order in the vicinity or even significantly above the room temperature.

Keywords: *DFT, Magnetic ordering, Janus Materials.*

NON-SPHERICAL ATOMIC EFFECTIVE PSEUDOPOTENTIALS APPLIED TO THE STUDY OF THE ELECTRONIC STRUCTURE OF SI NANOWIRES

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We discuss the development of effective pseudopotentials for systems where charge transfer processes between atomic species are strong enough to render the conventional spherical approximation of effective potential inaccurate [1]. We introduce a description and implementation of these nonspherical atomic pseudopotentials based on the classical multipole expansion of a localized charge distribution. Our results show that going beyond the spherical approximation allows for the proper passivation of semiconductor nanostructures, removing spurious virtual states that appear inside the energy bandgap when the pseudopotentials are implemented as spherical quantities (fig. 1). We apply the method to describe a set of hydrogen-passivated silicon nanostructures along different orientations, facet configurations and diameters and discuss their electronic properties [2]. In particular, we show that the (100) surface facet favors the presence of valence states, which can give ideas for device fabrication through the modulation of opto-electronic properties by surface modifications.

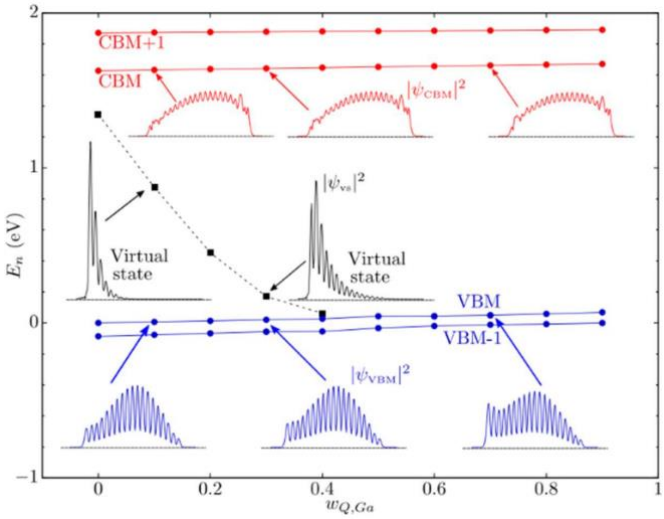

Fig. 1. Eigenvalues and squared wavefunctions for states around the bandgap for a long slab, where the occurrence of virtual spurious states inside the bandgap is shown. Taken from Ref. [1].

References:

[1] J. R. Cárdenas and G. Bester, "Atomic effective pseudopotentials for semiconductors," Phys. Rev. B 86, 115332 (2012). - J. Cárdenas, M. Bandera, and F. Nuñez-Murillo, "Multipole momento description of passivants and complex pseudopotentials for semiconductor surfaces," Computational Condensed Matter 33, e00765 (2022).

[2] F. Nuñez-Murillo and J. R. Cárdenas, "Influence of surface facets on the electronic structure of silicon nanowires and slabs from atomistic calculations," J. Appl. Phys. 134, 214302 (2023)

Keywords: *Atomistic calculations, electronic structure, semiconductor nanostructures*

LONG-TERM ANALYSIS OF ELECTROMECHANICAL PROPERTIES IN CEMENTITIOUS COMPOSITES WITH COPPER NANOPARTICLES

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This study investigates the electromechanical properties of cementitious composites incorporating copper nanoparticles. Unlike composites using copper slag, which have been shown to improve conductivity, mechanical strength, and durability, cement-based composites with copper nanoparticles have not yet been deeply explored in terms of their electrical and mechanical properties. In this research, cement specimens were fabricated with copper nanoparticle dispersions, synthesized using pulsed laser ablation in ultrapure water. Cylindrical samples were prepared following the ASTMC39M standard, with embedded desoldering copper wire electrodes and a dispersion-to-cement ratio of 0.47. The samples were labeled S1, S2, S3, and S4, each referring to the total laser exposure time in minutes (0, 5, 10, and 15 minutes, respectively). The electrical impedance spectroscopy (EIS) technique was employed to monitor the samples over a period of 140 days, generating Nyquist diagrams for each specimen. These diagrams were analyzed using computational tools and the Python 3 programming language to assess the polarization resistance and diffusive elements over time. It was observed that the heterogeneity parameter, representing the diffusive component, consistently decreased after the initial 28 days. Simultaneously, mechanical tests were performed on the samples, and current and voltage measurements were recorded using a DT-11 Potentiostat by DinTech. The findings revealed a significant increase in polarization resistance over time across all specimens, suggesting the inevitable oxidation phenomena occurring on the copper nanoparticles. Additionally, the heterogeneity parameter showed fewer changes between specimens with varying concentrations of copper nanoparticles, indicating that low concentrations may not have a significant impact on the electrical properties of copper-cement-based composites. The electrical properties were closely correlated with compressive mechanical strength, highlighting the complex interplay between mechanical and electrical characteristics. This study provides deeper insight into how copper nanoparticles influence the electrical and mechanical properties of cementitious composites, paving the way for future research and applications in advanced construction materials.

Keywords: *Copper Nanoparticles, Cementitious Composites, Electromechanical Properties.*

OPTIMIZATION OF PHOTOVOLTAIC CELL PROPERTIES AND EFFICIENCY BY INCORPORATING FUNCTIONAL GROUPS INTO Π-CONJUGATED TRIPHENYLAMINE MOLECULES

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This study focuses on optimizing the properties of photovoltaic cells by incorporating ethylenedioxythiophene and styrylnitroisoxazole into -conjugated triphenylamine molecules. The resulting compound, GC8, exhibits light absorption in the range of 400 nm to 700 nm and demonstrates a high hole mobility of $2x10^{-5}cm^2\ V^{-1}s^{-1}$, positioning it as an efficient donor material in organic photovoltaic cells. With a highest occupied molecular orbital (HOMO) energy level of 5.35 eV and a lowest unoccupied molecular orbital (LUMO) energy level of 2.94 eV, the calculated band gap is 2.41 eV, while the experimentally determined band gap is 1.9 eV, which is typical for small molecules. GC8 was utilized in planar heterojunction organic photovoltaic cells (PHJ-OPVs) using fullerenes (C60 and C70) as acceptors. The optimal active layer thickness of 20 nm for GC8 and a thermal annealing treatment of 5 minutes at 100 °C enhanced the power conversion efficiency (PCE) by 10%. C70, with its broader light absorption, further increased the efficiency to 6.15%. These enhancements are attributed to increased charge carrier mobility and improved optical absorption, highlighting the potential of chemical modifications in advancing renewable energy technologies.

Keywords: *Donor-acceptor systems, New π-conjugated push-pull molecule, Planar heterojunction, Organic photovoltaic cells, Post annealing*

DECOHERENCE EFFECTS ON QUANTUM TRANSPORT THROUGH TOPOLOGICAL DOMAIN WALLS

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The introduction of topology in condensed matter physics has led to the discovery of new and exciting materials such as topological insulators (TIs), in which robust edge states appear with energies that lie in the bulk band gap. The presence of robust edge states in a TI depends exclusively on the value of topological invariants that remain unaltered by adiabatic perturbations. A topological invariant can be non-uniform within a system, forming topological domains whose frontiers are known as domain walls (DWs) [1]. In recent years, DWs have been proposed for promising technological applications such as magnetic memories [2] and quantum information transfer [1]. For the DWs to be successfully utilized in electronic devices it is necessary to study the effects of conditions that are inevitable in realistic systems such as decoherence and non-zero temperature. In this work we propose a tight-binding-like model for a quantum Hall bar with multiple topological domains and calculate the resistance between different terminals by means of the recursive S-matrix method. The multidomain system is achieved by considering a two-dimensional electron gas with an applied magnetic field that is non-homogenous and allows the Chern number, which is a topological invariant, to take different values within the sample. The non-homogenous magnetic field is introduced into the model by means of a graphic algorithm to simplify the Peierls substitution. It is observed that when the local Chern number has different sign between adjacent domains, the longitudinal resistances oscillate and lose their quantized behavior. This effect is shown to be produced by interference as the oscillations are suppressed when decoherence is added into the DWs through Büttiker probes. The role of decoherence is further discussed by calculating the wave functions and current densities for both the coherent and decoherent DWs. Moreover, it is found that calculating the resistances for a finite temperature in the decoherent DWs results in quantized values that are in great agreement with the ones previously reported in experiments with intrinsic topological insulators [3].

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References:

[1] J. Zurita, C. E. Creffield, and G. Platero, Fast Quantum Transfer Mediated by Topological Domain Walls, Quantum 7, 1043 (2023).

[2] G. Venkat, D. A. Allwood, and T. J. Hayward, Magnetic Domain Walls: Types, Processes and Applications, J. Phys. D: Appl. Phys. 57, 063001 (2024).

[3] K. Yasuda, M. Mogi, R. Yoshimi, A. Tsukazaki, K. S. Takahashi, M. Kawasaki, F. Kagawa, and Y. Tokura, Quantized Chiral Edge Conduction on Domain Walls of a Magnetic Topological Insulator, Science (1979) 358, 1311 (2017)

Keywords: *Domain walls, topological insulator, decoherence.*

STUDY AND OPTIMIZATION OF ELECTRONIC AND STRUCTURAL PROPERTIES OF TWO-DIMENSIONAL MATERIALS (MXENES) FOR ENERGY GENERATION AND STORAGE THROUGH FIRST-PRINCIPLES CALCULATIONS

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In the ongoing search for innovative materials to address current energy and environmental challenges, MXenes have emerged as a promising class of two-dimensional materials. These materials exhibit a unique laminar structure primarily composed of layers of transition metal carbides, nitrides, or carbonitrides. These structural characteristics endow them with a wide range of properties that make them attractive for applications in various technological fields[1-3].

With this in mind, a high-throughput and high-performance search will be developed using databases, aiming to filter compounds that meet certain characteristics mentioned later for specific technological applications such as photocatalysis, photovoltaic effect, and lithium-ion batteries. The objectives are:

- To develop high-performance and high-throughput calculations to perform an initial study of the structural and electronic properties of the MXenes stored in the database, in order to select materials that meet general requirements for their application in photocatalysis, photovoltaic cells, and/or lithium-ion batteries using first-principles methods.
- Based on the materials from the database and materials found in the literature that meet the desired properties, study possible methods to enhance efficiency, performance, and longevity of MXenes for potential use in photocatalysis, photovoltaic cells, and lithium-ion batteries.

DFT calculations will be performed using the VASP (Vienna Ab-initio Simulation Package) code[4]. Additionally, complementary tools for structure analysis and visualization such as VTST (VASP Transition State Tools) and VESTA (Visualization for Electronic and Structural Analysis)[5], among others, will be used.

References:

[1] Naguib, M., Kurtoglu, M., Presser, V., Lu, J., Niu, J., Heon, M., Hultman, L., Gogotsi, Y., & Barsoum, M. W. (2011). Advanced Materials, 23, 4248-4253.

[2] Naguib, M., Mashtalir, O., Carle, J., Presser, V., Lu, J., Hultman, L., Gogotsi, Y., & Barsoum, M. W. (2012). ACS Nano, 6, 1322-1331.

[3] Khazaei, M., Ranjbar, A., Arai, M., & Yunoki, S. (2016). Physical Review B, 94, 125152.

[4] Kresse, G., & Hafner, J. (1993). Physical Review B, 47(1), 558-561.

[5] Momma, K., & Izumi, F. (2008). Journal of Applied Crystallography, 41, 653-658.

Keywords: *Mxenes, Energy, Photocatalysis, Photovoltaics, Lithium, Batteries*

FERROELECTRIC SWITCHING IN MONOLAYER WSE2 VIA CONCURRENT ANTISITE AND VACANCY DEFECTS. A DFT STUDY

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Room temperature multiferroicity in Te doped 2H WSe_2 samples has been reported recently [1]. First principles calculations showed that chalcogen vacancies trigger an electric polarization perpendicular to the layers of the material due to the rupture of its centrosymmetric character. The proposed mechanism for ferroelectric switching is the vertical displacement of the chalcogen atom located above a vacancy towards the vacancy position at the opposite side of WSe_2 monolayers. However, the calculated large energy barrier for such atomic displacements does not correspond to the experimental switching electric field. In this work an alternative mechanism for ferroelectricity is presented in which a Se atom antisite is placed above a chalcogen vacancy. First principles simulations based on density functional theory (DFT) and the modern theory of polarization [2] as implemented in the code Abinit [3,4], indicate this is a feasible mechanism for the ferroelectric switching given the reduced value of the energy barrier. The substitution of a Se atom by a W atom in the antisite together with the neighbor vacancy generate a group of four W atoms where the metallic bonds reduce the structural stiffness and hence decrease the energy barrier between the equilibrium positions at each side of the monolayer.

References:

[1] G. Cárdenas-Chirivi, et. al., Room temperature multiferroicity in a transition metal dichalcogenide. npj 2D Materials and Applications 7, 54 (2023).

[2] Resta, R. Macroscopic electric polarization as a geometric quantum phase. EPL 22, 133 (1993).

[3] X. Gonze. et al., The Abinit project: impact, environment and recent developments. Comput. Phys. Commun. 248, 107042 (2020).

[4] X. Gonze, et. al., Comput. Phys. Commun. 205, 106 (2016).

Keywords: *2D materials, Ferroelectricity, Density Functional Theory.*

Thermal, Optical, and Transport Properties

ENHANCING EXCITON LOCALIZATION IN TWO-DIMENSIONAL SEMICONDUCTORS THROUGH DIELECTRIC ENVIRONMENT MODIFICATION

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Low-dimensional semiconductors are known for their remarkable optical properties, which arise from the behavior of strongly confined charge carriers and the tunable excitations within their structures. Two-dimensional (2D) materials, in particular, have garnered significant interest due to their promising integration potential in optoelectronic applications [1, 2].

When the in-plane periodicity of an atomically thin semiconductor is disrupted, further reduction in system dimensionality can be achieved, leading to the creation of one-dimensional (1D) or zero-dimensional (0D) confined regions, where the carriers are fully localized.

In this study, we investigate the feasibility of exciton localization through the manipulation of the dielectric environment. Specifically, we model the impact of sandwiching a semiconductor monolayer between two non-homogeneous dielectric slabs.

We analyze how the screening of the electron-hole attraction is influenced by the dielectric properties of the surrounding materials. This modulation leads to the formation of regions where the Coulomb interaction is significantly enhanced, resulting in the localization of the exciton center of mass.

We calculate the energy discretization and radiative lifetime within both the Ritova-Keldysh and image-charge frameworks [3, 4, 5], as functions of the characteristic parameters of the materials encapsulating the semiconductor monolayer. Our findings offer insights into the ongoing challenge of fabricating controllable artificial atoms for high-quality quantum light emitters, which are critical components for the development of emerging photon-based quantum technologies.

References:

[1] S. Ayari, A. Smiri, A. Hichri, S. Jaziri, and T. Amand Phys. Rev. B 98, 235702 (2018).

[2] G.-H. Peng, et al. Nano Lett. 19, 2299 (2019).

[3] N. S. Rytova, Proc. MSU, Phys., Astron. 3, 30 (1967).

[4] L. V. Keldysh, Soviet Journal of Experimental and Theoretical Physics Letters. 29, 658 (1979).

[5] M. Kumagai and T. Takagahara, Phys. Rev. B. 40, 12359 (1989).

Keywords: *Exciton Localization, Two-Dimensional Semiconductors, Dielectric Environment Modulation.*

CUNBS3: A FIRST-PRINCIPLES EXPLORATION OF A POTENTIAL PHOTOVOLTAIC MATERIAL

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The escalating global energy demand underscores the critical need for efficient renewable alternatives. Photovoltaic materials, capable of converting sunlight into electricity, offer a promising solution. While perovskites [1,2] have garnered significant attention, copper-based chalcogenides like CuNbS3 emerge as potential candidates due to their intriguing electronic properties. This study provides a comprehensive first-principles investigation of $CuNbS_3$, focusing on its structural and electronic characteristics. We determined the ground-state crystal structure using the Birch-Murnaghan equation of state [3] and employed both GGA-PBEsol [4] and meta-GGA R2SCAN [5] functionals for electronic structure calculations as implemented the in VASP code [6]. To enhance band gap prediction accuracy, the G0W0 approximation was applied [7]. Our results indicate a band gap of 0.6 eV with R2SCAN and 1.04 eV with G0W0+PBEsol, suggesting CuNbS3 as a promising absorber material for photovoltaic applications. Further exploration of its optical properties and carrier transport characteristics is warranted to fully assess its potential.

Keywords: *GoWo, Band Structure, Chalcogenide*

NOVEL KAGOME KMN3SB5 METAL: CHIRAL MAGNETISM, LATTICE DYNAMICS, AND ANOMALOUS HALL CONDUCTIVITY

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Very recently, Kagome metals are reported to exhibit remarkable properties, including superconductivity, charge density wave order, and a large anomalous Hall conductivity (AHC), which facilitate the implementation of spintronic devices. All the latter promoted by the remarkable topological features shown by this family of crystals. In this work, we theoretically study a novel Kagome metal based on Mn magnetic sites in a KMn_3Sb_5 stoichiometry. By means of first-principles density functional theory calculations, we demonstrate that the studied compound is dynamically stable, locking the ferromagnetic order as the ground state configuration, thus preventing the charge-density-wave state as reported in its vanadium-based counterpart KV_3Sb_5. Our calculations reveal that KMn_3Sb_5 exhibits an out-of-plane (001) ferromagnetic response as the ground state, allowing for the emergence of topologically protected Weyl nodes near the Fermi level and nonzero AHC in this centrosymmetric system. We obtain a tangible AHC σ_{xy} = 314 $S \cdot cm^{-1}$ component, which is comparable to that of other Kagome metals. Finally, we explore the effect of the on-site Coulomb repulsion (+U) on the structural and electronic properties and find that, although the lattice parameters and σ_{xy} moderately vary with increasing +U, KMn_3Sb_5 stands as an ideal stable ferromagnetic Kagome metal with a large AHC response [1].

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References:

[1] S. Singh, A. C. Garcia-Castro, Kagome KMn3Sb5 metal: Magnetism, lattice dynamics, and anomalous hall conductivity, Phys. Rev. B 108 (2023) 245143. doi:10.1103/PhysRevB.108. 245143.

Keywords: *Kagome lattices, Chiral magnetism, Topology, Density-functional theory*

CONTROL OF THE SPIN-POLARIZED CONDUCTANCE IN A BILAYERED 2D MAGNETIC CRI3-BASED DEVICE

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In the last decade, 2D magnetic materials have garnered significant attention due to their unexpected behavior and potential next-generation applications, with particular interest in the field of spintronics. In this work, the electronic and magnetic structure of the CrI$_3$ bilayer-based device is theoretically studied, followed by its tunable transport properties under the presence of an external electric field. Due to its magnetically active behavior, the device demonstrates its capability to function as a spin-selective device. The appearance of the insulator-to-semimetal transition, induced by a perpendicularly applied electric field, is observed and explained. This phenomenon can be precisely controlled depending on the direction and intensity of the field. Each magnetic CrI$_3$ layer individually permits or restricts the spin-polarized electronic transport. Consequently, a spin-polarized transistor controllable via the electric field is proposed. To achieve a precise description of the system, a computational model based on density functional theory (DFT) was developed to investigate its electronic and magnetic structure, and their response under the effect of the electric field. This methodology was coupled to a maximally localized Wannier functions-based model, from which transport properties were obtained.

Keywords: *Spintronics, Two-dimensional materials, Two-dimensional Magnetism, Density-functional theory, Wannier functions.*

ELECTRICAL ANALYSIS OF CASEINATE-BORAX BIOFILMS

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In the search for new biodegradable polymeric materials, those based on caseinate emerge as an alternative to replace those from petrochemical sources. Efforts have been made to study the barrier properties to oxygen and moisture, and improvements in their rheological properties have been sought regarding their final processability, but little is known about their electrical behavior. In this work, we conducted a comprehensive analysis of different borax-modified biofilms using a range of advanced techniques, including electrical impedance spectroscopy, X-ray diffraction, infrared vibrational spectroscopy, and UV-Vis electron spectroscopy. This thorough approach allowed us to evaluate the effect that the incorporation of borax in the structure of the film had on these properties. The results found indicate that it is possible to modulate the electrical response with the systematic incorporation of borax. The trend of the real component of electrical conductivity indicated its decrease between 2.5-15% of added borax, while at concentrations higher than 15% the conductivity increases above the value for the pure calcium caseinate biofilm. The general behavior of conductivity presented three behaviors, between 0.1-102 Hz there was low frequency dispersion, between 102 -105 Hz there was long-range conductivity and at frequencies above 105 Hz, the biofilms presented short-range conductivity compatible with Johnsher's power law. The above agreed with the changes observed by XRD, Infrared and UV-Vis, demonstrating the comprehensive nature of our research.

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References:

[1] Franco-Bacca AP, Cervantes-Alvarez F , Becerra ME, Ávila AC, Giraldo Osorio O, Arias NP, Rodríguez-Gattorno G ,J. J. Alvarado-Gil G(1). Thermal, mechanical, and optical characterization of calcium caseinate biopolymers with borax as crosslinking agent. ICPPP21 - International Conference on Photoacoustic and Photothermal Phenomena

[2] Marina P. Arrieta, Mercedes A. Peltzer, María del Carmen Garrigós, Alfonso Jiménez, Structure and mechanical properties of sodium and calcium caseinate edible active films with carvacrol, Journal of Food Engineering, Volume 114, Issue 4, 2013, Pages 486-494,

Keywords: *caseinate biofilms, borax, electrical conductivity, impedance spectroscopy*

SOLID-STATE MECHANISMS ENHANCING FIRE RESISTANCE IN NIOBIUM AND BORON ALLOYED STRUCTURAL STEELS

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The stability of structural components at high temperatures, particularly above 600 °C, is crucial in maintaining the integrity of buildings and infrastructure during fire events. This study investigates the solid-state mechanisms by which boron (B) and niobium (Nb) alloying enhance the fire resistance of steels, focusing on their effects on microstructure and mechanical properties. Our research reveals that adding small amounts of boron (≈ 30 ppm) to Nb-microalloyed steels significantly improves their yield strength at elevated temperatures. The 66% yield-strength retention criterion, a benchmark for fire-resistant materials, is achieved at approximately 574 °C in boron-added alloys, compared to only 460 °C in boron-free counterparts. Quantum mechanical calculations demonstrate that boron reduces the vacancy formation energy by 11.7% in pure ferrite and up to 33.2% in Nb-containing steels. This reduction promotes the formation of higher-density vacancy-related crystalline defects, which are key to enhancing the material's high-temperature strength. We further analyze the effects of cooling rates on microstructural evolution, showing that slower cooling promotes ferrite transformation and (Nb, Ti)C precipitation, leading to a more equilibrium-phase microstructure. Rapid cooling induces upper bainite formation, with boron segregating at precipitate interfaces, effectively hindering coarsening kinetics and preserving yield strength during fire simulations. The coexistence of Nb and C solute clusters with NbC nanoprecipitates, observed under Atom Probe Tomography (APT) and transmission electron microscopy (TEM), further supports the role of boron in improving fire resistance through solid-state phenomena. This work contributes to the understanding of how boron and niobium alloying can be strategically utilized to develop cost-effective, high-performance fire-resistant steels. The insights gained from this study have broad implications for the design of safer structural materials, with a particular focus on optimizing alloy compositions and thermomechanical processing to exploit solid-state strengthening mechanisms.

References:

[1] Ferreira, P.P.; Carvalho, F.M.; Ariza-Echeverri, E.A.; Delfino, P.M.; Bauri, L.F.; Ferreira, A.M.; Braga, A.P.; Eleno, L.T.F.; Goldenstein, H.; Tschiptschin, A.P. Synergism between B and Nb Improves Fire Resistance in Microalloyed Steels. Metals 2023, 13, 84

Keywords: *Fire-resistant, Niobium and Boron alloying, Vacancy formation energy, Crystalline defects.*

PROPAGATION OF ELECTROMAGNETIC WAVES THRONGS A BI-PERIODIC 1D DIELECTRIC-GRAPHENE PHOTONIC CRYSTAL

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In this work, we study the photonic bands, the dispersion relation, and the macroscopic transmission and reflection spectra for a one-dimensional dielectric-graphene photonic crystal of a bi-periodic unit cell in the chemical potential. The unit cell consists of two graphene sheets separated by an isotropic dielectric medium, where the chemical potential for the first graphene sheet is μ a and the second sheet is μ b. The analytical equations for the photonic bands, the dispersion relation, and the transmission and reflection spectra of incident electromagnetic waves are derived using the transfer matrix formalism [1]. In addition, the optical conductivity of graphene is implemented taking into account both intraband and interband contributions [2]. We found that this bi-periodic photonic structure of chemical potential shows the formation of new photonic gaps compared to the conventional one-dimensional graphene dielectric photonic crystal [3]; likewise, new modes appear in the low-frequency graphene-induced band gap, but only in the TM polarization. Moreover, these non-propagating regions can be seen directly from the transmission and reflection spectra calculated from the found expressions. Finally, we have shown that the newly formed photonic gaps can modulate their thickness in frequency through the values of the chemical potential in the graphene sheets of the unit cell.

References:

[1] Zhan, X. Shi, Y. Dai, X. Liu, J. Zi, Transfer matrix method for optics in graphene layers, Journal of Physics: Condensed Matter. 10.1088/0953-8984/25/21/215301

[2] A. Falkovsky, Optical properties of graphene, Journal of Physics: Conference Series 129 (1) (2008) 012004. 10.1088/1742-6596/129/1/012004

[3] V. Bludov, N. M. R. Peres, M. I. Vasilevskiy, Unusual reflection of electromagnetic radiation from a stack of graphene layers at oblique incidence, Journal of Optics. 10.1088/2040-8978/15/11/114004

ENANTIOSPECIFIC ELECTRON TRANSPORT IN CHIRAL-MODIFIED MOLECULAR JUNCTIONS

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We shall disclose the theoretical dependence of electronic transport with geometrical chirality in a molecular electronic device in which the source electrode is modified by attaching a chiral gold cluster (chAu34) [1], and in the middle part, a chiral organic molecule (label as HB) is connected (see Fig. 1a,b). The presence of chAu34 in these devices triggers enantioselective transport, this means, a difference in transmission function (see Fig. 1c) and in the conductance: 43.4 μA/V for the R case vs. 34. 5 μA/V for the L case (see Fig. 1d). Also, we'll show that a change in orbital angular momentum between R and L systems underlies this phenomenon. It's worth mentioning that these devices could be an alternative to other chiral detection techniques, such as optical methods or those that depend upon the spin state of the system, as occurs in the Chiral-Induced Spin Selectivity (CISS) effect [2]. Also, this work could be a model that describes an intrinsically chiral STM dip, as is experimentally observed in Ref. 3. As a final comment, all calculations were performed in SIESTA and in Transiesta codes, which are based on DFT theory and Non-Equilibrium Green's Function method respectively.

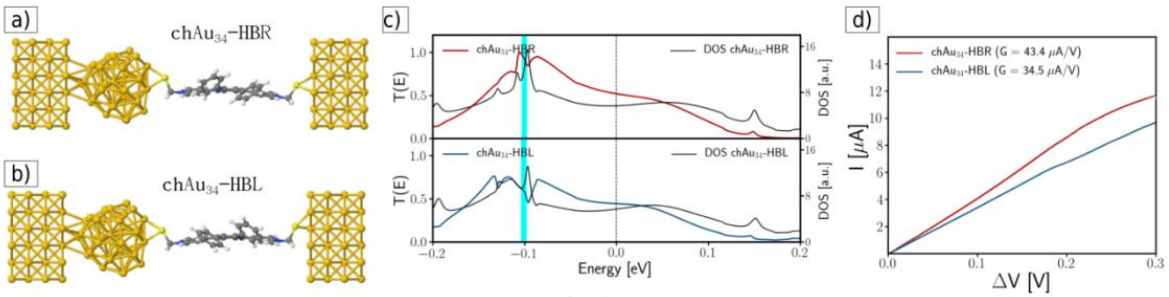

Fig. 1

References:

[1] J. J. Pelayo, I. Valencia, A. P. Garcá, L. Chang, M. López, A. Fortunelli, and I. L. Garzón (2018), "Chirality in bare and ligand-protected metal nanoclusters," Adv. Phys 3, 1509727.

[2] R. Naaman, Y. Paltiel and D. H. Waldeck (2020), "Chiral Molecules and the Spin Selectivity Effect", J. Phys. Chem. Lett., 11.

[3] H. L. Tierney, C. J. Murphy, and E. C. H. Sykes (2011), "Regular scanning tunneling microscope tips can be intrinsically chiral", Phys. Rev. Lett. 106, 010801.

Keywords: *Chirality, Quantum transport, DFT.*

Crystal Structure Prediction

CATALYTIC ACTIVITY AND SENSING PROPERTIES OF THE M-MOF74 (M=MN, FE, CO) METAL-ORGANIC FRAMEWORKS

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Metal-organic frameworks (MOFs) are crystalline materials characterized by porous structures formed through the coordination of organic ligands with metal-oxide clusters [1]. Specifically, MOF-74 is a honeycomb-like material with a pore size of approximately 1.2 nm, created by combining divalent metal ions with 2,5-dihydroxyterephthalic acid. This MOF, when combined with different transition metals, has demonstrated catalytic activity for the conversion of NH3, NO, and O2 into NO2, N2, and H2O [2]. In particular, Cu-MOF-74 has shown activity toward the oxygen reduction reaction (ORR) [3]. Other studies have reported sensing properties for Co-MOF-74, indicating that molecular interactions can alter the electronic band structure of MOFs, thereby enhancing their potential for toxic gas detection [4]. In this work, we employ spin-polarized density functional theory (DFT) calculations to investigate the electronic properties of M-MOF-74 (where M = Mn, Co, or Fe) and its interactions with O2, CO, and NO molecules. Additionally, we assess the activity of M-MOF-74 toward the oxygen reduction reaction (ORR) and the oxygen evolution reaction (OER), which are crucial electrochemical processes for clean energy technologies, particularly in metal-air batteries and fuel cells.

The calculations were performed using the VASP code, incorporating Hubbard (U) corrections to account for the on-site Coulomb interaction between M(3d) electrons. We used UMn=5.5 eV, UCo=5.3 eV, and UFe=6.5 eV. Additionally, we employed the meta-GGA exchange-correlation functional, including intermediate-range van der Waals interactions, as implemented in the SCAN+rVV10 functional. The electrocatalytic activity of M-MOF-74 for the oxygen reduction reaction (ORR) and the oxygen evolution reaction (OER) was assessed using the computational hydrogen electrode model proposed by Nørskov et al. [5]. This model depends on the adsorption strength of the ORR/OER reaction intermediates OH*, O*, and OOH* on the catalyst's active site, which is the metal center. Our results indicate that M-MOF-74 is a semiconductor with band gaps of 1.68 eV, 2.17 eV, and 2.10 eV for Mn, Co, and Fe, respectively. We also found that the interactions of O_2, CO, and NO with the MOF metal centers yield binding energies ranging from -0.33 eV to -0.54 eV. Both O_2 and NO introduce empty states within the band gap, whereas CO causes states to appear resonant in the conduction band. This suggests that M-MOF-74 could serve as a detector for O_2 and NO molecules, but not for CO. Regarding catalytic performance, the ORR evaluation reveals theoretical overpotentials of approximately 0.8 V for Co and Mn, and 1.0 V for Fe. For the OER, the overpotentials are 0.98 V for Co, 1.28 V for Mn, and 1.58 V for Fe. Considering that Pt(111)/C and IrO2(111) are the best commercial ORR and OER electrocatalysts, exhibiting

overpotentials of around 0.8 V, we conclude that Co-MOF-74 and Mn-MOF-74 are the best candidates for ORR, while Co-MOF-74 is the most suitable for OER.

References:

[1] Samuel et al., Chem. Rev. 2015, 115, 6051-6111

[2] Xie et al. ACS Appl. Mater. Interfaces 2020, 12, 48476-48485

[3] S. Rodriguez et al., J. Electroanal. Chem. 2022, 918, 116489-116497

[4] Strauss et al., ACS Appl. Mater. Interfaces 2019, 11, 14175-14181

[5] Nørskov et al., J. Phys. Chem. B 2004, 108, 17886-17892.

Keywords: *Metal-organic frameworks, Oxygen Reduction Reaction, Oxygen Evolution Reaction, Gas sensing, Density Functional Theory.*

EFFICACY OF VANADIUM OXIDE NANOPARTICLES DOPED WITH REDUCED GRAPHENE OXIDE IN THE PHOTOCATALYTIC DEGRADATION OF METHYLENE BLUE

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Water pollution from synthetic dyes is a critical global issue with severe implications for human health and ecosystem stability. This study focused on the Cundiboyacense region of Colombia, known for its high population density and agricultural significance, proposing an innovative solution through the use of vanadium oxide nanoparticles doped with reduced graphene oxide (V2O5+Nb+rGO) for the photocatalytic degradation of these pollutants. Preliminary analyses were conducted to identify the most affected areas by dye contamination and their socio-environmental impact. Subsequently, nanoparticles were synthesized and characterized, revealing fiber-like morphologies. Raman spectroscopy analyses identified the main vibrational modes associated with V2O5, while FTIR spectroscopy demonstrated the primary bonds associated with vanadium pentoxide. Additionally, X-ray diffraction (XRD) results indicated the formation of a secondary Nb2O5 phase. The effectiveness of the nanoparticles in degrading contaminants was evaluated based on their concentration, with results showing significant improvement in the degradation of methylene blue. This indicates the potential of this technology as a viable and sustainable alternative for wastewater treatment in the region. This advancement represents a crucial step towards mitigating water pollution, offering an effective strategy for the purification of wastewater contaminated with synthetic dyes, with positive implications for human consumption, agriculture, and environmental conservation in the Cundiboyacense region.

Keywords: *Photocatalytic degradation, vanadium oxide nanoparticles, reduced graphene oxide, synthetic dye pollution*

ADSORPTION AND DIFFUSION OF LITHIUM, SODIUM, GALLIUM, AND SULFUR ATOMS ON THE GAS MONOLAYER

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In this work, the adsorption and diffusion of lithium (Li), sodium (Na), gallium (Ga), and sulfur (S) atoms on the 2x2-GaS hexagonal monolayer surface are investigated using density functional theory (DFT) along with atomic pseudopotentials. The monolayer is modeled using the periodic slab approach. The slab includes a sufficiently large vacuum region (≈15 Å) to ensure that there are no interactions between the monolayer system and its image.

The calculated adsorption energy values indicate that the energetically most favorable site for the Li, Na, and Ga adsorbates is the H site (H is located right at the center of a hexagon formed by the projection of Ga and S atoms located in the top two layers of the GaS monolayer), while the most favorable site for the S adsorbate is the Ts site (Ts is located directly above a S atom belonging to the top layer of the GaS monolayer). The calculated adsorption energy values at the most favorable sites for the Li, Na, Ga, and S atomic adsorbates are -1.853 eV, -1.378 eV, -1.028 eV, and -1.525 eV, respectively.

The diffusion of Li, Na, Ga, and S atoms on the 2x2-GaS monolayer surface shows energy barriers of 28 meV, 40 meV, 72 meV, and 161 meV, respectively.

From the total (DOS) and partial (PDOS) density of states, it is established that, in all cases, the GaS+ads monolayer system acquires metallic behavior.

Finally, Bader charge analysis of the GaS+ads monolayer system at the energetically most favorable sites reveals that Li and Na atoms donate charge to the monolayer (cations), while the Ga atom neither donates nor acquires charge from the monolayer (it shares charge), and the S atom acquires charge from the monolayer (anion). From this electronic behavior, it is inferred that the GaS monolayer system with Li and Na adsorbates could be an excellent material for use as an anode in batteries.

Keywords: *h-AlN (0001) 4x4 monolayer, thermodynamic stability, DOS, Bader charge, Löwdin charge, DFT (GGA).*

EFFECT OF DEFECTS ON THE ENERGETICS AND ELECTRONIC PROPERTIES OF THE (4×4) ALN/(5×5) GRAPHENE HETEROBILAYER

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In this research, the energetics and electronic properties of the (4x4) AlN/(5x5) graphene heterobilayer with and without defects are studied. These defects are only considered in the (4x4) AlN monolayer. The (5×5) graphene monolayer is only considered as the substrate for the planar hexagonal (4x4) AlN monolayer.

The (4x4) AlN/(5x5) graphene heterobilayer is modeled using the periodic slab scheme: a (4x4) AlN monolayer is coupled to a (5×5) graphene monolayer, which presents a mismatch of 0.96%. To include the periodicity in the heterobilayer system, the slab contains a sufficiently large empty region (≈20 Å) so that no interactions occur between the heterobilayer system and its image. Here, two configurations are chosen: aluminum (AA) and nitrogen (AA') centered in a graphene hexagon, respectively; as far as is known, these configurations have not been reported in the scientific literature.

It is found that the values obtained for the binding energy, formation energies, adhesion work, and interface energy for the defect-free AA and AA' configurations are -19.13, -16.69, 19.13, and -46.42 meV/Å2, and -20.42, -16.77, 16.77, and -46.23 meV/Å2, respectively.

Additionally, for the AA and AA' configurations with aluminum vacancies, the values obtained are -18.94, -16.84, 16.84, and -46.30 meV/Å2, and -19.54, -17.40, 17.40, and -46.85 meV/Å2, respectively.

Finally, the values obtained for the AA and AA' configurations with nitrogen vacancies are -25.40, -27.49, 27.49, and -56.95 meV/Å2, and -26.99, -28.87, 28.87, and -58.32 meV/Å2, respectively.

The electronic properties of the (4x4) AlN/(5x5) graphene heterobilayers with and without defects are established via electronic density of states (DOS) and Bader charge.

Keywords: *(4x4) AlN/(5x5) graphene heterobilayers, binding energy, formation energies, adhesion work, interface energy, DFT (GGA).*

ELECTRONIC FLAT-BANDS ON TWISTED BILAYER PENROSE QUASICRYSTALS

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Since the discovery of high Tc superconductors, it has been recognized that the multiple layer structure of the system plays an important role in the arise of the superconducting state. The recent discovery of superconductivity in twisted bilayer graphene adds a twist to multiple layer systems, giving rise to flat bands, which are responsible of the correlated states along with the appearance of Moiré patterns [1]. Many multiple layer systems were discovered to be superconductors, one of them, the quasicrystals [2]. Quasicrystals were discovered in 1984 by D. Shechtman in a AlMn fast quenching alloy, presenting 5-fold axis and no translational symmetry [3]. A few years later after, it was discovered that these quasicrystals can be periodic in one dimension, and quasiperiodic in two dimensions, hence, a system consisting of a periodic staking of quasiperiodic layers. We investigate the electronic behaviour of two coupled quasiperiodic layers in perfect stacking, and when a Moiré pattern is present. In this work, we model the system using the tight binding Hamiltonian and the Penrose lattice. The electronic spectrum is analysed via the density of states and the wave function. We present the appearance of flat bands and electronic localizations when a Moiré pattern is formed. We also present briefly the behaviour of a trilayer twisted quasiperiodic system.

References:

[1] Y. Cao et al. Nature, 556, 43, (2018).

[2] K. Kamiya et al. Nature Communications, 9, 154, (2018).

[3] D. Shechtman et al. Physical Review Letters, 53, 1951, (1984).

Keywords: *Quasicrystal, flat-band, Moiré.*

MOF-5 ORGANOMETALLIC STRUCTURE AS A SENSOR FOR POLLUTANT GAS DETECTION

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Metal-organic frameworks (MOFs) constitute a class of crystalline porous materials in which metal ions or clusters are coordinated with organic ligands [1]. The exceptionally high porosity and extensive internal surface area render MOFs promising for applications, including clean energy technologies, electrocatalysis, and sensors [2]. Despite the wide range of physical properties exhibited by MOFs, there has been a limited number of studies on their electronic structure [3]. Nonetheless, it is well established that the electronic structure is crucial in determining the electronic, magnetic, optical, and chemical properties of these materials [4]. Indeed, the interaction and affinity between MOFs and various molecules can be effectively identified by observing changes in the band structures, work function, capacitance, and other electrical characteristics, thereby making these materials highly suitable for electronic sensors designed to detect small hazardous molecules [5]. One method to detect the presence of molecules within material structures is through X-ray photoemission spectroscopy (XPS). This technique allows one to extract information regarding the electronic structure of the absorbing atom and its local coordination environment, offering valuable insights into the sensing properties of MOFs [6]. Through density functional theory (DFT) studies and XPS simulations, we aim to theoretically investigate the potential of MOF-5 [$Zn_4O(BDC)_3$, BDC=benzodicarboxylate] as a sensor from a physics perspective. The calculation was performed by using the VASP code with the meta-GGA exchange-correlation functional, including intermediate-range van der Waals interactions (SCAN+rVV10). Our study focuses on the interaction of hazardous molecules like SO_2, CO_2, NO_2, and CO, within the the metal center of MOF-5. Pristine MOF-5 exhibits semiconductor characteristics, with a band gap energy of 3.44 eV. We observe that the adsorption of all molecules on the metal center is energetically stable. Except for CO, charge transfer from MOF-5 to the molecules was observed through the analysis of the Bader charge. Additionally, the organic ligands predominantly influence the states near the Fermi level. However, the CO and CO_2 molecules do not significantly affect the electronic structure of MOF-5. In contrast, a reduction in the band gap was observed for SO_2 and NO_2, with values of 2.6 eV and 1.8 eV, respectively. Notably, for NO_2, the magnetic moment of the nitrogen atom induces a spin-polarized band structure. Employing XPS simulations, a significant core-level shift (CLS) in the binding energy of Zn 2p near the NO_2 molecule was identified. The other molecules exhibit a CLS near the experimental limit, although still identifiable through XPS simulations. Therefore, our results indicate the potential for detecting NO_2 using MOF-5 as a photoemission sensor, contributing to applications in air and environmental monitoring and control.

References:

[1] S. L. James, "Metal-organic frameworks," Chem. Soc. Rev., vol. 32, pp. 276–288, 5 2003.

[2] H.-C. Zhou, J. R. Long, and O. M. Yaghi, "Introduction to metal–organic frameworks," Chem. Rev., vol. 112, no. 2, pp. 673–674, 2012.

[3] K. T. Butler, C. H. Hendon, and A. Walsh, "Electronic structure modulation of metal–organic frameworks for hybrid devices," ACS Applied Materials & Interfaces, vol. 6, no. 24, pp. 22 044– 22 050, 2014.

[4] B. Singh, A. Singh, A. Yadav, and A. Indra, "Modulating electronic structure of metal-organic framework derived catalysts for electrochemical water oxidation," Coord. Chem. Rev., vol. 447, p. 214 144, 2021.

[5] A. Chidambaram and K. C. Stylianou, "Electronic metal-organic framework sensors," Inorg. Chem. Front., vol. 5, no. 5, pp. 979–998, 2018.

[6] E. A. Dolgopolova, A. M. Rice, C. R. Martin, and N. B. Shustova, "Photochemistry and photophysics of mofs: Steps towards mof-based sensing enhancements," Chem. Soc. Rev., vol. 47, no. 13, pp. 4710–4728, 2018.

Keywords: *Density Functional Theory, X-ray Photoemission Simulation, MOF-5, Pollutant Molecule Sensor.*

AB-INITIO STUDY OF TOPOLOGICAL PROPERTIES OF A3BO ANTIPEROVSKITES

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In this work, we present an ab-initio study of the antiperovskite family A3BO (A = Ca, Ba; B = Sn, Pb, Ge), characterized by Pm3m space group. Employing density functional theory (DFT) calculations, we optimized lattice parameters and unveiled the electronic band structure. The inclusion of spin-orbit coupling (SOC) induced band inversion, a hallmark of topological materials. Calculated energy band gaps are in good agreement with experimental and theoretical reports [1]. Topological invariants derived from irreducible representations classify these materials as topological crystalline insulators. We further discuss the potential of these antiperovskites as higher-order topological insulators, with a particular focus on the possibility of realizing robust hinge states protected by crystalline symmetries.

References:

[1] Yuan Fang and Jennifer Cano. Phys. Rev. B 101, 245110 (2020)

Keywords: *Antiperovskites, Topological Crystalline Insulators, HOTI.*

HIGH FIELD MAGNETOTRANSPORT MEASUREMENTS OF THE TOPOLOGICAL SEMI-METAL AND CHARGE DENSITY WAVE COMPOUND TATE4

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The study of the coupling between topological states of matter and correlated states such as superconductivity or density waves in quantum materials has been an active field of research in experimental condensed matter physics in recent years. In this sense, TaTe4, a representative of the family of transition metal tetrachalcogenides, appears as a perfect standpoint to study this kind of interplay, since it is a long known-charge density wave system and a predicted topological semi-metal. Here we present a detailed study of the electronic band structure of this compound, through a combination of high field magnetotransport measurements via the Shubnikov de Haas effect, and density functional theory calculations. We provide evidence for the presence of Fermi surface sections not previously reported and analyze their connection with the predicted topological states for this compound.

Keywords: *Charge density wave, topology, magnetotransport measurements, Fermi surface.*

Magnetism, Strongly Correlated Systems, Collective Phenomena, Low-Temperature Physics

DISCONTINUOUS, COMPENSATION AND HYSTERESIS PHENOMENA IN A HIGH-SPIN ISING-TYPE FERRIMAGNET: S=3/ Q=7/2

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The research consists in describing qualitatively, through of an interaction Hamiltonian and a Monte Carlo method, the phenomena of discontinuity, compensation, and hysteresis in an Ising-type ferrimagnet of high spins (S=3 and Q=7/2), configured in a square lattice. The system undergoes this type of phenomena under the action of an external magnetic field, exchange interactions next-nearest neighbors, and the magnetocrystalline anisotropies of the sublattices that compose it. The increase in the modulus of the anisotropies of the sublattices implies a decrease in the temperatures at which the system presents compensation points and discontinuities in the magnetization. Likewise, the increase in the exchange interaction and the external field leads to a decrease in the compensation temperatures. The ferrimagnet exhibits multiple hysteresis loops and superparamagnetism, due to anisotropic and exchange effects.

References:

[1] Julio Cesar Madera, Nicolás De La Espriella, and Rhonald Burgos. Hysteresis and double-spin compensation behaviors in a ferroferrimagnetic model of high half-integer spins. physica status solidi (b), 260(4):2200517, 2023.

[2] Ying An, Shi-qi Xu,WeiWang, Zhen-yao Xu, and Bo-chen Li. An análisis of magnetic and hysteresis characteristics of a mixed spin ising-type borophene monolayer. Micro and Nanostructures, 183:207672, 2023.

[3] Bo-chen Li, Dan Lv, Wei Wang, Lei Sun, Zi-Ming Hao, and Jia Bao. Compensation temperature and hysteresis behaviors of a graphene-like bilayer: Monte carlo study. Communications in Theoretical Physics, 75(4):045702, 2023.

[4] Xiao-han Zhang, Wei Wang, Bo-chen Li, and Ying An. Exploring magnetic properties of an edge-modified kekulene multilayer cluster in an external magnetic field. The European Physical Journal Plus, 138(4):333, 2023.

[5] Mustafa Gençaslan and Mustafa Keskin. Dynamic magnetic hysteresis features of a mixed spin (2, 5/2) Ising system on a hexagonal lattice under an oscillating magnetic FIeld within the path probability method. International Journal of Modern Physics B, page 2450198, 2023.

[6] R. Masrour. Study of magnetic properties of Ising nanowires with core-shell structure. The European Physical Journal B, 96(7):100, 2023.

[7] M. Jerrari, R Masrour, and T Sahdane. Monte carlo study of magnetic and magnetocaloric properties of the graphene alternate layers of a ferrimagnetic mixed spins S = 3/2 and Q = 2. MRS Communications, 13(6):1171-1179, 2023.

[8] M Bessimou and R Masrour. Magnetocaloric e_ect and magnetic properties of dy2comno6: Monte carlo study. Philosophical Magazine, 103(1):56-66, 2023.

[9] Dan Lv, Hui-yi Li, De-zhi Zhang, and Bo-chen Li. Insights into magnetic behaviors of an ising graphene ladder-type chain structure applied in an external magnetic field. Micro and Nanostructures, 180:207609, 2023.

[10] J.C. Madera, M. Karimou, and N. De La Espriella. Effect of exchange, anisotropy, and external field interactions on the hysteresis and compensation of a two-dimensional ferrimagnet. Physica A: Statistical Mechanics and its Applications, page 129341, 2023.

Keywords: *Ferrimagnetic system, discontinuities, compensation temperatures, hysteresis*

FORMATION, GENERATION AND STABILITY OF MAGNETIC VORTEX IN INDIVIDUAL CO85NI15 NANOWIRES WITH TRANSVERSAL MAGNETIC ANISOTROPY

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Isolate cylindrical nanowires with transverse magnetic anisotropy exhibit remanent states composed of magnetic vortices, which can arrange transversely forming chains of vortices with alternating chirality, or longitudinally separated by states known as chiral domain walls [1]. The manipulation and control, both individually and collectively, of these magnetic configurations open new possibilities in information storage applications such as racetrack memory [2], as well as in logic gates [3]. Additionally, the rapid movement of domain walls suggests that a device leveraging these magnetic configurations could operate at exceptional speeds [4]. In this study, inspired by the work developed by Andersen et. al. [1,5], a computational model was performed using mumax3 [6,7], where a cylindrical geometry with dimensions of 70 nm in diameter and 1600 nm in length was established (see Figure 1), with a uniaxial magnetocrystalline anisotropy of 350 kJ/m^3 oriented at 78° with respect to the nanowire axis, for the hexagonal close-packed (Khcp) phase, and 100 kJ/m^3 oriented at 81° with respect to the axis of the nanowire, for the face-centered cubic (Kfcc) phase [8]. Additionally, an exchange stiffness constant of 26 pJ/m^3 and a saturation magnetization of 1273 kA/m for both phases were considered [9]. The external magnetic field was modelled with a sigmoid function, used to mimic the abrupt removal, and bring the system to remanence from a saturated state. Transversal vortex chains were obtained at both absolute zero (0 K) and room temperature (300 K) when saturation fields were applied oriented between -2° and 2° with respect to an axis perpendicular to the nanowire and the magnetocrystalline anisotropy. At larger angles, exotic configurations composed of longitudinal magnetic vortices are formed, which can be uniform at 0 K (see Figure 2) or very irregular at 300 K (see Figure 3). These results demonstrate that the stabilization of transverse magnetic vortices requires saturation fields remarkably close to an axis perpendicular to the nanowire, a result that is not affected by increasing temperature.

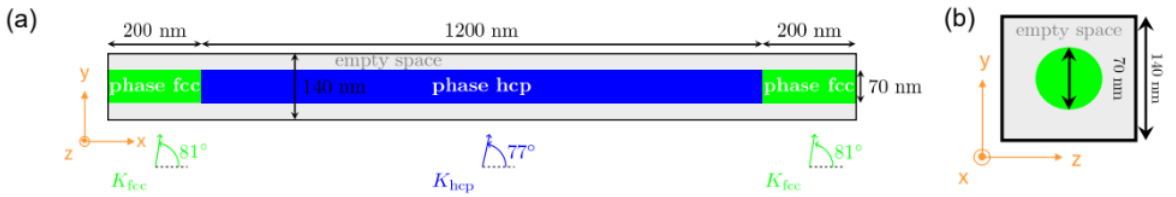

Figure 1. (a) Two regions are established in the nanowire: the blue region represents the hcp phase, where uniaxial anisotropy is set, and the green region represents the fcc phase, where cubic anisotropy is set. (b) Dimensions of the nanowire cross-section.

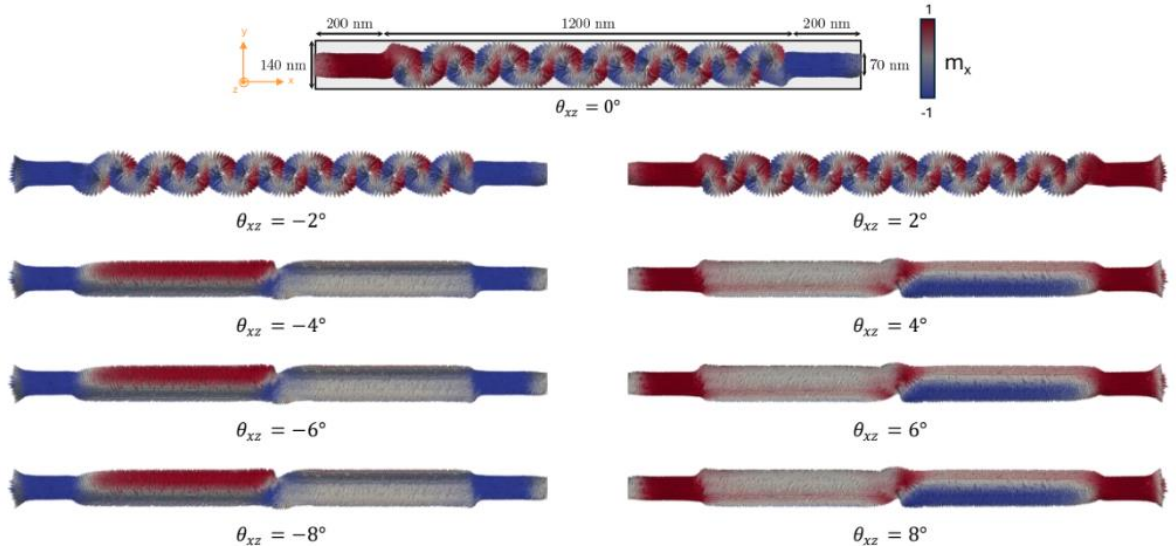

Figure 2. Micromagnetic simulations of Co85Ni15 nanowires as a function of the saturation magnetic field direction at 0 K. θXZ is an angle measured with respect to an axis perpendicular to the nanowire.

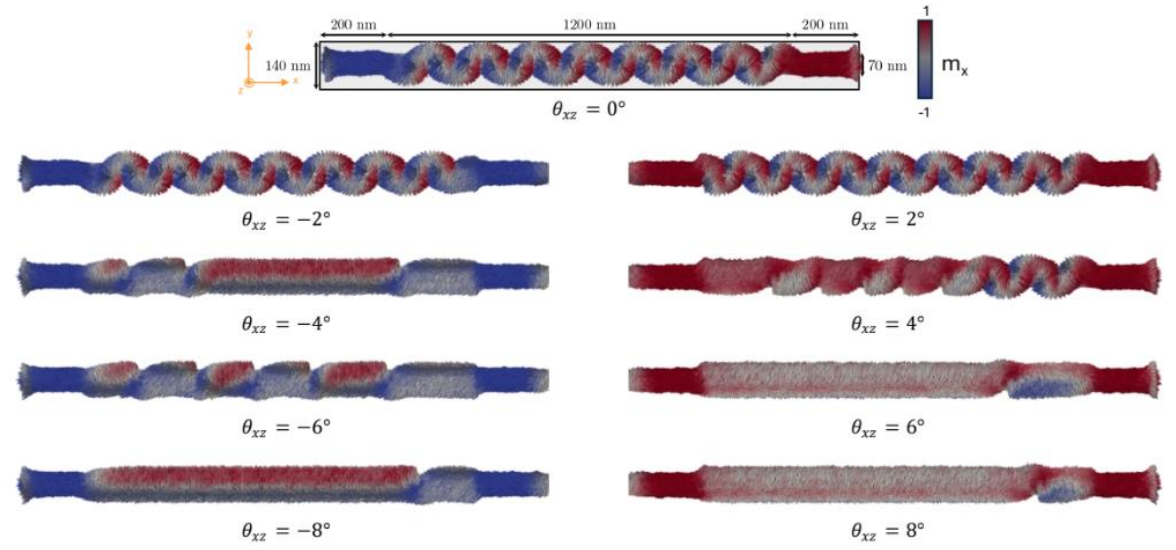

Figure 3. Micromagnetic simulations of Co85Ni15 nanowires as a function of the saturation magnetic field direction at 300 K. θXZ is an angle measured with respect to an axis perpendicular to the nanowire.

References:

[1] I. M. Andersen et al., Field Tunable Three-Dimensional Magnetic Nanotextures in Cobalt-Nickel Nanowires, Phys. Rev. Res. 3, 033085 (2021).

[2] S. S. P. Parkin, M. Hayashi, and L. Thomas, Magnetic Domain-Wall Racetrack Memory, Science 320, 190 (2008).

[3] J. Jaworowicz, N. Vernier, J. Ferré, A. Maziewski, D. Stanescu, D. Ravelosona, A. S. Jacqueline, C. Chappert, B. Rodmacq, and B. Diény, Magnetic Logic Using Nanowires with Perpendicular Anisotropy, Nanotechnology 20, 215401 (2009).

[4] R. Hertel, Ultrafast Domain Wall Dynamics in Magnetic Nanotubes and Nanowires, J. Phys. Condens. Matter 28, 483002 (2016).

[5] I. M. Andersen, L. A. Rodríguez, C. Bran, C. Marcelot, S. Joulie, T. Hungria, M. Vazquez, C. Gatel, and E. Snoeck, Exotic Transverse-Vortex Magnetic Configurations in CoNi Nanowires, ACS Nano 14, 1399 (2020).

[6] A. Vansteenkiste, J. Leliaert, M. Dvornik, M. Helsen, F. Garcia-Sanchez, and B. Van Waeyenberge, The Design and Verification of MuMax3, AIP Adv. 4, 107133 (2014).

[7] J. J. Joos, P. Bassirian, P. Gypens, J. Mulkers, K. Litzius, B. Van Waeyenberge, and J. Leliaert, Tutorial: Simulating Modern Magnetic Material Systems in Mumax3, J. Appl. Phys. 134, 171101 (2023).

[8] A. Carl, D. Weller, R. Savoy, and B. Hillebrands, HCP-FCC Phase Transition in Co−Ni Alloys Studied With Magneto-Optical Kerr Spectroscopy, MRS Online Proc. Libr. 343, 351 (1994).

[9] A. S. Samardak et al., Variation of Magnetic Anisotropy and Temperature-Dependent FORC Probing of Compositionally Tuned Co-Ni Alloy Nanowires, J. Alloys Compd. 732, 683 (2018).

Keywords: *Micromagnetic simulations, transverse anisotropy, nanowires, magnetic vortex, mumax3, vortex chain.*

PAIRS AND STRIPES PHASES IN AN ANTIFERROMAGNET WITHIN THE EXTENDED HUBBARD MODEL

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The conduction mechanism is the key to understanding superconductivity in materials. Cooper pairs are the charge carriers in superconductivity, but stripe-type phases are also found in type II superconductors [1,2] and might be important for high-temperature superconductivity [3]. In this work, we present a pairing mechanism in a two-dimensional antiferromagnetic material within the extended Hubbard model with repulsive electron-electron interaction and Ising-type spin interactions at different band occupancy levels. This model can show that charge transport is via hole pairs or stripe-type phases. The effects of repulsion and carrier concentration on the conduction mechanism are discussed. It is shown how the competition between kinetic energy, coulombic repulsion and antiferromagnetic order can lead to complex electronic structures and transport mechanisms.

References:

[1] Emery VJ, Kivelson SA, Tranquada JM. Stripe phases in high-temperature superconductors. Proc Natl Acad Sci U S A. 1999 Aug 3;96(16):8814-7

[2] Zheng, Bo-Xiao, Chia-Min Chung, Philippe Corboz, Georg Ehlers, Ming-Pu Qin, Reinhard M. Noack, Hao Shi, Steven R. White, Shiwei Zhang, and Garnet Kin-Lic Chan. 2017. "Stripe Order in the Underdoped Region of the Two-dimensional Hubbard Model". Science 358 (6367): 1155–60.

[3] Park, S., Kim, S.Y., Kim, H.K. et al. Superconductivity emerging from a stripe charge order in IrTe2 nanoflakes. Nat Commun 12, 3157 (2021).

Keywords: *Superconductivity, Hubbard model, Antiferromagnetism.*

STUDY OF EFFECT OF INCLUSION OF MULTIWALLED CARBON NANOTUBES (MWCNTS) IN STRUCTURAL AND ELECTRICAL PROPERTIES OF SAMPLES OF YBA2CU3O7−δ (YBCO)

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$YBa_2Cu_3O_{7-\delta}$ (YBCO) high temperature superconductor (HTSC) is a kind of ceramic superconductor which is very important due to its several applications some of them related with the production of strong magnetics fields make by superconductors coils to be used in numerous purposes as, for instance, in fusion energy [1–4]. To achieve high critical current density, Jc, at high magnetic fields, HTSCs can be embedded with nanostructure materials and carbon base compounds. Most of nanoparticles and carbon nanotubes (CNTs) can act as flux pinning centers because of their small sizes, or they can improve the grains boundary connections by localizing between HTSCs grains, and enhance pinning energy Uj and critical current density Jc [4–6]. In this work, we study the dependence of structural and electric properties of superconductor YBCO as a function of the inclusion of Multiwalled Carbon Nanotubes (MWCNTs) with a diameter between 4 and 10 times bigger than coherence length, ξ, of YBCO. For that purpose, we synthesized composites of 0.0, 0.2, 0.4, 0.6 and 0.8 %w/w MWCNTs (C00, C02, C04, C06, and C08 samples respectively). Additionally, we characterized the samples structurally using X-Ray Diffraction, and vibrationally with Raman and FTIR spectroscopy. Thanks to spectral and diffractograms obtained, we could conclude the presence of CuO phase in all samples, and Y_2BaCuO_5(Y-211) in all composites with WMCNTs [7]. Also, the presence of two superconductor phases ($YBa_2Cu_3O_{6.73}$ and $YBa_2Cu_{2.78}O_7$) in the C00 sample and presence of $YBa_2Cu_3O_{6.73}$ in the other composites (C02-C08). In this composites it was obtained a vibrational frequency ~600 cm^{-1} associated with a presence of Y-211 phase and the rupture of CuO_2 chains promoted for WMCNTs presence [8,9].

References.

[1] Gui, X.; Lv, B.; Xie, W. Chemistry in Superconductors. Chem. Rev. 2021, 121 (5), 2966–2991. https://doi.org/10.1021/acs.chemrev.0c00934.

[2] Chu, C. W.; Deng, L. Z.; Lv, B. Hole-Doped Cuprate High Temperature Superconductors. Physica C: Superconductivity and its Applications 2015, 514, 290–313. https://doi.org/10.1016/j.physc.2015.02.047.

[3] Sharma, R. G. Superconductivity: Basics and Applications to Magnets; Springer Series in Materials Science; Springer International Publishing: Cham, 2021; Vol. 214. https://doi .org/10.1007/978-3-030-75672-7.

[4] Sahoo, B.; Routray, K. L.; Mirdha, G. C.; Karmakar, S.; Singh, A. K.; Samal, D.; Behera, D. Investigation of Microhardness and Superconducting Parameters of CNTs Blended YBCO Superconductor. Ceramics International 2019, 45 (17, Part A), 22055–22066. https://doi.org/10.1016/j.ceramint. 2019.07.222.

[5] Hannachi, E.; Almessiere, M. A.; Slimani, Y.; Alshamrani, R. B.; Yasin, G.; Ben Azzouz, F. Preparation and Characterization of High-Tc (YBa2Cu3O7- δ)1-x/(CNTs)x Superconductors with Highly Boosted Superconducting Performances. Ceramics International 2021, 47 (16), 23539–23548. https://doi.org/10.1016/j.ceramint.2021.05.071.

[6] Dadras, S.; Liu, Y.; Chai, Y. S.; Daadmehr, V.; Kim, K. H. Increase of Critical Current Density with Doping Carbon Nano-Tubes in YBa2Cu3O7− δ . Physica C: Superconductivity 2009, 469 (1), 55–59. https://doi.org/10.1016/j.physc.2008.11.004.

[7] Antončík, F.; Sedmidubský, D.; Jiříčková, A.; Lojka, M.; Hlásek, T.; Růžička, K.; Jankovský, O. Thermodynamic Properties of Stoichiometric Non-Superconducting Phase Y2BaCuO5. Materials 2019, 12 (19), 3163. https://doi.org/10.3390/ma12193163.

[8] Liarokapis, E. Raman Spectroscopy, Structural Modifications, and Phase Transitions in the High Temperature Superconductors. Journal of Superconductivity 2000, 13 (6), 889–893. https://doi.org/10.1023/A:1026470316446.

[9] Ferraro, J. R. Practical Fourier Transform Infrared Spectroscopy: Industrial and Laboratory Chemical Analysis; Elsevier, 2012.

Keywords: *High Temperature Superconductors (HTS), Critical Current Density, Coherence length, Critical Temperature.*

MAGNETIC PROPERTIES OF SR2-XCEXFE1+X/2MO1-X/2O6 DOUBLE PEROVSKITE SYSTEM

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The ferromagnetic half-metallic Sr_2FeMoO_6 compound is considered a fundamental material to understand the electronic properties and high Curie temperature in double perovskites. This work presents the results of the structural and magnetic characterization of Ce doping in Sr_2FeMoO_6 compound. The samples were synthesized via solid-state reaction for Ce compositions from x= 0 to =0.5, with 0.05 increments. X-ray diffraction and Rietveld analysis for Ce concentrations showed a phase transition from tetragonal to monoclinic structure. The granular and percolated morphology of the samples was confirmed by scanning electron microscopy. Magnetic properties such as magnetic susceptibility, Curie temperature and the magnetoresistance were determined.

References:

[1] K. I. Kobayashi, T. Kimura, H. Sawada, K. Terakura, Y. Tokura, Nature 395, 677 (1998).

[2] T. E. Soto, J. L. Valenzuela, R. Mondragón, R. Morales, J. Lemus-Ruíz, O. Navarro, Phys. B: Cond. Matt. 455 (2014).

[3] B. Aguilar, T. E. Soto, J. de la Torre Medina and O. Navarro, Phys. B: Cond. Matt. 556, 108 (2019).

[4] Y. Ruiz, B. Aguilar, C. Carvallo, J. de la Torre Medina and O. Navarro, Int. J. Mod. Phys. 33, 1950344 (2019).

[5] M. Retuerto, J. A. Alonso, M. J. Martínez-López, N. Menendez, J. Tornero and M. García-Hernández, J. Mater. Chem. 16, (2006).

Keywords: *solid state, spintronic, magnetorresistence.*

ORDER-DISORDER DYNAMIC PHASE TRANSITION IN A MAGNETITE NANOPARTICLE AND ITS RELATIONSHIP WITH MAGNETIC HYPERTHERMIA: A MICROMAGNETIC APPROACH

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Magnetic nanoparticles (MNPs) have attracted recently a great interest in biomedical applications. One of them is magnetic hyperthermia for selective killing of cancer cells [1]. More concretely, MNPs can act as nanoheaters when they are under the influence of an alternating magnetic field (AMF). In this work, micromagnetic simulations have been used by solving the Landau-Lifshitz-Gilbert (LLG) equation to investigate the ground state of the magnetization dynamics of a single-domain nanoparticle of magnetite in an external AMF. Special attention has been paid to the circumstances dealing with a dynamic phase transition (DPT) when the amplitude and frequency of the AMF are varied. Moreover, we also focus on the influence of the orientation of the magnetic easy-axis of the MNP with respect to the direction of the external field, on the dynamic magnetic properties. Thus, by considering a wide range of orientations of the polar angle formed between the easy-axis and the field direction, it was possible to conclude that for amplitudes of the external AMF below a certain critical value, the system is not able to follow the magnetic field and it is found to be anchored in a dynamically ordered phase (DOP), whereas for larger amplitudes, the state corresponds to a dynamically disordered phase (DDP) where the magnetization is able to follow the external AMF, and for which dynamic hysteresis loops can be resolved [2]. From the area elapsed by the hysteresis loops it is possible to infer the energetic losses and therefore to obtain the Specific Loss Power (SLP), which is a relevant amount for determining the efficiency for magnetic hyperthermia. Our results suggest that the way the order-disorder DPT takes place and both the metastable lifetime as well as the SLP, are strongly dependent on the interplay between the orientation of the magnetic easy-axis and the amplitude and frequency of the external AMF. Our main results are summarized in a proposal of dynamic phase diagram.

References:

[1] Narayanaswamy, V.; Jagal, J.; Khurshid, H.; Al-Omari, I.A.; Haider, M.; Kamzin, A.S.; Obaidat, I.M.; Issa, B. Hyperthermia of magnetically soft-soft core-shell ferrite nanoparticles. Int. J. Mol. Sci. 2022, 23, 14825.

[2] Roa, N.; Restrepo, J. Micromagnetic Approach to the Metastability of a Magnetite Nanoparticle and Specific Loss Power as Function of the Easy-Axis Orientation. Physchem 2023, 3, 290-303. https://doi.org/10.3390/physchem3030020

Keywords: *Dynamic phase transitions, magnetic hyperthermia, Specific Loss Power, Magnetite Nanoparticles*

GE-NW/LATIO3 NANOSTRUCTURED MATERIALS

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The couple of nanostructured systems allows the development of innovative electrochemical systems, and this possibility motivated this work: to identify the electronic structure of the electrode/electrolyte interface of nanostructured materials. A germanium nanowire (Ge-NW) electrode, on a $LaTiO_3$ (LTO) perovskite oxide surface serving as an electrolyte, was modelled to study the electronic structure within the framework of the Density Functional Theory with the Hubbard-corrected Local Density Approximation. The shape of the Ge-NWs' cross-section changes and this depends on their orientation at the LTO electrolyte, as shown after the geometric optimization and due to the interactions between the Ge-NW and the LTO surface, evidenced by the electronic charge redistribution. The Ge-NW with the smaller diameter contact the LTO surface, it loses electronic charge. For larger Ge-NW, the depletion of electronic charge takes place either at the nanowire's surface or its cross-sectional center. The Ge/LTO systems with the smaller Ge-NWs exhibit metallic behavior. When the nanowire diameter increase, the systems turn into either a half-metal or a semiconductor, depending on the LTO electrolyte and Ge-NW relative orientation.

Keywords: *Electronic structure, Density Functional Theory, perovskite surface.*

LOCAL SYMMETRY OF CO, IN CO-DOPED ZNO NANOCRYSTALS

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Numerous physical and chemical methods have been used to produce ZnO or ZnO doped with transition metals (TM) [1-3]. In the process of doping this material, some studies suggest that the substitution of the doping metal occurs at the site where Zn is located. However, this may not be entirely accurate. It is possible that the TM is lodged in interstices within the wurtzite-like structure of ZnO or in places separate from where Zn is found in the crystal structure. This discrepancy could be due to differences in ionic radius between TM and Zn^{2+} or the preparation conditions of the doped samples, such as calcination temperature, acidity, etc., which may not allow for isomorphic substitution. Consequently, some magnetic and optical properties may vary based on the exact location of the dopant within the ZnO crystalline structure.

The objective of this work is, first, to evaluate the introduction of cobalt (Co) into the ZnO crystal structure at different Co concentrations, using X-ray diffraction (XRD) and electron paramagnetic resonance (EPR). The sol-gel method was used to prepare the single crystals. Secondly, the study aims to evaluate the magnetic characteristics of the interactions between neighboring magnetic ions. The results show that Co^{2+} replaces Zn^{2+} in the ZnO lattice, and the local symmetry where Co is accommodated in the ZnO lattice does not undergo deformation, preserving its undeformed axial symmetry. The EPR spectra were interpreted by considering four distinct paramagnetic centers, each experiencing single-ion anisotropy (D = 100 GHz). These centers include one comprising a Co^{2+} ion with a nearly isotropic g-tensor, two Co^{2+} ions exhibiting axial symmetry, and a fourth center attributed to two ferromagnetically coupled Co^{2+} ions (J = -6368 MHz).

References:

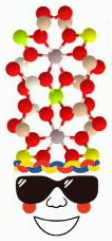
[1] S. Morasae, et al., Recent progress on doped ZnO nanostructures for visible-light photocatalysis. Thin Solid Films 605 (2016) 2–19. http://dx.doi.org/10.1016/j.tsf.2015.12.064

[2] F. Acosta-Humánez, C. Vargas-Hernandez, O. Almanza, Effect of sintering temperature on the structure and mean crystallite size of Zn1-xCoxO (x = 0.01 – 0.05) samples. Superficies y vacío, 27 (2) (2014) 43–48.

[3] R. Böttcher, et al., Local zincblende coordination in heteroepitaxial wurtzite Zn1-xMgxO:Mn thin films with 0.01 ≤ x ≤ 0.04 identified by electron paramagnetic resonance. Journal of Materials Chemistry C, 3 (45) (2015) 11918–11929. https://doi.org/10.1039/C5TC02720A.

Keywords: *ZnO, Electron Paramagnetic Resonance, DRX, nanocrystals.*

POSTERS



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Nanomaterials, Low-Dimensional Systems, and Novel Materials

ADSORPTION OF TOXIC GASES ON METAL-DECORATED SIGE NANOSHEETS: A DFT OUTLOOK

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Today, life is threatened by climate change and atmospheric pollution, which impacts worldwide flora and fauna. Toxic gases, such as CO and NO, mainly generated by combustion processes, also affect human health when exposed in large quantities. For this reason, there has been continuous research in the development of new and better materials that can detect toxic molecules, or, alternatively, new materials that can trap these molecules and thus remove them from the environment. Research in nanomaterials has opened a wide spectrum of applications in practically all fields of knowledge and, with the synthesis of graphene in 2004, there was a boom in the study of two-dimensional materials. Nowadays, siligene (SiGe), a two-dimensional material composed of Si and Ge atoms in equal quantities and with a honeycomb structure has not yet been synthesized; however, the results of theoretical simulations that have been reported are quite promising for the potential use of SiGe in the areas of energy storage and molecule detection [1,2]. In this work, Density Functional Theory calculations, addressing the adsorption of toxic gas molecules on SiGe monolayers decorated with Au, Ag, and Cu atoms, are presented and their potential use as gas traps or gas detectors is evaluated. The model used for this study was a 4×4×1 SiGe supercell with a lattice parameter a = b = 15.8 Å and a vacuum space of 40 Å between layers. The calculations were performed using the SIESTA code with Grimme's DFT-D2 dispersion correction to account for van der Waals interactions. The results suggest that the metal atoms are strongly bonded to SiGe with chemisorption energies, making the desorption of these atoms from the adsorbent system highly challenging. Additionally, the results show that the adsorption energies between the toxic gases and the metal-decorated monolayer range from 0.2 to 1.2 eV, indicating that the study of its potential as a material for detecting or capturing these molecules is highly promising.

References:

[1] Cid et al. (2023). Metal-decorated siligene as work function type sensor for NH 3 detection: A DFT approach. Applied Surface Science, 610, 155541.

[2] Cid et al. (2022). Enhanced reversible hydrogen storage performance of light metal-decorated boron-doped siligene: a DFT study. International Journal of Hydrogen Energy, 47(97), 41310-41319.

Keywords: *DFT, 2D materials, sensing.*

ANALYSIS OF THE ABSORPTION AND OPTICAL EMISSION SPECTRA OF CARBON DOTS OBTAINED FROM THE PEELS OF TWO FRUITS AT TWO STAGES OF RIPENING

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The composition of the carbon dots depends on the precursor source and, consequently, the photoemission is associated with the precursor. To understand the functional groups that contribute to the optical response, we synthesized carbon dots by the hydrothermal method from plantain and orange peels. These by-products, depending on the state of ripening, contain mainly cellulose when green and simple sugars when ripe. The analysis then focused on studying the influence of the precursor composition on the optical response. The parameters used for the synthesis were 217 °C, 15 h, 80% reactor filling, and water as solvent. The centrifugation process was at 4427 RCF at 4 °C, and the supernatant was filtered with 200 nm membranes. For the optical characterization of the synthesized dots, we measured the FTIR and UV-vis absorption and, with spectrofluorimetric, the emission spectra. The FTIR results showed that the cellulose band was maintained in the spectra of the carbon dots obtained from green peels, while new bands of nitrogen groups were present in the carbon dots obtained from mature peels. In these last spectra, the cellulose band is degraded. By UV-Vis, two absorption bands were observed at 230 nm corresponding to π-π* bonds and 280 nm to n-π*. Regarding the emission of the carbon dots, these present a redshift with a maximum emission of around 440 nm for the dots from the green precursor and a maximum emission of around 456 nm for the dots from the mature precursor.

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Keywords: *carbon dots, hydrothermal synthesis, optical properties, state of ripeness.*

ANALYSIS OF THE OPTICAL RESPONSE OF CHROMATOGRAPHIC FRACTIONS OF CARBON DOTS SYNTHESIZED FROM PLANTAIN PEEL

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Carbon dots are a type of nanoparticle of great interest due to their photoluminescent properties, good stability in aqueous media, and ease of synthesis. The emission characteristics are associated with the precursor, the dots obtained, and the synthesis conditions. In this work, we used a hydrothermal synthesis process, which generates a product with a great diversity of nanoparticles with different sizes and compositions, requiring separation or purification methods so the samples or fractions collected in a chromatographic column are homogeneous. Therefore, the aim was to study the characteristics of the optical responses of carbon dots associated with the different fractions. In the development of the work, carbon dots were synthesized under the same conditions, from "Hartón" variety plantain peel (Musa paradisiaca) in two extreme states of ripeness, green and ripe, to observe the differences between the optical responses associated with the change in the composition of the peels. From an aqueous solution, we separated the samples by column chromatography. We selected two of the eight fractions collected for each precursor to analyze the differences in their emission maxima. The wavelengths obtained using spectrofluorometry for the two fractions of carbon dots synthesized from ripe plantain peels are 402 and 472 nm, and for green plantain at 408 and 448 nm. According to the SEM micrographs, differences in the shapes of the dots were observed depending on the precursor used and differences in size depending on the selected fraction. The samples characterized by UV-vis absorption spectroscopy exhibited π to π^* and n to π^* electronic transitions, corresponding to C=C, C=O, and C=N bonds of the nanoparticle's core and surface. Likewise, FTIR showed that the fractions with emission maxima at low energies present bands corresponding to nitrogen and oxygen functional groups. In contrast, the fractions with emission maxima at higher energy present an intense band characteristic of epoxide groups. These results confirm that carbon dots may show differences in the emission response due to the precursor's composition and the nanoparticles' structure and size.

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Keywords: *carbon dots, hydrothermal synthesis, nanoparticles, optical properties, chromatography.*

ANISOTROPIC EFFECTS ON FERRIMAGNETIC FECO ALLOY QUASI-SPHERICAL NANOPARTICLE: A MONTE CARLO STUDY

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By means of Monte Carlo simulations, the thermomagnetic behavior of a nanoparticle of quasi-spherical geometry and size 2 nanometers, constituted by cubic structures centered on the body B2-type of ferrimagnetic FeCo alloys, is studied. The sublattices are configured with spins of values S =±3/2, ±1/2 for Co and Q=±2, ±1, 0 for Fe. Due to the action of the magnetocrystalline anisotropies of the system, the model presents pseudocritical and compensation temperatures, superparamagnetism and hysteresis loops for low temperatures.

References:

[1] Junaid Ul Ahsan, Harkirat Singh, Atomistic simulation study of FeCo alloy nanoparticles, Applied Physics A (2022) 128:443. doi.org/10.1007/s00339-022-05589-8.

[2] Kavita Kumari, Akshay Kumar, MinJi Shin, Shalendra Kumar, Seok Hwan Huh, Bon Heun Koo, Investigating the magnetocrystalline anisotropy and the exchange bias through interface effects of nanocrystalline FeCo, Journal of the Korean Physical Society (2021) 79:1180–1189. doi.org/10.1007/s40042-021-00315-8.

[3] T. Hasegawa, T. Niibori, Y. Takemasa, M. Oikawa, Stabilisation of tetragonal FeCo structure with high magnetic anisotropy by the addition of V and N elements, Scientific reports, 2019, 9, 1-9. doi: https://doi.org/10.1038/s41598-019-41825-7.

[4] K. Htoutou, A. Arbaoui, Effective-field theory with the probability distribution technique for a spin-3/2 core and spin-2 shell Ising nanowire: Thermodynamic properties and hysteresis behaviors, Physica B: Physics of Condensed Matter, 2022, 1-24. https://doi.org/10.1016/j.physb.2022.414095.

Keywords: *Nanoparticle, FeCo alloys, pseudocritical and compensation temperatures, hysteresis.*

ANISOTROPY AND SURFACE RECONSTRUCTION EFFECTS OF NANOPOROUS NONPOLAR SEMICONDUCTORS: A FIRST-PRINCIPLES STUDY

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Porous semiconductors have a wide range of applications in electronics, energy storage, and nanomedicine [1-2]. Although many investigations have been conducted over the years on the properties of these materials, almost none have examined the effects of pore anisotropy and surface reconstruction on the electronic properties of nonpolar porous semiconductors such as Si or Ge [3]. This work studies the impact of anisotropy and surface reconstruction in porous Si and Ge using the first-principles Density Functional Theory. The porous are modeled using the supercell scheme by removing columns of atoms in the [001] and [110] directions from an otherwise perfect Si or Ge bulk crystal. For the surface dangling bonds, two calculation schemes were implemented: one where all the dangling bonds are passivated with H, and the other where the structure is first geometry optimized to observe any surface reconstructions on the pore surface, then, the remaining dangling bonds are passivated with H. The results show significant differences in the electronic band gap with respect to the percolation direction, mainly due to the different quantum confinement, with the [001] direction having different gaps due to its denser structure and walls that could be regarded as interconnected nanowires. The passivation process shows that two nanostructures arise from different starting points, with the surface reconstruction scheme having lower formation energy than the other case. These results could be useful for understanding the effects of surface reconstruction and pore anisotropy in nonpolar nanoporous semiconductors, which could be of importance for applications in sensing electronics, energy storage and optoelectronics.

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Refrences:

[1] Israel González, et al., "Sodium effects on the electronic and structural properties of porous silicon for energy storage". International Journal of Energy Research 46(7), 8760-8780 (2022).

[2] Jose E. Santana, de Santiago, et al., "Fluorinated porous silicon as sensor material for environmentally toxic gases: a first-principles study", Materials Advances 2(3), 1072-1082 (2021).

[3] Ricardo Bermeo-Campos, et al., "Surface morphology effects on the mechanical and electronic properties of halogenated porous 3C-SiC: A DFT study", Applied Surface Science 631, 157481 (2023).

Keywords: *Silicon, germanium, porous, semiconductors, DFT*

CHARACTERIZATION OF GRAPHENE UV PHOTOFETS WITH ALUMINUM OXIDE PASSIVATION

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Graphene has emerged as a promising material for optoelectronics due to its high carrier mobility and in combination with other materials it is possible to enhance its light absorption in certain wavelengths. Improving its performance in the ultraviolet (UV) range could be crucial in aerospace, biological [1], and UV astronomy applications [2]. We focus on the characterization of graphene field-effect-transistors (GFETs) with aluminum oxide passivation in the UV region, with wavelengths ranging from 405 nm to 280 nm. Our objective is to understand the effect of the aluminum oxide on the device's responsivity. Our findings suggest that the aluminum oxide encapsulation not only improves the graphene's stability but also enhances its UV sensibility significantly, reaching a peak near 300 nm wavelength with a responsivity of up to 50 A W-1.

References:

[1] E. Monroy, F. Omn s, and F. Calle, "Wide-bandgap semiconductor ultraviolet photodetectors,"Semicond. Sci. Technol., vol. 18, no. 4, pp. R33–R51, Apr. 2003, doi: 10.1088/0268-1242/18/4/201.

[2] M. P. Ulmer, "A review of UV detectors for astrophysics: past, present, and future," presented at the SPIE OPTO: Integrated Optoelectronic Devices, M. Razeghi, R. Sudharsanan, and G. J. Brown, Eds., San Jose, CA, Jan. 2009, p. 722210. doi: 10.1117/12.810039.

Keywords: *Ultraviolet light, Photodetectors, Graphene Field-Effect-Transistors.*

CURRENT VS. VOLTAGE CHARACTERISTIC IN AN AL_0.1IN_0.9AS/INAS_0.09N_0.01/AL_0.1IN_0.9AS DOUBLE-BARRIER HETEROSTRUCTURE

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In this article We report the study of the characteristic behavior of current in function of applied voltage for a double-barrier heterostructure (DBH) of InAsAl/InAsN/InAsAl, considering low Nitrogen concentrations (< 1%) for different temperature values and with a magnetic field applied parallel and/or perpendicular to the double-barrier system. This work used the theory of non-equilibrium Green's function (NEGF). The current-voltage curves show a new resonant states due to the incorporation of Nitrogen in the quantum well and the intensity of these peaks diminishes with the increased temperature In addition, our results show that the effect of the applied magnetic field perpendicular to the current is stronger compared with the applied magnetic field parallel to the current, yielding a behavior similar to the experimental data by Di Paola [1].

References:

[1] D. M. Di Paola, M. Kesaria, O. Makarovsky, A. Velichko, L. Eaves, N. Mori, A. Krier, and A. Patanè, Sci. Rep. 2016; 6, 32039.

[2] O. Drachenko, A. Patanè, N. V. Kozlova, Q. D. Zhuang, A. Krier, L. Eaves, and M. Helm, Appl. Phys. Lett. 98, 162109 (2011).

Keywords: *tunneling, double barrier, impurity.*

DISEÑO Y ANÁLISIS DE UNIDADES DE MEMORIAS TIPO MEMRISTOR BASADAS EN NANOTUBOS DE TIO2

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Las tecnologías de almacenamiento de datos son fundamentales para el uso amplio de dispositivos electrónicos. La necesidad de recolección, almacenamiento y recuperación de información lleva al diseño de sistemas y/o mecanismos de resguardo cada vez mejores. Estos ofrecen una mayor densidad de almacenamiento, además, una mayor velocidad de escritura y lectura con un menor consumo energético. Dentro de ese contexto, los memristores se convierten en una alternativa interesante para potenciar el uso de memorias tradicionales, gracias a sus propiedades de conmutación resistiva que permiten el cambio súbito y no volátil de la resistencia eléctrica de un material dieléctrico. El dispositivo propuesto se fundamenta en el diseño de un sistema digital, el cual, individualmente por medio de etapas, realiza la recepción y procesamiento de una señal discreta que utiliza para escribir un valor resistivo en un memristor basado en nanoestructuras de TiO_2. El TiO_2, es un material que tiene una gran capacidad para cambiar de resistencia, en respuesta a las cargas eléctricas aplicadas, información que se conserva para luego obtener nuevamente la señal original. En cuanto al dispositivo objeto de estudio de este trabajo, su diseño está compuesto por una fase de carga que, utilizando un circuito lógico integrado, define dos estados lógicos. Uno equivalente a 5V igual a la alimentación del circuito, que representa un 1 lógico, y otro estado de 1V que es equivalente a un 0 lógico. La selección de estos estados fueron asumidos con la intención de obtener un cambio resistivo efectivo, pues la tensión aplicada se encuentra por encima de la tensión de umbral, lo que permite un cambio en el memristor. También se cuenta con una etapa de control donde por medio de multiplexores y demultiplexores, que funcionan como conmutadores análogos, que se separan los dos circuitos requeridos para cada, la escritura y la lectura, se requieren separar a cada proceso, con el fin de conservar íntegramente la información en el memristor. La fase de lectura consiste en el uso de amplificadores operacionales que por medio de una configuración de resistencias, incluido el memristor, se amplifica una pequeña señal que no afecta el valor resistivo, permitiendo obtener el estado lógico almacenado, el cual luego se ve representado en el estado de encendido o apagado de un diodo LED; lo anterior, puede ser representado como una salida paralela de datos que luego puede ser transformada en la señal original ingresada. El sistema desarrollado cuenta con un modo digital con entradas SET/RESET, con el fin de realizar un borrado común, o negado, de la información. Se realizaron pruebas físicas en un diseño para 2 bits donde se demostró la correcta escritura y lectura en el memristor, se reportan las ventajas del sistema propuesto y se comprueba su funcionamiento a escala, en comparación con otros diseños de memorias no volátiles, resaltando la simplicidad en el diseño y la escalabilidad del mismo. Dispositivos o sistemas de

resguardo de información basados en nanoestructuras de TiO_2 presentan potenciales aplicaciones en su capacidad de almacenar más información debido a su fabricación por nanotecnología.

References:

[1] Barella, M. (2018). Dispositivos de memoria basados en TiO2: fabricación y caracterización en ambientes hostiles mediante un controlador dedicado. https://ri.conicet.gov.ar/handle/11336/83239

[2] Quezada López, M. A. (2020). Emulador analógico de memristor [Tesis de maestría en ciencias, Centro de investigación y de estudios avanzados del instituto politécnico nacional]. https://repositorio.cinvestav.mx/handle/cinvestav/3448

[3.] Quiroz, H. P., Calderón, J. A., & Dussan, A. (2020). Magnetic switching control in Co/TiO2 bilayer and TiO2:Co thin films for Magnetic-Resistive Random Access Memories (M-RRAM). Journal Of Alloys And Compounds, 840, 155674. https://doi.org/10.1016/j.jallcom.2020.155674

Keywords: *Memristor, Memory, Digital system, nanoestructuras de TiO2.*

EFFECT OF THE ELECTROLYTE SOLVENT ON THE PERFORMANCE OF SULFUR-GRAPHENE COMPOSITE CATHODES OF LITHIUM SULFUR BATTERIES: A CLASSICAL MOLECULAR DYNAMICS STUDY

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Lithium-sulfur (Li-S) batteries have emerged as an alternative technology with higher capacity, performance, and lower cost compared to traditional lithium-ion batteries. The reason for the enhanced performance is the use of sulfur as the primary material in battery cathodes, generating an increase in the theoretical specific capacity from 372 mAh/g of graphite batteries to 1673 mAh/g of batteries with sulfur cathodes, which leads to achieving a higher energy density for Li-S batteries in the range of 2500–2800 Wh/kg (1). Therefore, using Li-S batteries as energy storage devices capable of mobilizing vehicles is a promising alternative. However, despite the advantages of Li-S batteries, using sulfur as a cathode of such a battery is not practical due to its diffusion in the form of polysulfides through the electrolytic solution that separates the cathode from the anode. This loss of polysulfides in diffusion is known as the "shuttle" effect, which is the leading cause of battery life depletion due to the loss of material capable of storing lithium. Finally, research efforts have focused on developing electrode and electrolyte systems that limit the transport of polysulfides from the cathode to the anode. For example, the use of carbonaceous materials in the cathode as a conductive matrix can achieve the goal of obstructing the diffusion of polysulfides through interactions of sulfur with graphitic carbon (2).

On the other hand, developing electrolytic solutions as a lithium-ion transport medium with adequate polysulfide solubility has facilitated the development of batteries with good charge/discharge cycles and high energy densities. However, the lack of understanding of diffusion processes in electrolytic solutions within the composite cathode represents a theoretical obstacle to developing electrode systems media that minimize the loss of active material by diffusion during charge/discharge cycles. Thus, we aim in this study the diffusivity of polysulfides in common electrolyte organic solvents such as 1,2-dimethoxyethane (DME) and 1,3-Dioxolane (DOL) at different proportions in bulk and confinement. The objective is to relate the batteries' cycling performance to the electrode systems' architecture and composition. We used classical molecular dynamics (MD) simulations to compute diffusion coefficients from the mean-squared displacements of polysulfides in the electrolyte solvents. Dynamic trajectories obtained from classical MD simulations allowed the identification of the optimal solvent concentrations and evaluation of the effect of the graphitic cathode matrix on the diffusivity of polysulfide during discharge.

References:

[1] Burgos, J. C., Balbuena, P. B., & Montoya, J. A. (2017). Structural dependence of the sulfur reduction mechanism in carbon-based cathodes for lithium–sulfur batteries. The Journal of Physical Chemistry C, 121(34), 18369-18377.

[2] Kim, H., Lim, H. D., Kim, J., & Kang, K. (2014). Graphene for advanced Li/S and Li/air batteries. Journal of Materials Chemistry A, 2(1), 33-47.

Keywords: *Lithium sulfur batteries, Composite cathodes, Energy storage.*

EFFECTS OF CARBON DOPING ON HEXAGONAL BORON NITRIDE: A VCA STUDY

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Hexagonal boron nitride (h-BN) is a material of outstanding interest because of its exceptional properties and diverse applications across various fields, including electronics, optoelectronics, and quantum technologies [1].

Theoretical investigations of h-BN have involved advanced numerical methodologies, including the density functional theory (DFT), to computationally address the material properties such as thermal and electrical conductivity, stability, and electronic structure [2].

In particular h-BN in its 2D monolayer form, has emerged as a promising emitter of quantum light due to its optical, chemical, thermal, and fabrication properties. Its emission spectrum spans from ultraviolet to infrared wavelengths, making it a compelling subject for investigating photon emission properties toward applications in quantum computing, quantum crystallography, and quantum metrology [3].

An important aspect of material characterization involves understanding the role of defects in the crystalline structure. From the theoretical point of view, this is typically studied using the supercell method, which has a high computational cost, especially with increasing system complexity. To address these challenge, we explore an alternative approach for small substitutions using the Virtual Crystal Approximation (VCA). By incorporating virtual atoms into DFT calculations, VCA provides results comparable to those obtained with the supercell method, but at a significantly reduced computational cost [4].

By means of the VCA we obtain the band structure of slightly Carbon-doped h-BN, and observe how the monolayer emission can be tuned along a wide range of frequencies, with small changes in the doping. This underscores the versatility of h-BN as photon emitter for multiple applications, highlighting its importance in the current landscape of emerging quantum technologies.

References:

[1] Shaik, A. B. D. A. J. W. I., & Palla, P. (2021). Optical quantum technologies with hexagonal boron nitride single photon sources. Scientific reports, 11(1), 12285.

[2] Cahangirov, S., Topsakal, M., Aktürk, E., Şahin, H., & Ciraci, S. (2009). Two-and one-dimensional honeycomb structures of silicon and germanium. Physical review letters, 102(23), 236804.

[3] Mendelson, N., Chugh, D., Reimers, J. R., Cheng, T. S., Gottscholl, A., Long, H., ... & Aharonovich, I. (2021). Identifying carbon as the source of visible single-photon emission from hexagonal boron nitride. Nature materials, 20(3), 321-328

[4] Bellaiche, L., & Vanderbilt, D. (2000). Virtual crystal approximation revisited: Application to dielectric and piezoelectric properties of perovskites. Physical Review B, 61(12), 7877.

Keywords: *DFT, hBN, VCA.*

ELECTRONIC SPECTRUM OF GE-CORE/SI-SHELL NANOWIRES DETERMINED BY MEANS OF ATOMIC EFFECTIVE POTENTIAL CALCULATIONS

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Core/shell nanowires gain attention in current research due to their diverse technological applications [1]. In this realm, SiGe-based nanostructures offer the additional benefit of a direct implementation in modern devices [2]. In this work, we conduct atomistic calculations of the electronic structure of Ge-core/Si-shell nanowires. We consider structures grown along the [100] direction with different surface facet configurations. Moreover, we set the samples diameter to approximately 5 nm and set the Ge-core diameter to values ranging from 0.7 nm to 3.8 nm. The calculation process involves 1) setting the Si and Ge nonlocal effective atomic pseudopotentials [3] to reproduce the band offset reported by recent experimental reports, 2) defining and optimizing the atomic structure to consider the strain (fig. 1a) using classical elastic theory, and 3) solving the single particle Schrödinger equation. Our results show the formation of type-II heterostructures, where the VBM and CBM are localized in the core and shell, respectively (fig. 1b), and band gaps in the range from 0.5 eV to 1 eV approximately.

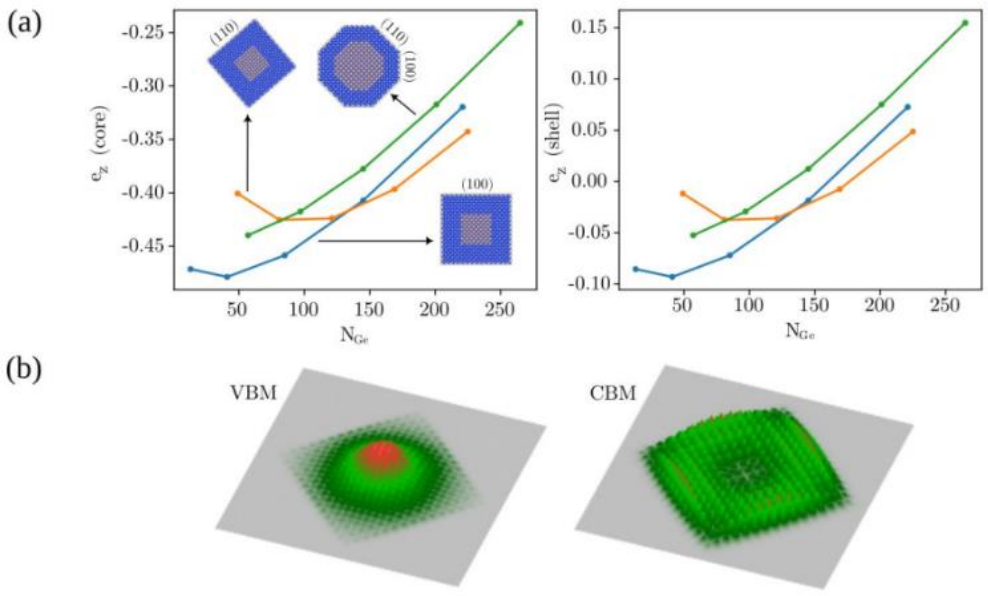

Fig 1: (a) Core and shell strains along the structure axis according to the number of Ge atoms. (b) Square-averaged wavefunctions of the valence band maximum (VBM) and conduction band minimum (CBM).

References:

[1] Ray, S. K., Katiyar, A. K. y Raychaudhuri, A. K. "One-dimensional Si/Ge nanowires and their heterostructures for multifunctional applications-a review". Nanotechnology 28, 092001 (2017).

[2] Bhuyan, P.D., Kumar, A., Sonvane, Y. et al. "Si and Ge based metallic core/shell nanowires for nano-electronic device applications". Sci Rep 8, 16885 (2018).

[3] J. R. Cárdenas and G. Bester, "Atomic effective pseudopotentials for semiconductors,"Phys. Rev. B 86, 115332 (2012). - J. Cárdenas, M. Bandera, and F. Nuñez-Murillo, "Multipole momento description of passivants and complex pseudopotentials for semiconductor surfaces," Computational Condensed Matter 33, e00765 (2022).

Keywords: *Atomistic calculations, electronic structure, Ge-core/Si-shell nanowires.*

ESTUDIO DE LAS PROPIEDADES VIBRACIONALES DE LOS DICALCOGENUROS DE METALES DE TRANSICIÓN WSE2 Y VSE2

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En este trabajo se presentan los estudios teóricos de las propiedades vibracionales de los dicalcogenuros de metales de transición WSe2 y VSe2. El estudio de los materiales se realizó en su fase 2H y 1T respectivamente, mediante aplicación de cálculos de primeros principios basados en la teoría del funcional de la densidad (DFT) y en la teoría de perturbaciones del funcional de la densidad (DFPT) implementada en el paquete Abinit [1]. Se empleó el funcional de intercambio y correlación PBE [2], para las interacciones de van der Waals se tuvo en cuenta la corrección semi empírica de Grimme DFT-D3 sin incluir correcciones de 3 cuerpos [3].

Se realizó un estudio de las frecuencias vibracionales empleando una malla de puntos q 12X 12X1 para cada uno de los materiales, utilizando dos bandas para el buffer de la estructura de bandas con fin de evitar las frecuencias imaginarias que son frecuentes en este tipo de materiales [1]. En las estructuras de bandas fonónicas obtenidas se observan nueve modos vibracionales en el centro de la zona de Brillouin. En el punto gama se observa una diferencia mayor de las frecuencias entre los modos ópticos y acústicos para el WSe2, 61.24cm^ 1 (7.6 meV). No se obtienen frecuencias de fonones imaginarias lo que indica estabilidad dinámica de las dos monocapas.

Referencias:

[1] Gonze, X., Jollet, F., Araujo, F.A., Adams, D., Amadon, B., Applencourt, T., Audouze, C., Beuken, J.M., Bieder, J., Bokhanchuk, A. and Bousquet, E., 2016. Recent developments in the ABINIT software package. Computer physics communications, 205, pp.106-131.

[2] John P Perdew. Unified theory of exchange and correlation beyond the local density approximation. Electronic structure of solids' 91, 11, 1991

[3] Stefan Grimme. Semiempirical gga-type density functional constructed with a long-range dispersion correction. Journal of computational chemistry, 27(15):1787–1799, 2006

Keywords: *DFPT, vibraciones*

EVALUATION OF THE DIFFUSION OF HEAVY METALS IN AQUEOUS MEDIUM ON GOLD SURFACES BY MEANS OF CLASSICAL MOLECULAR DYNAMICS SIMULATIONS

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The presence of contaminants in water bodies is a problem that demands high efforts in detection and remediation. Currently there are very efficient mechanisms for detecting pollutants, but they are high cost and difficult to port, in addition, it is not always possible to monitor the concentrations of pollutants "in situ" and in real time. This disadvantage has driven the generation of optical and electrochemical sensors that can work remotely and constantly during the day, sending information periodically. However, synthesizing materials for sensors that present a physicochemical response in the presence of contaminants is one of the most exciting challenges in materials science today.

In this work, we propose to take advantage of classical molecular dynamics simulations based on empirical force fields to predict the behavior of heavy metal ions in the presence of a gold surface that makes up fiber optic sensors. This gold surface was functionalized with molecules of 1,6-hexanodithiol, cysteamine, and L-cysteine, to evaluate the effect of functionalization on the affinity of heavy metal ions towards the sensors' surface. For the classical molecular dynamics simulations, the OPLS and Sutton-Chen forcefields and the SPC-E water model represented the interactions of the system components. The mean-squared displacement allowed the calculation of the diffusion coefficients of heavy metal ions in bulk, non-functionalized surface, and functionalized surface systems. The local density profiles along the z-axis allowed the affinity of heavy metal ions to gold surfaces to be analyzed.

Molecular dynamics simulations showed that the diffusion coefficients of heavy ions are strongly perturbed with the presence of the gold surface, considerably decreasing their values compared to when they are dissolved in water (bulk). With the insertion of the ligand molecules on the surface, we can observe that they remain bound to the surface by the thiol group due to a high affinity between this group and the gold atoms. The computational results allowed us to observe that ligand molecules have a substantial incidence on the diffusion coefficients of heavy metals, finding in most cases that the molecule of 1,6-hexanodithiol generates an even more significant decrease in the diffusion coefficients of heavy metals.

References:

[1] Zhang, Y. nan, Sun, Y., Cai, L., Gao, Y., & Cai, Y. (2020). Optical fiber sensors for measurement of heavy metal ion concentration: A review. In Measurement: Journal of the International Measurement Confederation (Vol. 158). Elsevier B.V. https://doi.org/10.1016/j.measurement.2020.107742

[2] Lee, J. S., Han, M. S., & Mirkin, C. A. (2007). Colorimetric detection of mercuric ion (Hg2+) in aqueous media using DNA-functionalized gold nanoparticles. Angewandte Chemie - International Edition, 46(22), 4093–4096. https://doi.org/10.1002/anie.200700269

[3] Liu, J., & Lu, Y. (2007). Rational Design of "Turn-On" Allosteric DNAzyme Catalytic Beacons for Aqueous Mercury Ions with Ultrahigh Sensitivity and Selectivity. Angewandte Chemie - International Edition, 46(40), 7587–7590. https://doi.org/10.1002/anie.200702006

[4] Wang, L., Zhang, J., Wang, X., Huang, Q., Pan, D., Song, S., & Fan, C. (2008). Gold nanoparticlebased optical probes for target-responsive DNA structures. Gold Bulletin, 41(1), 37–41. https://doi.org/10.1007/BF03215621

[5] Todorov, I. T., & Smith, W. (n.d.). THE DL POLY 4 USER MANUAL.

EXPLORING NEW 3D AND 2D STRUCTURES OF TIO2: THROUGH DFT

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In this work, the thermodynamic (formation energy), dynamic (phonon dispersion relation), and mechanic (elastic constants) stability of titanium dioxide TiO2 in its trigonal phase are established in bulk and monolayer forms, using Density Functional Theory (DFT) with the GGA-PBE approximation, along with atomic pseudopotentials and a plane wave basis. Additionally, D2 and D3 dispersion corrections are used to account for Van der Waals interactions. The monolayer is modeled using a periodic slab scheme, with a sufficiently large vacuum region (≈15 Å) to ensure that there are no interactions between the monolayer system and its image.

From the results, the formation energies of Ef = -2.542 eV/Cell and Ef = -2.509 eV/Atom for the bulk and monolayer T-TiO2 systems, respectively, shows that both systems are thermodynamically stable, making their growth in the laboratory theoretically possible.

The results of the second-order elastic constants (SOEC) indicate that both the bulk T-TiO2 system and the monolayer are mechanically stable. Additionally, the phonon dispersion relation indicates that the monolayer is dynamically stable.

From the DOS and electronic band structure, it is established that trigonal TiO2 is a non-magnetic semiconductor with an indirect bandgap. The bulk TiO2 presents an indirect bandgap of 2.487 eV, while the monolayer exhibits an indirect bandgap of 2.660 eV. Finally, the charge distribution in the bulk and monolayer systems shows an ionic bond between the constituents of the system due to the transfer of approximately two electrons from titanium to the pair of oxygen atoms to which it is bonded.

Keywords: *TiO2, DFT, formation energy, phonon dispersion relation, elastic constants, Bader charge.*

FERROIC ORDER ANALYSIS FOR W(S_(1-X) TE_X)_2(1- δ) CRYSTALS

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Transition metal dichalcogenides (TMDs), are chemical compounds of the form MX_2, with M being a transition metal (as for example W and Mo) and X being a chalcogenide (Te, Se and S) [1]. These specific materials exhibit interesting properties such as ferroelectricity, ferromagnetism and multiferroicity [2].

Recently, it has been found that in solid solutions of TMDs such as $W(Se_{1-x}\ Te_x)_{2(1-\delta)}$ multiferroic properties can be obtained, with x being the tellurium doping and δ being the vacancy doping [2]. The promotion of vacancies is such solid solutions permit us to envisage a strategy of design for new 2D multiferroic composites. In this context, we want to explore the solid solution of $W(S_{1-x}\ Te_x)_{2(1-\delta)}$, in search of multiferroic properties and their correlation with the formation of vacancies in the solid. This considering that WS2 is ferromagnetic [2,3-4]and WTe2 is ferroelectric [2,5].

In this work, $W(S_{1-x}\ Te_x)_{2(1-\delta)}$ crystals were grown using the chemical vapor transport (CVT) technique. Various spectroscopy techniques such as Raman, X-ray diffraction (XRD) and X-ray fluorescence (XRF) were used for their respective characterization. For the analysis of ferroic orders, a vibrating-sample magnetometer (VSM) was used to measure ferromagnetism and a piezoresponse force microscopy (PFM) was used to measure ferroelectricity.

Thus, in this poster we present the results obtained from the analysis of the ferroic properties in $W(S_{1-x}Te_x)_{2(1-\delta)}$ crystals that were synthesized.

References:

[1] Manzeli, S., Ovchinnikov, D., Pasquier, D., Yazyev, O. V. & Kis, A. 2D transition metal dichalcogenides. Nat Rev Mater 2, 1–15 (2017).

[2] Cardenas-Chirivi, G. et al. Room temperature multiferroicity in a transition metal dichalcogenide. npj 2D Mater Appl 7, 1–10 (2023).

[3] Luxa, J. et al. Origin of exotic ferromagnetic behavior in exfoliated layered transition metal dichalcogenides MoS2 and WS2. Nanoscale 8, 1960–1967 (2016).

[4] Ding, X. et al. Enhanced ferromagnetism in WS2 via defect engineering. J. Alloys Compd. 772, 740–744 (2019).

[5] Sharma, P. et al. A room-temperature ferroelectric semimetal. Science Advances 5, eaax5080 (2019).

Keywords: *Transition metal dichalcogenides, TMDs, ferroelectricity, ferromagnetism, multiferroicity, ferroic order.*

GERMANIUM NANOWIRES AS ACETONE-ADSORPTION MEDIUM FOR DIABETES DIAGNOSIS

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One key aspect of the successful treatment of diabetes, a global issue, is early detection. Acetone is a waste product of fat metabolism, which occurs when the body substitutes fat for sugar to generate energy. Individuals with diabetes produce excess acetone when there is insufficient insulin to transport glucose into cells; hence, acetone serves as a reliable indicator of diabetes. Germanium nanowires offer a set of properties that make them highly versatile and promising for various applications in electronics. Their high: chemical reactivity, surface-to-volume ratio, flexibility, and sensitivity, make them ideal materials for the adsorption and detection of chemical agents through a variety of mechanisms. In this work, an undoped and B-, Al-, or Ga-doped, germanium nanowire was studied as the base material for potential acetone molecule detection and diabetes diagnosis. The nanowires were modelled using the supercell scheme by removing atoms outside a circumference of the [111] direction from a perfect Ge crystal. First-principles calculations were used to determine the molecular adsorption geometries, adsorption energies, and electronic properties of these nanowires with adsorbed acetone. The results suggest that the acetone molecule undergoes chemisorption when interacting with the Ge nanowires, achieving adsorption energies ranging from 0.49 eV to 1.61 eV. The estimated desorption time of the molecule suggests that to desorb the molecule, a temperature above 400°K is needed for the Al- and B-doped cases, while for the undoped case even at room temperature the desorption time is in the range of microseconds. Modulation of the work function of the nanowire upon acetone adsorption was found, in the order of tenths of eV, being largest in the case of the undoped nanowire. This research may offer valuable insights for the development of biosensing devices based on germanium nanostructures. [1-3]

References:

[1] J. E. Santana, K. J. García, I. J. Hernández-Hernández, Á. Miranda, M. Cruz-Irisson, and L. A. Pérez, "Urea adsorption and detection using silicon nanowires doped with B, Al, C, Ge, N, and P: A DFT investigation," Physica B: Condensed Matter, vol. 691, p. 416332, 2024/10/15/ 2024, doi: https://doi.org/10.1016/j.physb.2024.416332.

[2] I. J. Hernández-Hernández, F. de Santiago, A. L. Marcos-Viquez, Á. Miranda, M. Cruz-Irisson, and L. A. Pérez, "A comparative DFT study of CO and NO capture by copper- and titanium-

functionalized SiC and GeC monolayers," Materials Letters, vol. 370, p. 136805, 2024/09/01/ 2024, doi: https://doi.org/10.1016/j.matlet.2024.136805.

[3] F. De Santiago, J. E. Santana, Á. Miranda, L. A. Pérez, R. Rurali, and M. Cruz-Irisson, "Silicon nanowires as acetone-adsorptive media for diabetes diagnosis," Applied Surface Science, vol. 547, p. 149175, 2021/05/01/ 2021, doi: https://doi.org/10.1016/j.apsusc.2021.149175.

Keywords: *Germanium nanowires, acetone, DFT, sensors*

GOLD NANOPARTICLES AS CHARGE CARRIERS IN PIEZOELECTRIC CEMENT-BASED COMPOSITES

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This study investigates the use of gold nanoparticles (Au NPs) as charge carriers in piezoelectric cement-based composites. These composites have the potential to monitor the strain state of structural elements or function as self-powered materials for structural health monitoring (SHM) applications. However, the low electrical conductivity of the hydrated cement matrix presents a limitation. Au NPs offer a promising solution by increasing the free electric charge within the matrix, thereby enhancing both the electrical conductivity and the piezoelectric response of the composite. The study explores the effects of incorporating low concentrations of Au NPs (442 and 658 ppm) on the electrical and piezoelectric properties of cement-based composites. It also examines the impact of curing the material under a constant electric field. Electrical impedance spectroscopy was used to evaluate the polarization resistance and piezoresistive properties of the material, while open-circuit potential (OCP) measurements were conducted during mechanical loading to assess piezoelectric activity. The results showed a significant reduction in the composite's total electrical resistance, down to $1.5 \pm 0.2\ k\Omega$, nearly four times lower than reference samples. In terms of piezoelectricity, the piezoelectric voltage coefficient g33 improved remarkably, increasing by a factor of 57 compared to the reference specimens. This substantial enhancement is attributed to both the Au NP concentration and the electrical curing process. In conclusion, the study demonstrates the feasibility of creating a highly conductive cement matrix with low concentrations of Au NPs and highlights the potential piezoelectric behavior of the composite materials.

Keywords: *Gold Nanoparticles (Au NPs), Piezoelectric Cement Composites, Structural Health Monitoring (SHM).*

IMPACT OF DOPING WITH MONO AND DIVACANCIES ON THE STRUCTURAL AND ELECTRONIC PROPERTIES OF SIC MONOLAYER

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Two-dimensional (2D) materials have attracted attention in the scientific community since the discovery of graphene due to their unique properties, such as their surface-to-volume ratio, of great importance for applications in sensing and energy storage [1, 2]. In addition, recent research shows that electronic properties can be modified by impurities, such as doping, vacancies, and antisite defects [3]. In general, these impurities can modify the electronic band structure and modulate the band gap, as well as enhance the interaction with adsorbates. In this work, we present a density-functional-theory study on the effects of single and double vacancies on the electronic properties of doped silicon carbide monolayers (SiC-ML). Where B, Al, Ga, N, P, and As, were used as substitutional dopants. The interaction of these dopants with single and double vacancies were also investigated. Single vacancies were created by removing one Si or C atom. The results show that the most energetically favorable substitution is for a Si atom. The lattice parameter of the supercell was found to increase with the dopant atomic size. Also, only n-type dopants (N, P, and As) exhibit a spin-polarized ground state. The most stable dopant species is B. Vacancies cause larger reconstructions when interacting with heavier dopant species. By fine-tuning the band gap through the interactions between vacancies and dopants, 2D SiC may have a wide range of applications, such as molecular sensing, photocatalysis, energy storage, and radiation detection.

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References:

[1] M. González et al., "Exploring the electronic and mechanical properties of lithium-decorated silicon carbide nanowires for energy storage", Journal of Energy Storage 62, 106840 (2023).

[2] F. De Santiago et al., "First principles study of hydrogen storage on B-doped SiC monolayers through light transition metal atoms," Int J Hydrogen Energy, vol. 63, pp. 668–676, Apr. 2024, doi: 10.1016/J.IJHYDENE.2024.03.133.

[3] Lucia G. Arellano et al., "Theoretical prediction of two-dimensional II-V compounds semiconductors", Physical Review Materials 7, 014006 (2023)

Keywords: *Silicon Carbide, Monolayer, Vacancy, DFT*

IMPLEMENTATION OF A LOW-COST ANODIZING PROCESS FOR OBTAINING NANOPOROUS TEMPLATES FOR NANOWIRE GROWTH

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The study of zinc oxide (ZnO) and copper oxide (CuO) nanowires has attracted attention in recent years due to their potential technological applications. Previous research has highlighted various synthesis methods for these nanostructures, primarily through the use of porous templates, such as porous anodic alumina (PAA). These methods involve techniques like two-step anodization, which is typically carried out at low temperatures (0°C). High-purity aluminum is used as the template, and acids such as sulfuric, hydrochloric, phosphoric, or oxalic acid are employed to control the anodization process. Additionally, an inert counter electrode (cathode), such as platinum, is used to ensure the formation of a well-defined porous structure. However, these methods face challenges, including high costs associated with high-purity aluminum, the platinum electrode, and the cooling system. Furthermore, there are environmental contamination issues due to the use of these strong acids. To overcome these limitations, a different approach to the anodizing process is proposed. The use of pulsed voltage is suggested, allowing the process to be conducted at room temperature, thereby eliminating the need for a cooling system and optimizing processing time. Moreover, the use of commercial aluminum is proposed to reduce the high costs associated with high-purity aluminum. Similarly, replacing the platinum counter electrode with one made of commercial aluminum is proposed, resulting in a cost reduction of over 1500 times. Finally, phosphoric acid is suggested as a less contaminating alternative.

The implementation of the low-cost anodizing process enabled the fabrication of nanoporous templates from commercial aluminum. Morphological characterization using scanning electron microscopy (SEM) revealed the formation of nanopores in the aluminum molds with features similar to those reported in the literature, showing uniform and acceptable pore size, which demonstrates the feasibility of this approach. These templates were subsequently used for the growth of ZnO and CuO nanowires via the electrodeposition technique. The same experimental setup used in the anodizing process was employed for this procedure.

References:

[1] M. M. Rahman, T. H. Reshmi, "Inexpensive and highly controlled growth of zinc oxide nanowire: Impacts of substrate temperature and growth time on synthesis and physical properties," Current Applied Physics, vol. 41, pp. 32-40, 2022.

[2] Calderón, C. L. L., Nal, S. M., Saavedra, D. C. P., Silveyra, J., Socolovsky, L. M., Pampillo, L. G., & García, R. M. (2016). Fabricación de alúmina anódica porosa de bajo costo: Un estudio comparativo de la morfología producida por uno y dos pasos de anodizado. Matéria (Rio de Janeiro), 21, 677-690.

[3] NEMES, D., MOLDOVAN, V., BRUJ, E. et al., "Porous anodic alumina films obtained by two step anodization", In: Bulletin of the Transilvania University of Braşov, v. 4, n. 2, Series I: Engineering Sciences, Transilvania University Press, Brasov, Romania, pp. 75-80, 2011.

[4] B. Patella, S. Piazza, C. Sunseri, and R. Inguanta, "Anodic Alumina Membranes: From Electrochemical Growth to Use as Template for Fabrication of Nanostructured Electrodes," Applied Sciences, vol. 12, no. 2, p. 869, Jan. 2022, doi: 10.3390/app12020869.

[5] Chung, CK., Liu, T.Y. & Chang, W.T. Effect of oxalic acid concentration on the formation of anodic aluminum oxide using pulse anodization at room temperature. Microsyst Technol 16, 1451–1456 (2010). https://doi-org.ezproxy.unal.edu.co/10.1007/s00542-009-0944-9

[6] C. L. Londoño Calderón, "Fabricación de nanohilos magnéticos a base de compuestos de hierro," Tesis de Doctorado, Buenos Aires, Argentina, septiembre de 2017.

Keywords: *Anodizing, Porous Anodic Alumina (PAA), nanowires, electrochemical cell, scanning electron microscopy (SEM).*

NANOMATERIALS IN AGRICULTURE: A STUDY ON THE STRUCTURAL PROPERTIES OF TITANIUM DIOXIDE, ZINC OXIDE, AND ZEOLITE NANOFERTILIZERS

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This work presents the characterization of nanofertilizers based on titanium dioxide, zinc oxide, and zeolite. Various advanced analytical techniques were employed, such as scanning electron microscopy (SEM), X-ray diffraction (XRD), dynamic light scattering (DLS), and X-ray photoelectron spectroscopy (XPS). These methods allowed for the study of the morphological, structural, and chemical properties of the nanomaterials obtained through high-energy milling. The results demonstrated a significant reduction in particle size, improving their effectiveness as fertilizers. Zeolite nanoparticles showed notable changes in morphology and size, while TiO2 maintained its anatase structure. In the case of ZnO, a wurtzite-type crystalline structure with particle sizes below 100 nm was detected. These findings highlight the potential of these nanofertilizers to enhance fertilization efficiency in agriculture.

NICKEL CATALYSTS FOR CO2 METHANATION: A GREEN SYNTHESIS APPROACH VIA PULSED LASER DEPOSITION

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CO2 hydrogenation is a key alternative for reducing the environmental impact of industrial activities, with methanation standing out as a process that converts CO2 into methane (CH4), a renewable energy source. Nickel (Ni)-based catalysts are commonly used in this reaction due to their high hydrogenation capacity and low cost. However, traditional synthesis methods produce toxic waste. To address this, physical methods are proposed for cleaner and more efficient synthesis. In this study, catalysts were synthesized using pulsed laser deposition (PLD), varying energy and deposition time to study their influence on material properties. The catalysts were tested in CO2 methanation and showed catalytic performance comparable to those synthesized by wet impregnation, while requiring less hydrogen consumption for activation prior to the reaction.

OPTICAL CHARACTERIZATION OF GRAPHENE FIELD-EFFECT TRANSISTORS MODIFIED WITH PORPHYRIN MOLECULES

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Incorporating organic molecules into electronic devices has proven to be an effective strategy for improving their optoelectronic properties [1]. Graphene has emerged as a promising material for optoelectronics; however, its limited visible light absorption (2.3%) necessitates hybrid structures to enhance performance. Porphyrins are promising materials for optoelectronic applications due to their exceptional structural and functional characteristics. This study investigates the effects of tetrakis pentafluorophenyl porphyrin iron chloride (FeTPPCl) on the optoelectronic properties of graphene field-effect transistors (GFETs) encapsulated with aluminum oxide (Al2O3) [2]. A FeTPPCl solution in dichloromethane (DCM) was applied to the graphene channel using a microdrop technique with a pulled glass capillary and micromanipulator. We systematically measured the modified GFETs' response to wavelengths from near-ultraviolet (NUV) to near-infrared (NIR) at varying incident power levels. The results show increased responsivity with a local minimum around 418 nm, where FeTPPCl exhibits maximum absorption. These findings suggest that porphyrin molecules can enhance the photoresponse of GFETs at specific wavelengths, even when encapsulated. This methodology supports future research into the effects of porphyrins and other organic molecules on GFETs for high-performance optoelectronic applications.

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References:

[1] Garg, M., Tak, B. R., Rao, V. R., & Singh, R. (2019). Giant UV photoresponse of GaN-based photodetectors by surface modification using phenol-functionalized porphyrin organic molecules. ACS applied materials & interfaces, 11(12), 12017-12026.

[2] K Dockx, M D Barnes, D J Wehenkel, R van Rijn, H S J van der Zant, and M Buscema. Strong doping reduction on wafer-scale cvd graphene devices via al2o3 ald encapsulation. Nanotechnology, 35:395202, 9 2024.

Keywords: *Graphene Photodetector, Porphyrins, Surface Modification.*

PHYSICAL PROPERTIES CHARACTERIZATION OF THE CRI2 MONOLAYER

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Two-dimensional magnetic materials have captivated the academic and technological world for their unique properties resulting from quantum confinement and surface effects within their confined geometries, emerging as promising candidates to revolutionize technology and research by offering new possibilities in fields such as spintronics, nanoscience, and nanotechnology [1,2]. In this context, the CrI_2 monolayer presents itself as a fascinating and underexplored system, combining intrinsic magnetic properties with the versatility of 2D materials. The CrI_2 monolayer comprises an atomic layer of chromium atoms sandwiched between two layers of iodine atoms, forming a unique crystalline structure. This material exhibits intrinsic antiferromagnetic behavior, distinguishing it from other more studied magnetic 2D materials such as CrI_3 [3] and making it an ideal candidate for investigating fundamental magnetic phenomena at the atomic scale.

In this work, a comprehensive study of the physical properties of the CrI_2 monolayer was carried out using first-principles computational methods. Its crystal structure was characterized in detail, revealing similarities between the monoclinic and orthorhombic phases at the monolayer level. Magnetic anisotropy was analyzed, identifying the axes of easy magnetization. In addition, a detailed analysis of the vibrational properties of the system was carried out, including calculating the phonon dispersion ratio and the phonon density of states. This study revealed the dynamic stability of the monolayer and allowed the identification of the specific contributions of Cr and I atoms to the vibrational modes. Also, theoretical Raman and infrared spectra were calculated, providing crucial predictions for future experimental verifications. These spectra not only confirm the stability of the system but also provide a unique vibrational "fingerprint" of the CrI_2 monolayer, facilitating its identification and characterization in future experiments. The study was complemented by an analysis of thermodynamic properties, such as specific heat and entropy, revealing the crucial influence of phonons on the thermal behavior of the material. This comprehensive analysis provides a solid basis for understanding and predicting the behavior of this promising magnetic 2D material, paving the way for its potential application in advanced devices and stimulating future experimental investigations.

References:

[1] S. Kumari, D. K. Pradhan, N. R. Pradhan, and P. D. Rack, "Recent developments on 2d magnetic materials: challenges and opportunities," Emergent Materials, vol. 4, no. 4, pp. 827–846, 2021.

[2] D. L. Cortie, G. L. Causer, K. C. Rule, H. Fritzsche, W. Kreuzpaintner, and F. Klose, "Two-dimensional magnets: forgotten history and recent progress towards spintronic applications," Advanced Functional Materials, vol. 30, no. 18, p. 1901414, 2020.

[3] D. Staros, G. Hu, J. Tiihonen, R. Nanguneri, J. Krogel, M. C. Bennett, O. Heinonen, P. Ganesh, and B. Rubenstein, "A combined first principles study of the structural, magnetic, and phonon properties of monolayer cri3," The Journal of Chemical Physics, vol. 156, no. 1, 2022.

Keywords: *low-dimensional, magnetic materials, anisotropy, phonons, Raman and infrared spectra,*

PHYSICAL-STATISTICAL MODEL FOR IMPEDANCE ANALYSIS OF CARBON NANOTUBES CEMENT-BASED COMPOSITES

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The study of the electrical properties of cement composites with the addition of nanoparticles has mainly focused on the use of circuit models. However, in the case of carbon nanotubes, a lack of precision has been observed in fitting these types of models. In response to this, Triana-Camacho and collaborators proposed an adaptation of the generalized effective medium theory of induced polarization (GEMTIP) to apply it to cylindrical inclusions, modeling experimental data obtained through electrical impedance spectroscopy (EIS) for these types of samples (Triana-Camacho et al., 2022). In this work, we build on this model, combining it with Bayesian methods for parameter inference and the Markov Chain Monte Carlo (MCMC) method. For this purpose, a MATLAB code was implemented that integrates the Metropolis-Hastings MCMC routine (Laine, 2021) and the GEMTIP model. The code allows the inference of parameters that describe the electrical impedance curves of cement samples with the addition of carbon nanotubes, prepared under an applied electric field. The computational analysis made it possible to study the influence of the applied field on the orientation of the carbon nanotubes and how this affects the electrical properties of the samples.

References:

[1] Triana-Camacho, D. A., Miranda, D. A., García-Macías, E., Mendoza Reales, O. A., & Quintero-Orozco, J. H. (2022). Effective medium electrical response model of carbon nanotubes cement-based composites. Construction and Building Materials, 344, 128293. https://doi.org/10.1016/j.conbuildmat.2022.128293

[2] Laine, M. (2021). MCMCRUN: Metropolis-Hastings MCMC simulation for nonlinear Gaussian models [Repositorio de Github]. https://github.com/mjlaine/mcmcstat/blob/master/mcmcrun.m

Keywords: *Carbon Nanotubes, Impedance Spectroscopy, Markov Chain Monte Carlo.*

SÍNTESIS Y CARACTERIZACIÓN DE NANOPARTÍCULAS DE FE3O4 Y BAO UTILIZANDO EL EXTRACTO DE LA HOJA DE AZADIRACHTA INDICA PARA APLICACIONES MEDIOAMBIENTALES

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La contaminación del agua por metales pesados y colorantes orgánicos es uno de los desafíos más apremiantes que afecta tanto a la sociedad como al entorno ambiental. Colombia es un país rico en recursos hídricos; sin embargo, no está exento de contener contaminación en sus cuerpos de agua [1]. Las nanopartículas (NPs) a base de metal pueden usarse como catalizadores, por el tamaño de su superficie tienen la propiedad de adsorber moléculas orgánicas y pueden unirse con varias moléculas [2]. Con el propósito de contribuir a minimizar la contaminación por colorantes orgánicos y metales pesados en el agua, se sintetizaron nanopartículas de magnetita y óxido de bario por medio del método de coprecipitación, empleando el extracto de las hojas de Azadirachta indica como agente estabilizante y protector. Con el fin de analizar las propiedades y características fisicoquímicas de las nanopartículas de BaO y Fe3O4 obtenidas y estimar las posibles aplicaciones medioambientales en las que pueden emplearse, las NPs fueron caracterizadas por medio de las técnicas de Termogravimetría, Microscopía Electrónica de Barrido y Espectroscopía Infrarroja por Transformada de Fourier; las NPs de magnetita también fueron caracterizadas por Magnetometría de Muestra Vibrante.

Referencias:

[1] Gobierno de Colombia (2021). Informe Nacional De Calidad Del Agua Para Consumo Humano Inca 2021. Calidad del agua para el consumo humano, 1-147.

[2] Das, C. S. (2020). Green Synthesis, Characterization and application of natural product coated magnetite nanoparticles for wastewater treatment.

SYNTHESIS AND CHARACTERIZATION OF CARBON-BASE MATERIAL AND ITS APPLICATION AS SOIL AMENDMENT

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The current environmental challenges facing our planet require a multifaceted approach to their resolution. One area of focus is the development of technologies based on sustainable and environmentally friendly materials. In recent years, there has been a resurgence of interest in biochar among the scientific community, with its proven applications in water decontamination and, more recently, soil amendment attracting particular attention [1,2]. Biochar is a carbon-based material derived from the thermochemical transformation of biomass. It can be produced from a variety of organic wastes, including agricultural and industrial sources, offering significant economic, social, and environmental benefits and contributing to the implementation of a sustainable circular economy.

In light of the aforementioned considerations, our research is centered on the thermochemical transformation of agricultural residues from the Colombian Caribbean Region (plantain rachis and cassava peel) into biochar through the use of the slow pyrolysis method. This approach offers a low-cost alternative that does not generate greenhouse gas emissions, making it an environmentally sustainable option. This study focused on analyzing the impact of specific pyrolysis process parameters (type of biomass, pyrolysis temperature) on the physical characteristics (morphology, structure, and surface functional groups) of the biochar. Furthermore, this study presents a comprehensive study of the impact of these biochars on the amendment of arid soils in the region. To this goal, we conducted an analysis of soil parameters, including pH, humidity, and the content of nitrogen (N), potassium (K), phosphorus (P), and carbon (C), regarding the type of biochar and its concentration in the soil. It is of great importance to note that the soils of the Colombian Caribbean are severely degraded, compacted, and desertified due to the impact of extreme climatic conditions (high temperatures and drought) and poor agricultural practices. This has led to significant challenges in food security in the region, which we aim to address through our contribution.

References:

[1] A. A. Collins et al., Restoration of soil quality using biochar and brown coal waste: A review, (2020) Science of the Total Environment 722, 137852

[2] M. Guo et al., Biochar-Facilitated Soil Remediation: Mechanisms and Efficacy Variations, (2020) Frontiers in Environmental Science 8, 521512

Keywords: *Carbon-based materials, Biochar, Slow Pyrolysis.*

SYNTHESIS AND CHARACTERIZATION OF NANOCRYSTALLINE FERRITES FROM THE MN1- XZNXFE2O4 SYSTEM (X = 0, 0.2, 0.4, 0.6, 0.8 AND 1.0) OBTAINED VIA HYDROTHERMAL PROCESS USING ALOE BARBADENSIS MILL (ASPHODELACEAE) EXTRACT FOR THE TREATMENT OF CONTAMINATED WATERS

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The synthesis of nanocrystalline spinel ferrites has become an important part of novel materials research. The study of these materials has great relevance in modern technological applications in various industrial and biological fields [1]. It is well known that the preparation method can strongly affect the composition and microstructure of spinel-type nanocrystalline ferrites, and therefore, their chemical, structural and magnetic properties. Among the existing physical and chemical methods for the synthesis of spinel nanocrystalline ferrites, as high energy mechanical alloy [2], sol-gel method, polyol process, co-precipitation method, solid state reaction method, auto-combustion method, ceramic processing method [3]. However, recent research has reported the synthesis of spinel nanoferrites via hydrothermal, using eco-friendly solvents from plant extract.

In this work, the MnZn nanocrystalline ferrites were synthesized by the hydrothermal method, the Mn1-xZnxFe2O4 (x=0, 0.2, 0.4, 0.6, 0.8 and 1.0) system varying the compositions of Mn and Zn, using the extract of the aloe barbadensis mill plant as a solvent environmental friendly. The influence of the composition on the morphology, microstructure and its optics properties of the final product obtained were studied through the characterization of the samples by X-Ray Diffraction (XRD), Scanning Electron microscopy (SEM), Transmission Electron Microscopy (TEM), Vibrating Sample Magnetometer (VSM) and UV visible spectroscopy (UV-VIS). It will be evaluated which of the compositions of the Mn – Zn system is the most effective for the treatment of water contaminated with dyes. The ferrite powders obtained were spinel phase, with secondary phases (hematite) except for x = 0.6, the synthesized Mn-Zn ferrite had the best performance, which was a pure spinel-type crystalline structure. The average crystallite size, estimated from Scherrer equation, the size was on the order of nanometers. For SEM and TEM, it was observed that the ferrites are agglomerated, and their structure is quasispherical. From the hysteresis loops, it can be observed that the considered magnetic nanoparticles present a narrow loop tendency of soft magnetic materials. The UV–Vis spectroscopy determines the direct energy bandgap which increases from ~2.47 to ~2.57 eV.

References:

[1] Sharma I and Garg E. A Review on Nanoferrites in Biomedical Applications. IJBAS. 2022; volume 11: pages 1-4.

[2] Younes A. Kherrouba N, Bouamer A. Magnetic, optical, structural and thermal properties of copperferrite nanostructured synthesized by mechanical alloying. MNA2 2021; Volume16: Pages 251-256

[3] Preeti T, Deepika C, Shilpa T, Nikhil B, Atul T. A review on MnZn ferrites: Synthesis, characterization and applications. JCeramint 2020 Volume 46: Pages 15740-15763. Key words: nanocrystalline ferrites, hydrothermal, XRD, SEM, TEM UV-Vis.

THEORETICAL STUDY OF H2 AND CO ADSORPTION ON GRAPHENE SUPPORTED CO13 AND FE13 CLUSTERS

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Energy consumption has experienced a steady growth in recent years, driven by population growth and industrial activity. Additionally, most of the energy currently produced comes from non-renewable and polluting sources, which has generated significant interest in the search for new energy sources. Recently, research has been conducted on gas capture for its subsequent use as energy sources or raw materials, with the aim of finding alternative energy sources and reducing greenhouse gas emissions. Among these gases are H_2, used in the generation of green hydrogen, and CO, which can be employed in the production of synthetic fuels. In this work, a theoretical study was conducted using density functional theory (DFT) to analyze the adsorption capacity of H_2 and CO on Co and Fe metal clusters. An analysis was performed to identify the preferred adsorption sites for these molecules, as well as the energies associated with these sites.

Keywords: *CO adsorption, H2 Adsorption, graphene supported cluster, Density Functional Theory.*

THERMOELECTRIC PROPERTIES IN PERIODIC AND APERIODIC MAGNETIC SILICENE STRUCTURES

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The versatile structures based on silicene have an effective magnetoresistive response and at the same time have the ability to polarize spins and valleys. Simple magnetic junctions and periodic and aperiodic magnetic structures are useful as versatile structures [1-3]. Despite these efforts, there are few studies on this type of structures related to thermoelectricity. In this sense, we investigate the transmission and transport properties as well as the thermoelectric properties in periodic and aperiodic magnetic silicene structures. These systems are generated by placing a layer of silicene on a supporting dielectric substrate as SiO_2, the silicene is covered with a protective substrate to prevent degradation. Ferromagnetic electrodes (FMEs) are located and distributed in a periodic and aperiodic fashion on silicene. In particular, we focus on the thermoelectric properties in complex Cantor structures. Our methodology is based on the transfer matrix method, the Landauer-Büttiker formalism, and the Cutler-Mott formula to calculate the transmittance, the conductance, the Seebeck coefficient, and the power factor. Our main results show that the Cantor structures for the PM configuration have a better fragmentation and redistribution of states than the periodic ones, as a consequence, the thermoelectric properties exhibit higher values. On the contrary, for the AM configuration, the system with the best values is the periodic structures due to the accumulation of states at the edges of the gaps.

References:

[1] D. Wang, Z. Huang, Y. Zhang, and G. Jin, Phys. Rev. B 93, 195425 (2016).

[2] J. G. Rojas-Briseño, M. A. Flores-Carranza, P. Villasana-Mercado, S. Molina-Valdovinos, and I. Rodríguez-Vargas, Phys. Rev. B 103, 155431 (2021).

[3] P. Villasana-Mercado, J. G. Rojas-Briseño, S. Molina-Valdovinos, and I. Rodríguez-Vargas, J. Phys.: Condens. Matter 35, 085302 (2022).

Keywords: *Silicene, Cantor, Conductance, Seebeck coefficient, Power factor.*

Thermal, Optical, and Transport Properties

¿WHAT KIND OF RELATIONSHIP ARE BETWEEN ELECTRICAL LOSSES AND RHEOLOGICAL PARAMETERS SUCH AS LOSS FACTOR AND LOSS MODULUS? A POINT OF VIEW FROM POLYSACCHARIDE FILMS

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In recent years, increased research has focused on more sustainable packaging aimed at environmental preservation and conscious consumption. Starch and casein salts are widely explored polysaccharides due to their abundance, thermoplasticity and low cost. The high starch content in cassava (Manihot esculenta Crantz), compared to other starch sources, significantly facilitates its production on an agroindustrial scale by using its roots to produce derived products that in turn become base raw materials for other industries. Various biopolymers derived from polysaccharides such as starch have been used as polymeric matrices to obtain biodegradable packaging, as well as to develop films from renewable sources. The potential of these polysaccharides to replace conventional packaging is a beacon of hope, with properties (stability, mechanical and barrier) that can be tailored to each application. Many of the applications of these polysaccharides as smart materials can be applied as hybrid materials, sensors, photonic devices, smart composite materials whose properties such as optical, electrical, mechanical and rheological can be modulated or present different behaviors depending on the stimulus applied to them. For example, when analyzing the rheological properties of these polysaccharides, it is interesting to observe characteristics such as stabilizers, and binding agents of samples which is responsible for their use in food, pharmaceutical, and cosmetic industries. On the other hand, less known properties for polysaccharides such as electrical properties are important for the development of sensors and/or electrochromic materials, among others. In this work, polysaccharide films such as starch and caseinate were prepared and modified with Borax (17.5, 20, 25%). So far, comprehensive studies in these two areas are scarce and data relating to rheological properties such as loss factor and modulus could help to understand more deeply the behavior of this type of films in search of advanced applications.

References:

[1] Nayda Patricia Arias Duque, Jose de Jesús Agustín Flores -Cuautle, Pablo Fernando Grajales Carrillo, Oscar Hernán Giraldo Osorio, Gemima Lara Hernández., 2023 Cogent Food & Agriculture, 9:1, DOI: 10.1080/23311932.2023.2221104

[2] Adriana Paola Franco-Bacca,Fernando Cervantes-Alvarez, Juan Daniel Macías,Joan Alexis Castro-Betancur,Reynell Junior Pérez-Blanco,Oscar Hernán Giraldo Osorio,Nayda Patricia Arias Duque,Geonel Rodríguez-Gattorno and Juan José Alvarado-Gil. Polymers 2021, 13(23), 4106

[3] Yu Li, Fan Wang, Jieru Xu, Tong Wang, Jinling Zhan, Rongrong Ma, Yaoqi Tian. Improvement in the optical properties of starch coatings via chemical-physical combination strategy for fruits preservation, Food Hydrocolloids,Volume 137,2023,108405, https://doi.org/10.1016/j.foodhyd.2022.108405.

[4] Mejía-Manzano, L.A.; Vázquez-Villegas, P.; Prado-Cervantes, L.V.; Franco-Gómez, K.X.; Carbajal-Ocaña,

S.; Sotelo-Cortés, D.L.; Atehortúa-Benítez, V.; Delgado-Rodríguez, M.; Membrillo-Hernández, J. Advances in Material Modification with Smart Functional Polymers for Combating Biofilms in Biomedical Applications. Polymers 2023, 15, 3021. https://doi.org/10.3390/polym15143021

Keywords: *Polysaccharides, rheological properties, electrical losses*

ALUMINIUM OXIDE ALD GRAPHENE ENCAPSULATED PHOTODETECTORS

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Optoelectronics is a vast field with applications in communication, imaging, and aerospace industries. Since its isolation in 2004, graphene has emerged as a promising material for optoelectronics [1; 2] due to its broad wavelength absorption, fast response times, and high mobility [3; 4]. However, its limited visible light absorption (2.3% of incident light [4; 5]) necessitates hybrid structures to enhance performance, and passivation is required to maintain its electrical properties under ambient conditions. We present a systematic study of graphene field-effect transistors (GFETs) passivated with aluminum oxide, examining their response to wavelengths from near-ultraviolet (NUV) to near-infrared (NIR) at different incident powers in ambient conditions, obtaining up to 1.5 A/W of responsivity. Our findings show that these devices retain their properties for months, revealing a gating mechanism upon illumination that can be linked to deep traps within the oxide. We propose varying the passivation layer's thickness can fine-tune the devices' response.

References:

[1] F. Kusmartsev, W. Wu, M. Pierpoint, and K. Yung, "Application of graphene within optoelectronic devices and transistors," Applied spectroscopy and the science of nanomaterials, pp. 191–221, 2015.

[2] F. Bonaccorso, Z. Sun, T. Hasan, and A. C. Ferrari, "Graphene photonics and optoelectronics," Nature photonics, vol. 4, no. 9, pp. 611–622, 2010

[3] F. Koppens, T. Mueller, P. Avouris, A. Ferrari, M. S. Vitiello, and M. Polini, "Photodetectors based on graphene, other two-dimensional materials and hybrid systems," Nature nanotechnology, vol. 9, no. 10, pp. 780–793, 2014.

[4] J. Li, L. Niu, Z. Zheng, and F. Yan, "Photosensitive graphene transistors," Advanced Materials, vol. 26, no. 31, pp. 5239–5273, 2014.

[5] S. Kim, M. S. Jang, V. W. Brar, K. W. Mauser, L. Kim, and H. A. Atwater, "Electronically tunable perfect absorption in graphene," Nano letters, vol. 18, no. 2, pp. 971–979, 2018.

Keywords: *Graphene, Optoelectronics, Responsivity.*

COMPUTATIONAL MODEL FOR THE ACOUSTIC EVALUATION OF ONION (ALLIUM CEPA) AND QUINCE (CYDONIA OBLONGA)

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The loss of agricultural products due to factors such as pests, diseases, adverse weather conditions, overproduction, and inadequate post-harvest management represents a significant challenge for the agricultural sector, resulting in food waste and economic losses. This work presents a computational model that simulates the acoustic and morphological properties of onions (Allium cepa) and quinces (Cydonia oblonga), providing an alternative tool for determining the quality of these products. The research was based on the application of low-intensity acoustic waves and the analysis of their propagation to obtain intrinsic parameters such as acoustic phase velocity, among others. An exhaustive study of the morphological and rheological properties of onions and quinces was conducted, which was fundamental for developing an accurate physical model. Subsequently, the model was solved using the finite element method (FEM), from which the wave travel time, acoustic phase velocity, and stiffness modulus were obtained, allowing for the analysis and understanding of acoustic wave behavior in these media. The developed computational model enables the optimization of storage time, the establishment of better shelf conditions, and the alternative and automated determination of food quality without causing damage during the analysis process. This tool facilitates quick and efficient sampling, significantly contributing to the reduction of losses in the agricultural production chain. The implementation of this computational model represents a major advancement in determining the quality of agricultural products, offering a practical and efficient solution to one of the sector's main challenges. The application of this technology can lead to a significant reduction in food waste and improve the economic efficiency of post-harvest management.

DEVELOPMENT AND IMPLEMENTATION OF A LONGITUDINAL SPIN SEEBECK EFFECT MEASUREMENT SETUP

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This work focuses on the developing a setup to measure the longitudinal spin Seebeck effect (LSSE), which generates a spin current or spin angular momentum flux in a magnetic material due to a temperature gradient [1]. Additionally, conventional thermoelectric effects, as well as direct and inverse spin Hall effects, are explored to understand the processes involved in SSE measurement. The measurement setup is divided into two phases: simulation and experimental setup. Thermal simulations using Autodesk software analyze temperature differences and heat flow, establishing design criteria such as heat conductor block size, heater/Peltier cell temperatures, sample positioning, heat sink base, and reference materials (Cu, brass, AlN). The experimental setup includes the fabrication of type K thermocouples, as well as the electrical and thermal characterization of each system component to perform LSSE experiments. This phase highlights the technical challenges encountered during the process and provides crucial information for optimization by integrating the results of the previous simulations. Applying the design parameters resulted in the successful operation of a device to study the spin Seebeck effect in magnetic materials. The device operates effectively within a temperature range of 25 ± 3 to 50 ± 0.5 °C, while the magnetic field can be varied from -800 ± 0.1 Oe to 800 ± 0.1 Oe. The LSSE voltage is measured using a nanovoltmeter, temperature is recorded by an Arduino-based data acquisition system, the magnetic field is generated by an electromagnet and measured by a Hall probe. Finally, the SSE was studied in a ZnFe2O4 thin film with Pt layer, yielding a Seebeck coefficient of 0.040 ± 0.004 μ V/K, which is comparable to those of the other ferrites reported in the literature [2].

References:

[1] Uchida, K., Takahashi, S., Harii, K. et al. Observation of the spin Seebeck effect. Nature 455, 778–781 (2008).

[2] Gil-Monsalve, J., et al. "Influence of substrate type and magnetic anisotropy on the spin Seebeck effect in ZnFe2O4 thin films." Applied Physics A 129.4 (2023): 270.

Key words: *Spin Seebeck Effect, spintronics, caloritronics.*

EFFECT OF BORAX ON ELECTRICAL CONDUCTIVTY AND STRUCTURE OF STARCH BIOFILMS

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Currently, society requires the manufacture and access to more environmentally friendly materials and technologies to face the challenges of food security, energy transition, circularity in production and sustainability. Therefore, it is necessary to involve transdisciplinary efforts that allow these challenges to be addressed in a comprehensive manner. In this work, the effect of incorporating Borax into native starch and fermented starch biofilms was analyzed. Native starch presented a low-frequency conductivity of the order of $10^{-10}\ \Omega^{-1}\ cm^{-1}$ at 0.1 Hz, while for fermented starch this value was of the order of $10^{-9}\ \Omega^{-1}cm^{-1}$. For native starch, a decrease in the real component of conductivity of up to 4 orders of magnitude was found at low frequencies, while this effect was two orders of magnitude for fermented starch. The structure of biofilms by XRD shows it is amorphous to the extent of the increase in borax in the structure. This opens the possibilities of developing biodegradable films.

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References:

[1] Franco-Bacca, Adriana Paola, Cervantes-Alvarez, Fernando, Macías, Juan Daniel, Castro-Betancur, Joan Alexis, Pérez-Blanco, Reynell Junior, Giraldo Osorio, Oscar Hernán, Arias Duque, Nayda Patricia, Rodríguez-Gattorno, Geonel, Alvarado-Gil, Juan José. Polymers 2021, 13(23), 4106; https://doi.org/10.3390/polym13234106

[2] Lozano, M.J., Arias Duque, N.P., Mendoza, J.S., Aristizábal-Marulanda, V. Challenges for biorefineries in Latin America: A prospective analysis. In The Future of Biorefineries, 2023, pp. 53–108

Keywords: *starch, electrical conductivity, impedance spectroscopy*

ELECTROCHEMICAL CHARACTERIZATION OF MICROBIOLOGICAL CORROSION IN NI2+XMN1−XGA ALLOYS

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This research aims to examine the biocorrosion in Ni-Mn-Ga alloys in the presence of Pseudomonas aeruginosa. The alloys will be exposed to nutrient solutions and evaluated using Open Circuit Potential, Linear Polarization Resistance, Electrochemical Impedance Spectroscopy, and SEM-EDX analysis. The electrochemical tests will be carried out using a Gamry Interface 1000E Potentiostat, with Framework TM Data Acquisition software for data analysis. It is expected that the results will demonstrate the influence of nickel (Ni) on corrosion resistance, with higher concentrations of this element leading to increased resistance. The presence of bacteria is anticipated to result in biofilm formation and micropitting, indicating an intensified corrosive effect attributed to Pseudomonas aeruginosa. Differences in the corrosion potential, Ecorr, and the average corrosion rate, vcorr, are expected to reflect the influence of alloy composition. The system's impedances will be modeled to characterize and quantify the phenomena present at the electrochemical interface. This study will focus on the early evolution of corrosion, with tests lasting two hours. The expected results will contribute to a better understanding of how microbial corrosion affects shape memory alloys, highlighting changes in structure, oxide film formation, and accelerated corrosion in the presence of bacteria.

Keywords: *Biocorrosion, Ni-Mn-Ga Alloys, Pseudomonas aeruginosa, Electrochemical Impedance Spectroscopy, Shape Memory Alloys.*

ENERGY ANALYSIS OF A BIOMASS GASIFICATION PROCESS THROUGH THE INTEGRATION OF AN OPTIMIZED PHENOMENOLOGICAL MODEL

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In this study, the transport mechanisms involved in the gasification of residual biomass are analyzed by establishing energy, mass, and momentum balance equations. The behavior of the process is examined by considering mixtures in different proportions of three types of agro-industrial residues generated in the department of La Guajira. The main objective is to identify the mixture that maximizes the energy content of the gas and minimizes the carbon footprint of the process. The model solution is compared with the results obtained in a biomass gasification pilot plant located at the facilities of the University of La Guajira.

References:

[1] Kushwah, A., Reina, T.R., Short, M. (2022). Modelling approaches for biomass gasifiers: A comprehensive overview. Science of The Total Environment. Volume 834, 2022, 155243, ISSN 0048-9697

[2] Kushwah, A., Reina, T.R., Short, M. (2022). Modelling approaches for biomass gasifiers: A comprehensive overview. Science of The Total Environment. Volume 834, 2022, 155243, ISSN 0048-9697

Keywords: *Transport mechanisms, Biomass gasification, Optimal mixture.*

FIRST HYPERPOLARIZABILITY OF BENZOXAZOLE DERIVATIVES IN THE CONTEXT OF DFT (DENSITY FUNCTIONAL THEORY).

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Linear optics (LO) is widely used but has limitations in microscopy and OLED devices due to light dispersion and wavelength, affecting resolution and efficiency [1-3]. Nonlinear optics (NLO) offers solutions through effects like hyperpolarizability and two-photon absorption (TPA), advancing technologies such as two-photon microscopy and medical treatments [4-5]. First hyperpolarizability enables applications in optoelectronic devices and biomedical sensors [6-7]. Density Functional Theory (DFT) is crucial for studying optical properties and designing advanced materials [8]. Benzoxazole and oxazole derivatives stand out for their optical and chemical properties, with potential in medicine and nanomaterials [9]. There is a need to find new materials with good nonlinear optical properties to optimize OLED and fluorescence microscopy technologies for medical diagnostics and new technologies. This theoretical study calculates the nonlinear property of first hyperpolarizability in π-conjugated organic compounds derived from 2,5-Diphenyl-1,3-oxazol-4-yl-(2-phenyl-1,3-benzoxazole). Four organic compounds were examined in the gas phase, methanol, and toluene. The substituents used are -NH2 and -NO2, individually and simultaneously on the phenyl ring at the end of the parent molecule. Methodologically, hybrid functionals and Gaussian basis sets were used in computational quantum chemistry software. Results reveal a significant increase in dipole moment, polarizability, and static and dynamic first hyperpolarizability for 1064 nm in solvents, suggesting a greater nonlinear optical response of the compounds. The best results are from measurements in methanol, where dynamic first hyperpolarizability values $\beta(-2\omega ; \omega, \omega)$ range from 10.89 × 10−30 esu to 21.84 × 10−30 esu, indicating a superior nonlinear optical response compared to the gas phase and toluene.

References:

[1] Vermeulen, N., Espinosa, D., Ball, A., Ballato, J., Boucaud, P., Boudebs, G., Campos, C. L. A. V., Dragic, P., Gomes, A. S. L., Huttunen, M. J., Kinsey, N., Mildren, R., Neshev, D., Padilha, L. A., Pu, M., Secondo, R., Tokunaga, E., Turchinovich, D., Yan, J., ... Van Stryland, E. W. (2023). Post-2000 nonlinear optical materials and measurements: data tables and best practices. Journal of Physics: Photonics, 5(3), 035001.

[2] Castillejo, M., Oujja, M., Agua, F., Sanz, M., Morales-Martin, D., García-Heras, M., & Villegas, M. Á. (2021). Study of historical glass grisailles by nonlinear optical microscopy. [3] Mahmoudi, C., Chouk, R., Baatout, K., Jaballah, N. S., Khalfaoui, M., & Majdoub, M. (2022). Synthesis, characterization and DFT study of new anthracene-based semiconducting polyethers for OLED application. Journal of Molecular Structure, 1251, 131993.

[4] Valencia, J., Rubio, V., Puerto, G., Vasquez, L., Bernal, A., Mora, J. R., Cuesta, S. A., Paz, J. L., Insuasty, B., Abonia, R., Quiroga, J., Insuasty, A., Coneo, A., Vidal, O., Márquez, E., & Insuasty, D. (2023). QSAR Studies, Molecular Docking, Molecular Dynamics, Synthesis, and Biological Evaluation of Novel Quinolinone-Based Thiosemicarbazones against Mycobacterium tuberculosis. Antibiotics, 12(1), 61.

[5] Li, T., Li, F., Altuzarra, C., Classen, A., & Agarwal, G. S. (2020). Squeezed light induced two-photon absorption fluorescence of fluorescein biomarkers. Applied Physics Letters, 116(25).

[6] Zhao, G., Yan, W., Wang, Z., Kang, Y., Ma, Z., Gu, Z. G., Li, Q. H., & Zhang, J. (2023). Predict the Polarizability and Order of Magnitude of Second Hyperpolarizability of Molecules by Machine Learning. Journal of Physical Chemistry A, 127(29), 6109–6115.

[7] Boyd, R. W., Gaeta, A. L., & Giese, E. (2023). Nonlinear Optics. Springer Handbooks, 1097–1110.

[8] Datar, M., Dhanwad, R., Javeed, M., Gunavanthrao Yernale, N., & Suliphuldevara Mathada, B. (2024). Synthesis, Structural Investigations, DFT Calculations, and Molecular Docking Studies of Novel 2-(Substituted-Aryloxymethyl)-5-(Pyridin-4-yl)-1, 3, 4-Oxadiazoles: Highly Potential InhA and Cytochrome c Peroxidase Inhibitors. Polycyclic Aromatic Compounds.

[9] Costa, T. M. da, & Corrêa, D. S. (2021). Síntese e caracterização de novos derivados benzoxazol e naftoxazol. Revista de Iniciação Científica Da ULBRA, 1(19), 2021.

Keywords: *Benzoxazole, First Hyperpolarizability, Density Functional Theory.*

NON-LINEAR HALL RESPONSE IN TWO DIMENSIONAL PT SYMMETRIC SYSTEMS

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We study the non-linear Hall effect in two dimensional PT-symmetric systems by means of the density matrix theory. We analyse the effect of scalar disorder in the system and find that, to leading order in impurity density, there are Berry curvature dipole, skew scattering and side jump contributions [1,2]. An electric field correction to the collision integral is included in the theory, whose effect is to double the side jump contribution.

References:

[1] Phys. Rev. Research 4, 013001

[2] Phys. Rev. B 96, 035106

Keywords: *Density matrix theory, nonlinear response, anomalous Hall effect.*

PERFORMANCE PARAMETERS OF AN SPR BIOSENSOR WITH 2D MATERIALS AS A FUNCTION OF THE CHEMICAL POTENTIAL OF GRAPHENE

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Recently, optical biosensors, especially surface plasmon resonance biosensors, have been widely used for the detection of biomolecules due to their plasmonic advantages [1-4]. For these biosensors, there are several methods of surface plasmon excitation, one of them is the prism coupling in Kretschmann configuration [2], which uses the phenomenon of attenuated total reflection to detect optical changes. Also, there has been much research on biosensors based on 2D materials due to their exceptional optical and electronic properties [5-7]. In this work, we study the performance parameters of a surface plasmon resonance biosensor with a gold/2D material/graphene structure in Kretschmann configuration as a function of the chemical potential of graphene. The attenuated total reflection of the surface plasmon resonance is studied for different 2D materials and calculated using the transfer matrix method. We found that there is a value of the chemical potential of graphene, which we called the critical point, at which the performance parameters of a biosensor change abruptly for any type of 2D material used in its structure. In the case of sensitivity, we found a sudden increase around the critical point, but in the case of detection accuracy and quality factor we found a deep drop at the critical point. Moreover, as the number of graphene sheets increases, the change in the values of the biosensor performance parameters at the critical point is more abrupt. Lastly, we derive an analytical expression for the sensitivity that help us to explain its behavior for the different 2D materials used in the biosensor structure.

References:

[1] S. Pal, Y. K Prajapati, J. P. Saini, Influence of graphene's chemical potential on SPR biosensor using ZnO for DNA hybridization, Opt. Rev. 27 (1) (2020) 57–64. doi:10.1007/s10043-019-00564-w.

[2] A. Panda, P. D. Pukhrambam, G. Keiser, Performance analysis of graphene-based surface plasmon resonance biosensor for blood glucose and gas detection, Appl. Phys. A Mater. Sci. Process. 126 (3) (2020). doi:10.1007/s00339-020-3328-8.

[3] K.M. Ibrahimi, R.Kumar,W. Pakhira, Early detection of cancer cells using high-sensitivity dual-side polished photonic crystal fiber biosensors based on surface plasmon resonance, Optical and Quantum Electronics 56 (5 2024). doi:10.1007/s11082-024-06782-0.

[4] K.M. Ibrahimi, R.Kumar,W. Pakhira, Early detection of cancer cells using high-sensitivity dual-side polished photonic crystal fiber biosensors based on surface plasmon resonance, Optical and Quantum Electronics 56 (5 2024). doi:10.1007/s11082-024-06782-0.

[5] S. Wang, H. Tian, C. Ren, J. Yu, M. Sun, Electronic and optical properties of heterostructures based on transition metal dichalcogenides and graphene-like zinc oxide, Scientific Reports 8 (12 2018). doi:10.1038/s41598-018-30614-3.

[6] J. Wu, M. Gong, ZnO/graphene heterostructure nanohybrids for optoelectronics and sensors, Journal of Applied Physics 130 (2021) 070905.doi:10.1063/5.0060255.

[7] Z. L. Lei, B.Guo, 2D Material-Based optical biosensor: Status and prospect, Advanced Science 9 (2 2022). doi:10.1002/advs.202102924.

Keywords: *SPR biosensor, 2D materials, chemical potential, performance parameters.*

PROXIMAL AND OPTICAL CHARACTERIZATION OF ORANGE PEELS, PLANTAIN PEELS, AND CORN HUSKS AS PRECURSORS OF FLUORESCENT DOTS

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Carbon dots are nanoparticles made up of a primarily amorphous carbon core and functional groups on the surface. The formation of the dots depends on the polymers contained in the sample, from which, by the hydrothermal method (bottom-up), pyrolytic, aldol, and self-condensation reactions are generated, giving rise to a wide variety of intermediates, which, depending on their abundance, polymerize and form the core scaffold. This work consisted of comparing the absorbance response by infrared spectroscopy and the emission by photoluminescence with a proximal analysis to understand the variations in the composition of the precursors used to synthesize carbon dots, also taking into account the variety of plant material. For this, banana peels, orange peels, and corn husks were obtained from the northern region of Valle del Cauca and the department of Caldas. The precursors, after being washed, were disinfected and taken to an oven for dehydration. The precursors were subsequently pulverized to a particle size of 106 µm, and, finally, the pulverized precursor was optically and chemically analyzed. The FTIR results indicated that the main differences in composition are observed between precursors and that the influence of the variety is not significant; it was also observed that the C=O band of fats and the O-C-O band of epoxy groups are those that are modified and, therefore, are characteristic vibration modes of the sample. The emission patterns of each precursor were obtained by photoluminescence, observing that the banana has a particular line shape that may be related to its majority hemicellulose content as indicated by the proximate analysis.

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Keywords: *carbon dots, hydrothermal synthesis, vegetable sources.*

SOLID SOLUTIONS OF TRANSITION METAL DICHALCOGENIDES FOR THERMOELECTRIC APPLICATIONS

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Nowadays, alternatives in energy generation are being explored to reduce dependence on hydrocarbons. One promising solution is the use of thermoelectric materials, which can harness waste heat and convert it into electricity. Although several types of thermoelectric materials exist, their market availability is limited, and they do not compete effectively with other energy sources like solar or hydroelectric power. This limitation drives the search for new materials that can outperform traditional alternatives. In this context, the family of transition metal dichalcogenides emerges as a promising alternative, as these materials have shown potential to improve their thermoelectric properties through chemical doping or vacancy variations in their crystal structure. In this work, we present our strategies for optimizing the thermoelectric properties of solid solutions of transition metal dichalcogenides, specifically from WSe2 to WTe2, by direct measurement of the thermoelectric figure of merit (ZT) using the Harman method both in and out of plane.

Keywords: *Thermopower, transition metal dichalcogenides, thermoelectric figure of merit (ZT), thermoelectric materials. low dimensional materials*

SPR BIOSENSORS TO MEASURE GLUCOSE LEVELS IN THE SKIN

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Surface Plasmon Resonance (SPR) optical sensors are based on the excitation of surface plasmons. In this work, we propose the use of the SPR optical technique for the modelation of a biosensor capable of directly measuring glucose in the skin in a non-invasive manner, allowing for continuous monitoring. According to Homola [1], a large part of the SPR, wave's electromagnetic field is located in the dielectric medium, so the propagation constant is highly sensitive to changes in the refractive index. In this work, we employed the Kretschmann configuration, using metals such as Au and Ag in combination with TMDCs (Transition Metal Dichalcogenides), such as MoS2, MoSe2, WS2, and WSe2. We also sought to add graphene to each of these combinations, changing the number of layers and chemical potential. The SPR biosensor system consists of a prism, metal, TMDCs, and skin. We also analyzed bimetallic sensors using both Au and Ag, and all these configurations were analyzed with and without graphene. We evaluated performances parameters such as sensitivity, spectral full width at half maximum (FWHM), detection accuracy (DA), and quality factor (QF), using the reflectance calculated with the transfer matrix method. The skin's refractive index used was 1.445, based on the report by Anuj K. Sharma [3] of a refractive index of 1.445 + 0.01i, where only the real part was used since skin absorption was not considered. Assuming that glucose levels are reflected in changes in the skin's refractive index, this study sought to examine the biosensor's behavior by varying the refractive index in the third decimal place, based on the increments reported in the studies of Mudgalc [4] and Mostufa [5], which measured glucose concentration in urine, as these increments showed changes in the observed concentrations. The biosensors that showed the best performance were those to which Au was added, such as the biosensor composed of Au and WS2, which showed a sensitivity range of 140 to 162 °/RIU, FWHM of 14.2 to 17 °, QF of 8 to 9, and DA of 0 to 0.3. When incorporating graphene into the systems, the biosensor that presented the best behavior was composed of Au and MoSe2, along with a single layer of graphene and a chemical potential of 0.25, achieving a sensitivity of 120 to 155 °/RIU, FWHM of 14.5 to 16 °, QF of 7.5 to 10, and DA of 0 to 0.21.

References:

[1] Jiří Homola. "Present and future of surface plasmon resonance biosensors". En: Analytical and bioanalytical chemistry 377 (2003), págs. 528-539.

[2] Sachin Singh, Pravin Kumar Singh, Ahmad Umar, Pooja Lohia, Hasan Albargi, L Castañeda y DK Dwivedi. "2D nanomaterial-based surface plasmon resonance sensors for biosensing applications". En: Micromachines 11.8 (2020), pág. 779.

[3] Anuj K Sharma y Gerhard J Mohr. "Plasmonic optical sensor for determination of refractive index of human skin tissues". En: Sensors and Actuators B: Chemical 226 (2016), págs. 312-317.

Keywords: *SPR biosensors, skin, glucose measurement.*

SPR OPTICAL BIOSENSOR BASED ON 2D MATERIALS FOR GLUCOSE DETECTION

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Modern life demands the development of high technology aimed at providing human beings with devices that allow them to improve their quality of life through real-time information that allows them to make decisions in their daily lives, as well as in industrial life. A technology that allows us to achieve this is based on sensors of different types and uses, such as chemical, mechanical, pressure, acoustic and optical, among others. Surface plasmon resonance (SPR) sensors have been used for the detection of a wide range of compounds, from ions, proteins, viruses, and even small molecules; this allows them to be applied in environmental monitoring, water quality analysis, food quality, industrial safety, clinical diagnosis, etc. With the synthesis of graphene, and a wide range of 2D (atomic order thickness) materials, which have extraordinary optical properties, it has been possible to improve the quality of traditional SPR sensors [1-3]. On the other hand, diabetes mellitusis a chronic degenerative disease that is on the rise and is considered a public health problem, there are 537 million people living with diabetes today. It is estimated that by 2045 the mortality rate could reach 700 million globally, according to the International Diabetes Federation (IDF). Diabetesis known to involve complex metabolic disorders and is characterized by elevated blood glucose levels that can lead to serious medical complications, including chronic kidney disease, limb amputation, premature death, and numerous other complications. In this project, we seek to improve the performance parameters of SPR sensors applied to the detection of different glucose concentrations. These parameters quantify the quality of the sensor, its feasibility, and its detection capability. The SPR sensors to be analyzed are prism-coupled sensors in Kretschmann configuration, formed by different heterostructures based on 2D materials, metals and dielectrics. Among the 2D materials to be considered are graphene, transition metal dichalcogenides, black phosphorene, MXenes, among others. The study is performed by attenuated total reflection (ATR), calculated through the transfer matrix method. The theoretical results we have obtained improve the sensitivity by 30% and the quality factor and detection accuracy by approximately 40%.

References:

[1] Zong-Lin Lei and Bo Guo, 2D Material-Based Optical Biosensor: Status and Prospect. Advanced Science. 2022, 9, 2102924. doi: 10.1002/advs.202102924

[2] Naresh, V.; Lee, N. A Review on Biosensors and Recent Development of Nanostructured Materials-Enabled Biosensors. Sensors 2021, 21, 1109. https://doi.org/10.3390/s21041109

[3] N. Mudgal, A. Saharia, A. Agarwal, J. Ali, P. Yupapin, G. Singh, Modeling of highly sensitive surface plasmon resonance (SPR) sensor for urine glucose detection, Optical and Quantum Electronics (2020) 52:307. https://doi.org/10.1007/s11082-020-02427-0

Keywords: *SPR biosensor, 2D materials, performance parameters.*

STUDY OF THE ELECTRONIC TRANSPORT AND THE THERMOELECTRIC EFFECT IN APERIODIC GATED PHOSPHORENE SUPERLATTICES

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Recently, the nano-structuring techniques in low-dimensional materials has acquired great relevancy due to the potential improvement in the capabilities and efficiency of electronic devices. In the case of electrostatic and magnetic gated superlattices in two-dimensional (2D) materials like graphene [1], it is possible to manipulate the electronic transport properties and observe phenomena such as magnetoresistance, thermoelectric effect and spin-valley polarization [2, 3]. Phosphorene, another 2D material, is formed by phosphorus (P) atoms distributed in a puckered honeycomb layer. The band structure of phosphorene exhibits moderate bandgap (~1.5 eV) in the gamma (Γ) point and high anisotropy, which differentiates the propagation between zigzag (Γ-X) and armchair (Γ-Y) directions [4]. The behavior of charge carriers (holes and electrons) can be explained by the low-energy effective Hamiltonian derived from the tight binding model [5, 6]. In this work, we theoretically explore the ballistic transport properties in aperiodic superlattices applied to a phosphorene monolayer. The aperiodicity of the electrostatic barriers is implemented by using Fibonacci and Thue-Morse type sequences [7, 8]. Transmission probability and conductance is calculated by the matrix transfer method under the Landauer-Büttiker formalism [9]. Additionally, the study of thermoelectric properties is carried out by calculating the Seebeck coefficient and the power factor using the Cutler-Mott formula. Our results showed that the aperiodicity promotes strong fragmentation of the valence and conduction mini-bands as well as high modulation of the transport and thermoelectric properties in contrast to the case of periodic superlattices.

References:

[1] A. Zhao, B. Wang, APL Materials, 8, 030701(2020).

[2] I. Choudhuri, P. Bhauriyal, B. Pathak, Chem. Mater. 31, 8260 (2019).

[3] O. Oubram, J. Phys.: Condens. Matter 36, 225302 (2024).

[4] A. N. Rudenko, M. I. Katsnelson, Phys. Rev. B 89, 201408 (2014).

[5] M. Ezawa, New J. Phys. 16, 115004 (2014).

[6] E.J. Guzmán, O. Oubram, O. Navarro, I. Rodríguez-Vargas, Phys. Rev. B 107, (4), 045407 (2023).

[7] S. Molina-Valdovinos, E.J. Guzmán, I. Rodríguez-Vargas, J. Appl. Phys. 127, 154302 (2020).

[8] E.J. Guzmán, S. Molina-Valdovinos, O. Oubram, I. Rodríguez-Vargas, J. Appl. Phys. 128, 224302 (2020).

[9] E.J. Guzmán, O. Navarro, O. Oubram, I. Rodríguez-Vargas, J. Appl. Phys. 124, 144305 (2018).

Keywords: *phosphorene, aperiodic superlattices, ballistic transport, thermoelectric effect.*

SURFACE-BINDING MOLECULAR MULTIPODS STRENGTHEN THE HALIDE PEROVSKITE LATTICE AND BOOST LUMINESCENCE

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Rationally designed organic chemical structures and terminal moieties are widely employed to achieve defect-less perovskite crystals, passivate grain boundaries, and improve energy alignment at perovskite/transport layers interfaces; thus, enabling high-efficient solar technology [1]. However, the effect of these compounds on perovskite lattice dynamics is poorly understood. Herein, we show that the soft structure of halide perovskites can be hardened through non-covalent interactions with π-conjugated molecular additives [2]. DFT predictions underpinning a diluted screening effect on injected carriers by lattice dynamics, drive experimental findings on an enhancement of charge recombination, thus boosting the external quantum efficiency of perovskite LEDs (PeLEDs). Study of Ab initio molecular dynamics-based vibrational spectra and low-frequency Raman experiments support these findings.

References:

[1] Kim, YH., Kim, S., Kakekhani, A. et al. Comprehensive defect suppression in perovskite nanocrystals for high-efficiency light-emitting diodes. Nat. Photonics 15, 148–155 (2021). https://doi.org/10.1038/s41566-020-00732-4

[2] Kim, DH., Woo, SJ., Huelmo, C.P. et al. Surface-binding molecular multipods strengthen the halide perovskite lattice and boost luminescence. Nat Commun 15, 6245 (2024). https://doi.org/10.1038/s41467-024-49751-7

Keywords: *PeLEDs, DFT, Raman spectroscopy*

SYNTHESIS AND CHARACTERIZATION OF BI25FEO40 IRON-SILLENITE AT DIFFERENT CALCINATION TEMPERATURES

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A theoretical and experimental study of the properties of the iron sillenite has been done. Different samples were synthesized at five different temperatures from 550 °C to 750 °C to find the best calcination temperature according to its phase formation which were quantified using X rays diffractometry (XRD). Crystal structure characterization allows to establish that the material belongs to the I23 space group. Morphological characterization using a scanning electron microscope (SEM) and microstructure analysis show uniform particle size. Semi-quantitative compositional studies (EDS) prove the structure in the pure crystallographic phases. An optical band gap matching with literature was found using Kubelka-Munk's method over UV-Vis spectroscopy. A Physical Properties Measurement System (PPMS) was used to measure heat capacity and a transition was found at 163K. An electronic paramagnetic resonance (EPR) was done and its results match the ones found in literature.

References:

[1] H. Jebari, , N. Tahiri, M. Boujnah, O. El Bounagui, L. Boudad, M. Taibi, H. Ez-Zahraouy (2022). Structural, optical, dielectric, and magnetic properties of iron-sillenite Bi25FeO40.

[2] Oussama Baaloudj, Hamza Kenfoud, Ahmad K. Badawi , Achraf Amir Assadi, Atef El Jery, Aymen Amine Assadi, Abdeltif Amrane (2022). Bismuth Sillenite Crystals as Recent Photocatalysts for Water Treatment and Energy Generation: A Critical Review.

Keywords: *Sillenite, calcination temperature, photocatalysis.*

TRANSPORT THROUGH A DOUBLE QUANTUM DOT IN THE PAULI SPIN BLOCKADE REGIME

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Quantum dots are 0D few-electron (or hole) systems that allow for the study and manipulation of individual electrons (or holes) at low temperatures. Due to the possibility of employing the spin degree of freedom of an electron (or hole) as the building block of a qubit, they constitute one of the most promising candidates for spin-based quantum computing in semiconductor devices. Inspired by recent experiments in germanium-silicon core-shell nanowires hole double quantum dots (DQD), we simulate the dc (current) and ac (parametric capacitance) transport signatures of Pauli spin blockade (PSB), a phenomenon in which, due to the Pauli exclusion principle, current is suppressed when the bias voltage is negative. Our preliminary results are consistent with (unpublished) data involving transport through a DQD in the PSB regime. The present work is currently been developed in collaboration with Simon Svab, Rafael Eggli, Miguel Carballido, Pierre Chevalier Kwon, Taras Patlatiuk and Dominik Zumbühl (University of Basel), Ang Li and Erik Bakkers (TU Eindhoven), Stefano Bosco (QuTech and Kavli Institute of Nanoscience) and William Coish (McGill University).

References:

[1] Burkard, G., Ladd, T. D., Pan, A., Nichol, J. M., & Petta, J. R. (2023). Semiconductor spin qubits. Reviews of Modern Physics, 95(2), 025003.

[2] Hanson, R., Kouwenhoven, L. P., Petta, J. R., Tarucha, S., & Vandersypen, L. M. (2007). Spins in few-electron quantum dots. Reviews of Modern Physics, 79(4), 1217-1265.

[3] Eggli, R. S., Svab, S., Patlatiuk, T., Trüssel, D. A., Carballido, M. J., Chevalier Kwon, P., Geyer, S., Li, A., Bakkers, E.P.A.M., Kuhlmann, A.V. & Zumbühl, D. M. (2023). Cryogenic hyperabrupt strontium titanate varactors for sensitive reflectometry of quantum dots. Physical Review Applied, 20(5), 054056.

Keywords: *double quantum dot, Pauli spin blockade.*

Crystal Structure Prediction

COMPUTATIONAL MODELING OF THE OPTICAL PROPERTIES OF METALLIC NANOPARTICLES FOR POTENTIAL AGRICULTURAL APPLICATIONS

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Due to their significant optical properties and the various methods available for their synthesis, metallic nanoparticles are currently a major focus of both theoretical and experimental research by scientists worldwide. In this research, we conduct a theoretical characterization of Ag and Au nanoparticles through computational simulation. Specifically, we analyze the optical properties (absorbance, transmittance, and reflectance) of single and paired nanoparticles using the finite element method. Simulations are performed by varying the geometry (spherical and cylindrical), sizes, and materials of the nanoparticles to characterize their optical behavior. The results are compared with those reported in the literature, and finally, the potential of the nanoparticles for agricultural applications is evaluated.

Keywords: *Metal nanoparticles, Optical properties, Agricultural applications.*

DFT DETERMINATION OF STRUCTURAL PROPERTIES OF MOLECULES WITH POTENTIAL USE IN SENSORS USING QUANTUM ESPRESSO AND AIIDA

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In this work, we present a computational study focused on determining the structural geometries of four molecules using density functional theory (DFT) combined with the Quantum ESPRESSO package. To manage and automate the calculations, we used AiiDA, an advanced tool that not only optimizes data management but also ensures result reproducibility, a crucial aspect of contemporary scientific research. The molecules selected for this study were 1,6-hexanedithiol, 4-mercaptopyridine, diglycolic acid, and cysteine, which have been reported as potential candidates for sensor fabrication for detecting contaminants in aqueous media. Structural optimization calculations were performed using ultrasoft pseudopotentials and the Perdew-Burke-Ernzerhof correlation and exchange approximation for solids (PBEsol) within the DFT framework. AiiDA facilitated the efficient management of multiple calculations, allowing detailed workflow monitoring and automated result collection. The obtained results show significant agreement with theoretical data found in the literature, demonstrating the effectiveness of the DFT approach for accurate molecular structure prediction. Furthermore, the implementation of AiiDA provided a highly reproducible environment, highlighting the importance of automated management tools in modern computational research. This study underscores the potential of DFT and Quantum ESPRESSO, together with AiiDA, as powerful tools for research in computational chemistry and materials science, enabling not only precise prediction of structural properties but also efficient management and replication of complex calculations.

References:

[1] Giannozzi, P., et al. (2009). Quantum ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics: Condensed Matter, 21(39), 395502. DOI: 10.1088/0953-8984/21/39/395502

[2] Pizzi, G., et al. (2016). AiiDA: Automated interactive infrastructure and database for computational science. Computational Materials Science, 111, 218-230. DOI: 10.1016/j.commatsci.2015.09.013

Keywords: *DFT, Structural properties, Quantum Espresso, AiiDA.*

ESTIMATION OF SUITABLE UPPER-LIMITS FOR TEMPERATURE IN STABILITY COMPARISONS BETWEEN SOLID PHASES AT HIGH PRESSURES: STUDY CASES OF CARBON, OXYGEN, AND FLUORINE

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For most solid materials, the Quasi-Harmonic Approximation (QHA) is expected to remain valid across a wide temperature range, which extends further as pressure increases, sometimes surpassing the melting temperature of the material. Therefore, it becomes crucial to establish additional criteria to define the maximum temperature at which it is still meaningful to compare the stability of different crystalline phases, ideally without the high computational cost of accurately calculating the melting curve for each solid phase. In this study, we demonstrate that for crystalline systems where QHA holds true at elevated temperatures, an alternative and computationally efficient phenomenological approximation can effectively identify the region in the pressure-temperature (P-T) space where melting is likely to occur, based on Lindemann's criterion. By quantifying the deviation of atoms from their equilibrium positions as temperature increases in the solid phase, we were able to define their stability region in the P-T space, constrained by a line representing an 11% average deviation of atomic positions relative to interatomic distances. This approach provides a reliable lower limit for the melting line, offering a practical and accessible alternative, especially when accurate experimental data is lacking or when existing calculations are inconclusive.

References:

[1] Montoya JA, Cogollo-Olivo BH. Estimation of suitable upper-limits for temperature in stability comparisons between solid phases at high pressures. Study cases: carbon, oxygen, and fluorine. Revista de la Academia Colombiana de Ciencias Exactas, Físicas y Naturales. 47(182):37-50, enero-marzo de 2023

Keywords: *Lindemann; Melting; DFT; QHA; High Pressure; Diamond.*

ESTUDIO DE LA ESTABILIDAD EN LA DINÁMICA NO LINEAL PARA HACES ÓPTICOS PROPAGÁNDOSE EN UNA RED STUB

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Este trabajo se centra en la investigación de la dinámica no lineal de haces ópticos en sistemas periódicos no lineales, específicamente en una red fotónica stub. La red, compuesta por guías de onda acopladas con geometría stub, se analiza teóricamente mediante simulaciones numéricas en Python. La implementación del modelo teórico en la red Stub se lleva a cabo con precisión mediante el método de Newton-Raphson. El objetivo principal de la investigación es analizar la estabilidad de la propagación de las ondas no lineales en función de la potencia óptica. Las simulaciones realizadas durante el estudio permiten no solo examinar detalladamente las soluciones no lineales, sino también calcular los estados estacionarios y analizar la estabilidad resultante. Los resultados ofrecen una comprensión detallada de la estabilidad de la propagación de ondas no lineales en esta configuración, contribuyendo así al avance del conocimiento en este campo de investigación.

Referencias:

[1] A. M. G. Hernández, "Óptica y fotónica: ciencia y tecnología de la luz," Revista de la Academia Colombiana de Ciencias Exactas, Físicas y Naturales, vol. 46, (2022).

[2] B. Real, C. Cantillano, D. López-González, A. Szameit, M. Aono, M. Naruse, S. J. Kim, K. Wang, and R. A. Vicencio, "Flat-band light dynamics in stub photonic lattices", Scientific Reports, vol. 7, no. 1, pp. 1–7, (2017).

Keywords: *Modos acoplados, Fotónica, Red Stub.*

STUDY OF THE MECHANISM OF FLUORINE-INDUCED MAGNETISM IN GRAPHENE

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Different types of adsorbed atoms can induce magnetism on graphene. Among all the atoms studied, the magnetism induced by light atoms such as H, F and C on graphene has received great attention because it does not involve d or f orbitals. In the case of an isolated fluorine atom on graphene, the experimental results obtained so far are not sufficient to clarify the induced magnetism [1,2,3]. In this work, we carried out a comprehensive study using Density Functional Theory (DFT) with different functionals (HSE, PBEsol and ACBN0) and also DFT + U + V calculations to investigate the adsorption and magnetic properties of isolated fluorine atoms on graphene. Our results reveal that the gradient corrected functionals erroneously predict a non-magnetic ground state, while more accurate calculations such as hybrid functionals and DFT + U + V calculations predict a magnetic moment of 1 Bohr magneton per cell for the graphene system with adsorbed fluorine. We then develop tight-binding models based on our DFT results, using Wannier functions, that accurately reproduce the observed electronic structure and magnetic order. This allows us to elucidate the physical origins and identify the key factors influencing the magnetic behavior of these covalent systems, paving the way for a deeper understanding of the system and providing a computationally efficient tool to explore the electronic structure and magnetic behavior of the system. Our work demonstrates the crucial importance of an accurate treatment of electronic correlations to capture the magnetic ground state in these systems, contributing to the understanding of light atom-induced magnetism in graphene.

References:

[1] Hong et al., Physical Review B 83, 085410 (2011)

[2] Nair et al., Nature Physics 8 199–202 (2012)

[3] Hong et al., Phys. Rev. Lett. 108, 226602 (2012)

Keywords: *ACBN0, DFT, hybrid functionals.*

HEUSLER ALLOYS: STRUCTURAL FEATURES AND PHYSICAL PROPERTIES EXPLORED

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Heusler alloys are materials composed of two or more 3d transition metals combined with one 3p element. The properties of these compounds can be tuned by substituting or replacing one of them. These properties, including shape memory, ferromagnetism, half-metallicity, half-ferromagnetic behavior, and Hall anomalous effect make Heusler alloys suitable for applications in actuators, sensors, and spintronic devices. The Ni_2MnGa compound and its Ni-excess alloys are among the most extensively studied. These alloys exhibit higher martensite-austenite transformation temperatures and lower Curie temperatures when Ni is in excess, and Mn is reduced. Increasing the Ni concentration from 0 to 1.0 tends to increase the thermal hysteresis during the martensite-austenite phase transition, which can affect magnetocaloric effect applications.

We found that in the martensite phase, the crystal structure is tetragonal. Considering, the compatibility between the martensite and austenite phases, crystal parameters are used to derive factors and . These factors are used to evaluate this compatibility. The theoretical prediction of no thermal hysteresis is valid when either and .

On the other hand, substituting Fe into this alloy can increase ductility. However, this substitution not only affects the bonds, bulk modulus, and shear modulus but also alters relaxation frequencies. Measurements of impedance as a function of temperature reveal that when these materials are subjected to time-variant fields, the relaxation frequencies can range from low to high depending on the Fe content in the alloys.

INFLUENCE OF NON-HERMITIAN POTENTIALS ON THE MOBILITY PROBLEM OF NONLINEAR BEAMS

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In the study of nonlinear optical systems, the goal is to counteract the problem of diffraction in the propagation of optical information through non-deforming solutions (optical solitons). These solitons have been observed throughout history in various fields of physics and can arise in optical systems due to a balance between beam diffraction and the nonlinearity of the medium.

In this work, the analysis of the evolution of optical beams in a nonlinear periodic medium is presented using the nonlinear Schrödinger equation, where the interaction of light with the medium is described by a potential that extends throughout the space where the light propagates. Specifically, the existence and stability of stationary solutions were investigated when the periodicity of the array corresponds to a one-dimensional lattice. Subsequently, the numerical propagation of these solutions was implemented to corroborate their stability through the simulation of different experimental conditions.

Additionally, the mobility regimes of the solutions in a 1D system in the presence of PT symmetry have been studied, and how this affects the transport of light within the waveguides.

References:

[1] Carl M Bender. "Introduction to PT-symmetric quantum theory". En: Contemporary Physics 46.4 (2005), págs. 277-292. DOI: 10.1080/00107500072632. eprint: https://doi.org/10.1080/00107500072632. URL: https://doi.org/10.1080/00107500072632.

[2] Yaroslav V. Kartashov, Boris A. Malomed y Lluis Torner. "Solitons in nonlinear lattices". En: Rev. Mod. Phys. 83 (1 abr. de 2011), págs. 247-305. DOI: 10.1103/RevModPhys.83.247. URL: https://link.aps.org/doi/10.1103/RevModPhys.83.247.

[3] Z. H. Musslimani et al. "Optical Solitons in PT Periodic Potentials". En: Phys. Rev. Lett. 100 (3 ene. de 2008), pág. 030402. DOI: 10.1103/PhysRevLett.100.030402. URL: https://link.aps.org/doi/10.1103/PhysRevLett.100.030402.

[4] Sean Nixon, Lijuan Ge y Jianke Yang. "Stability analysis for solitons in PT-symmetric optical lattices". En: Phys. Rev. A 85 (2 feb. de 2012), pág. 023822. DOI: 10.1103/PhysRevA.85.023822. URL: https://link.aps.org/doi/10.1103/PhysRevA.85.023822.

[5] M. Skorobogatiy y J. Yang. Fundamentals of Photonic Crystal Guiding. Cambridge University Press, 2009. ISBN: 9780521513289. URL: https://books.google.com.co/books?id=-GPNWG5I-dkC.

[6] Jianke Yang. Nonlinear Waves in Integrable and Nonintegrable Systems. Society for Industrial and Applied Mathematics, 2010. DOI: 10.1137/1.9780898719680.

Keywords: *Optical solitons, PT symmetry, Nonlinear periodic media, Diffraction.*

MODOS NO LINEALES LOCALIZADOS EN UNA RED RHOMBIC

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En las últimas décadas, ha surgido un creciente interés en el campo de la óptica no lineal, tanto en ámbitos científicos como industriales, debido a las ventajas que los dispositivos fotónicos ofrecen en comparación con los electrónicos, destacando su amplio ancho de banda y su potencial reducido consumo energético [1]. Estos dispositivos poseen una respuesta no lineal que permite la generación de uno de los fenómenos con enorme relevancia en la fotónica: los solitones ópticos. En este trabajo, se introduce una red fotónica de geometría romboédrica (rhombic) compuesta por arreglos periódicos de guías de ondas acopladas evanescentemente. Este tipo de acoplamiento entre guías adyacentes da lugar a la formación de dos bandas de dispersión y una banda plana [2]. Se examina específicamente la generación de solitones como resultado de la interacción entre la difracción de la luz y la respuesta no lineal del medio (efecto Kerr), al excitar estas bandas. Se propone un sistema conservativo que asume un medio no lineal de tipo Kerr, infinito y discreto, compuesto por guías de onda que forman una geometría romboédrica. Este sistema se utiliza para modelar la propagación de haces ópticos, empleando la Ecuación no Lineal de Schrödinger Discreta (ENLSD).

Referecias:

[1] Jeff Hecht, The Breakthrough Birth of Low-Loss Fiber Optics, Optics and Photonics News 31(3), 26-33 (2020).

[2] Sebabrata Mukherjee and Robert R. Thomson, Observation of robust flat-band localization in driven photonic rhombic lattices, Opt. Lett. 42, 2243-2246 (2017).

Keywords: *Óptica no lineal; Guías de onda; ENLSD.*

THEORETICAL ANALYSIS OF THE OPTICAL PROPERTIES OF TIO2 NANOPARTICLES USING COMPUTATIONAL ELECTROMAGNETISM TECHNIQUES

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The use of nanoparticles such as zinc, titanium, zirconium, and silver has enabled the development of nanomaterials with superior chemical, mechanical, and physical properties compared to conventional materials. Among metallic nanoparticles, titanium dioxide (TiO_2) is widely used in various technological applications due to its unique optical properties, making it ideal for photocatalysis, solar cells, and optoelectronic devices. At the nanoscale, these optical properties are strongly influenced by the crystalline structure and morphology of TiO_2. This study provides a theoretical characterization of the optical properties of TiO_2 nanoparticles with different geometries and dimensions, using computational electromagnetism methods to analyze their ability to absorb and scatter an electric field. Initially, the optical properties of the nanostructures are examined through Maxwell's equations, along with numerical methods to solve electromagnetism problems, primarily focusing on the finite element method. Additionally, considering that metallic nanomaterials are being recently studied for potential antimicrobial and antifungal applications, as well as for photocatalysis, solar cells, and optoelectronic devices, a possible application in one of these fields is evaluated.

Keywords: *Metal nanoparticles, Optical properties, Optoelectronic devices.*

THEORETICAL AND EXPERIMENTAL STUDY OF THE PEROVSKITE-TYPE FERRO-MANGANITE LA0.5CA0.5MN0.5FE0.5O3

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Synthesis and characterization of the structural and electrical properties of the perovskite-type ferro-magnetite $La_{0.5}Ca_{0.5}Mn_{0.5}Fe_{0.5}O_3$ are reported. Structural analysis reveals crystallization of the material in an orthorhombic structure, space group Pbnm (#62). The optical response suggests semiconductor-type behavior with bandgap E g =2.3 eV. Band structure calculations around the Fermi level result in two different band gap values for the two spin up and spin down polarizations, as expected in ferromagnetic semiconductor materials. The hybridizations observed in the density of states curves as a function of energy suggest that the ferromagnetic character is due to double exchange mechanisms, coexisting with antiferromagnetic super-exchange, which is essentially due to the disorder of Fe^{3+} and Mn^{4+} cations in the octahedra along the three crystallographic axes.

Keywords: *DRX, DFT, semiconductor.*

TUNING MAGNETIC AND SEMICONDUCTING PROPERTIES OF CR-DOPED CATIO3 PEROVSKITES FOR ADVANCED SPINTRONIC APPLICATIONS

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The physical properties of perovskite-type materials are sensitive to their chemical composition and crystallographic structure, which makes them highly versatile for various advanced technological applications. In this theoretical study, density functional theory (DFT) is employed to investigate the electronic properties of the perovskite-like material $CaTiO_3$, focusing on the substitution of Ti^{4+} with the magnetic transition metal Cr^{4+}. The results reveal a systematic increase in the effective magnetic moment and a gradual decrease in the bandgap with increasing Cr^{4+} content in the $CaTi_{1-x}Cr_xO_3$ system (x=0.0, 0.25, 0.5, 0.75, 1.0). The interactions between electronic orbitals associated with Ti-O-Cr inter-octahedral bonds modify the magnetic response of the material, leading to hybridizations between valence and conduction states that alter its semiconductor character. This tunability in electronic and magnetic properties underscores the potential of these materials for applications in spintronics. The study offers novel insights into the design of new magnetic semiconductor materials with tailored functionalities, contributing to the development of next-generation spintronic devices.

Keywords: *DFT; spintronic; first principles calculation; magnetic semiconductor material*

UNDERSTANDING NOBLE GAS INCORPORATION IN MANTLE MINERALS: AN ATOMISTIC STUDY

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Ab initio calculations in forsterite (Mg_2SiO_4) are used to gain insight into the formation of point defects and incorporation of noble gases. We calculate the enthalpies of incorporation both at pre-existing vacancies in symmetrically non-equivalent sites, and at interstitial positions. At high pressure, most structural changes affect the MgO_6 units and the enthalpies of point defects increase, with those involving Mg and Si vacancies increasing more than those involving O sites. At 15 GPa Si vacancies and Mg interstitials have become the predominant intrinsic defects. We use these calculated enthalpies to estimate the total uptake of noble gases into the bulk crystal as a function of temperature and pressure both in the presence and absence of other heterovalent trace elements. For He and Ne our calculated solubilities point to atoms occupying mainly interstitial sites in agreement with previous experimental work. In contrast, Ar most likely substitutes for Mg due to its larger size and the deformation it causes within the crystal. Incorporation energies, as well as atomic distances suggest that the incorporation mainly depend on the size mismatch between host and guest atoms. Polarization effects arising from the polarizability of the noble gas atom or the presence of charged defects are minimal and do not contribute significantly to the uptake. Finally, the discrepancies between our results and recent experiments suggest that there are other incorporation mechanisms such as adsorption at internal and external interfaces, voids and grain boundaries which must play a major role in noble gas storage and solubility.

Keywords: *Noble gases, ab-initio study, point defects*

USING SURFACE-FACET TRANSITIONS TO TUNE THE ELECTRONIC SPECTRUM OF COLLOIDAL SILICON QUANTUM RODS

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The idea of inducing controlled changes in the electronic structure of nanometric devices via surface modifications has been proposed in the last few years by different authors [1]. In this work, we show that the judicious combination of surface facets on silicon colloidal quantum rods leads to strong modifications of the electronic structure. In this work, we propose a silicon nano rod structure where the ratio of surface facets (100)/(110) is modified along the system (fig. 1). Our results, obtained by means of atomistic calculations and effective pseudopotentials [2], show an energy bandgap more closely related to the symmetry rather than to the number of atoms or size of the system (fig. 2), exhibiting a reduction of the bandgap, in comparison to more uniform nanostructures, which may be convenient for opto-electronic application. Moreover, the wave function localization of the LUMO and HOMO states can be associated to a type-II heterostructure, which is unexpected considering that there is only one atomic species present all over the structure.

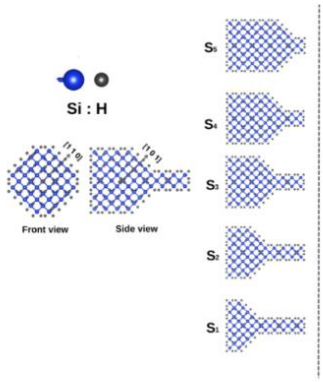

Fig. 1. Nanorod structures showing the atomic composition. The left-hand side shows the crystallographic orientations.

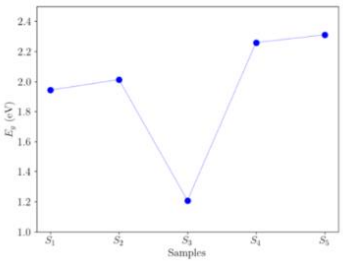

Fig. 2. Energy bandgap according to the shown in Fig. 1.

References:

[1] T. Vo, A. J. Williamson, and G. Galli, "First principles simulations of the structural and electronic properties of silicon nanowires," Phys. Rev. B 74,045116 (2006).

[2] J. R. Cárdenas and G. Bester, "Atomic effective pseudopotentials for semiconductors,"Phys. Rev. B 86, 115332 (2012). - J. Cárdenas, M. Bandera, and F. Nuñez-Murillo, "Multipole moment description of passivants and complex pseudopotentials for semiconductor surfaces," Computational Condensed Matter 33, e00765 (2022).

Keywords: *Atomistic calculations, electronic structure, semiconductor nanostructures*

Magnetism, Strongly Correlated Systems, Collective Phenomena, Low-Temperature Physics

AB INITIO STUDIES OF ELECTRONIC AND MAGNETIC PROPERTIES OF XGETE3 MONOLAYERS (X=CR, MN, FE)

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This study employed the Vienna Ab initio Simulation Package (VASP), utilizing various functionals to comprehensively describe the electronic and magnetic properties. To correct the magnetic part of transitions metals Cr, Mn, and Fe, a GGA+U scheme was employed. Significant findings emerged regarding the stability of ferromagnetic phases in the initial two monolayers, Cr2Ge2Te6 (CGT) and Mn2Ge2Te6 (MGT), alongside the stability of the antiferromagnetic phase in Fe2GeTe6 (FGT). Phonon calculations conducted via Phonopy provided valuable insights into the dynamical stability of these monolayers. It was observed that CGT and MGT monolayers exhibited robust stability, while FGT monolayers displayed instability. Additionally, magnetic alloys of each monolayer, including CGT, MGT, and FGT, were performed and studied using the special quasi-random structures (SQS) methodology to understand their properties and behavior These results underscore the importance of further electronic computational studies on transition-metal trichalcogenides (TMTCs) to elucidate the underexplored realm of magnetism in 2D systems. This exploration was prompted by the experimental synthesis of magnetic monolayers in 2017 [1,2].

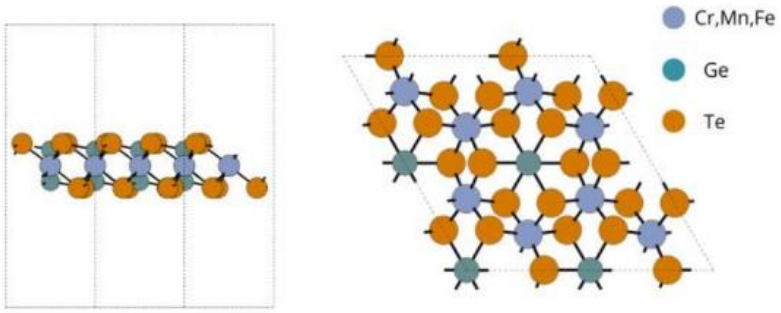

Fig. 1. Side and top view of XGeTe3 monolayers.

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References:

[1] Cheng Gong et al. Discovery of intrinsic ferromagnetism in two-dimensional van der Waals crystals. In: Nature 546.7657 (2017), pp. 265–269.

[2] Bevin Huang et al. Layer-dependent ferromagnetism in a van der Waals crystal down to the monolayer limit'. In: Nature 546.7657 (2017), pp. 270–273.

ANGULAR DEPENDENCE OF FERROMAGNETIC RESONANCE IN FECO THIN FILMS

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In this work, magnetic anisotropies in a FeCo thin film grown on a MgO substrate were studied. The ferromagnetic resonance (FMR) technique was used to determine the magnetic parameters of the thin film at room temperature, such as the g factor, magnetic anisotropy fields, and effective magnetization. The angular dependence of the FMR spectra was attributed to the presence of an uniaxial anisotropy superimposed on the fourfold anisotropy, which was confirmed by the in-plane and out-of-plane hysteresis curves, revealing a hard out-of-plane magnetic axis. Analysis of the FMR linewidth dependence on the orientation of the applied magnetic field and the excitation frequency in FMR experiments revealed exceptionally low damping values for ferromagnetic conductors (α ~ 5 × 10−3). These findings suggest that the FeCo/MgO system is a promising candidate for future applications in thermomagnetic effects.

Keywords: *Angular dependence, ferromagnetic resonance, damping*

DENSITIES IN BOSE-EINSTEIN CONDENSATES FROM ALKALINE ATOMS TO SUPERSOLID SYSTEMS.

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The Bose-Einstein condensate (BEC) was theoretically predicted by Albert Einstein and Satyendra Nath Bose in 1924, but the first atomic BEC was experimentally observed only after several decades. The BEC is a macroscopic quantum phase transition in which a large number of bosons condensate in the lowest-energy single-particle state when the system is cooled below a critical temperature Tc [1]. In a remarkable realization, Anderson et. al. [2] achieved one of the first experimental observations for a BEC. In the experiment, a vapor of rubidium-87 atoms was confined in a magnetic trap and cooled down to extremely low temperatures in the order of nano-kelvins. Recently, atoms with larger (magnetic) dipole moments, such as ^{164}Dy [3], have become available for experimental studies of quantum phenomenon. Thus, the so-called dipolar Bose-Einstein condensates open up new avenues in the research for the static and dynamic properties of such systems, where the anisotropic long-range dipolar interaction plays an important role.

It is well known that many of the static and dynamic properties of an atomic BEC are studied by solving the mean-field Gross-Pitaevskii (GP) equation, which is a nonlinear partial differential equation for short-range atomic interaction. In the case of a dipolar BEC, it is necessary to include an additional term in order to give an accurate description of the dipole-dipole interaction potential that does not have a trivial evaluation form. In the last case, the GP equation becomes a nonlinear partial integro-differential equation, which is much more complex to solve. The evaluation of the dipolar integral term in the coordinate space is not straightforward due to the divergence at short distances. However, this can be done by evaluating the dipolar term in the momentum (k) space using the convolution theorem. Moreover, a dipolar BEC collapses for strong dipolar interaction beyond a critical value, and a Lee-Huang-Yang-type (LHY-type) beyond-mean-field quantum-fluctuation interaction is necessary to stabilize a strongly dipolar droplet against collapse [4]. A high-density droplet formation was observed experimentally in a dipolar BEC under a strong trap of 164 Dy, for a number of atoms above a critical value and for an appropriate mixture of dipolar and contact interactions [5].

In this work we study the difference in the density profiles for the next three cases: i) BEC, ii) dipolar BEC and iii) a dipolar BEC including the quantum-fluctuation Lee–Huang–Yang interaction. The effects of quantum-fluctuation interaction is modeled as a quartic nonlinearity term in the beyond mean field model of description of the system. We use, as long as possible, similar values of nonlinearities for all cases in the range of the experimental interest. Finally, we emphasize that the

value of our work is towfold: on one side, it is analyzed the consequences in the density profiles as a result of the quantum-fluctuation interactions and the dipolar interaction term, and on the other side, our work provides an example of efficient algorithm to use in the study of the beyond-mean-field theory in ultra-cool atoms [6].

References:

[1] A. J. Leggett. Quantum Liquids. Bose Condensation and Cooper Pairing in Condensed-Matter Systems. Oxford Univ. Press, Oxford, 2006.

[2] M. H. Anderson et. al. Observation of Bose-Einstein condensation in a dilute atomic vapor. Science, 269:198, 1995.

[3] M. Lu et. al. Strongly dipolar Bose-Einstein condensate of dysprosium. Phys. Rev. Lett., 107:190401, 2011.

[4] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. 106, 1135, 1957; A. R. P. Lima and A. Pelster, Phys. Rev. A 84, 041604, 2011; A. R. P. Lima and A. Pelster, Phys. Rev. A 86, 063609, 2012; F. Wächtler and L. Santos, Phys. Rev. A 93, 061603, 2016.

[5] M. Schmitt, M. Wenzel, F. Böttcher, I. Ferrier-Barbut, and T. Pfau, Nature (London) 539, 259, 2016.

[6] Vladimir Lončar, Luis E. Young-S., Srdjan Škrbić, Paulsamy Muruganandam, Sadhan K. Adhikari and Antun Balaž, Comput. Phys. Commun. 195, 117, 2015; ibid. 200, 406, 2016.

Keywords: *Bose-Einstein condensate, dipolar interaction, quantum-fluctuation.*

EFFECT OF SM-DOPING PROCESS INTO THE YIG SLABS ON STRUCTURAL AND MAGNETIC PROPERTIES

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Yttrium Iron Garnet (YIG) $Y_3Fe_5O_{12}$ is a material of significant interest due to its ferromagnetic properties; it is magnetically soft, has high saturation magnetization (Ms), and low coercive fields (HC). Additionally, being an electrical insulator makes it a good candidate for ferromagnetic resonance (FMR) studies and spin-caloritronics applications. In addition, the replacement of a small fraction of the yttrium ions in YIG garnet by samarium (Sm) provides distinct benefits towards manipulating its magnetic and optical properties, which are key features for the development of microwave devices and spintronic applications. In this work, we report the results of Sm doping in YIG slabs synthesized by solid-state reaction, hereinafter namely $Y_{3-x}Sm_xFe_5O_{12}$ with x values of 0.0, 0.1, 0.2, 0.3, 0.4, 0.5 and 0.6. The structural analysis by X-ray diffraction showed the cubic phase garnet structure (Ia-3d) for all compositions without the presence of secondary phases. The Sm substitution induced slight changes in the lattice parameter as a consequence of similar ionic radio between Sm(III) and Y(III) ions (NC=6). The mean grain size around 4 to 9 μ m was determined from the scanning electron micrographs, and the grains exhibited an uniform growth with well-defined grain boundaries. Magnetic properties for all samples were analyzed through magnetization (M) against field (H) curves through vibrating sample magnetometer (VSM) at 300K. M(H) loops showed as expected a ferromagnetic soft behavior with Hc values around 1 Oe. A steady decrease for the Ms was observed as a function of the doping concentration, reaching a ~6% reduction for the highest concentration. A large number of magnetostatic modes were exited by ferromagnetic resonance using broadband FMR spectroscopy based on a coplanar waveguide spectometer. FMR absorption spectra showed that both surface and volumen modes were drastically affected by Sm introduced into the lattice, leading to an overlapping of all modes at 8 GHz for x = 0.6.

References:

[1] Li, H. (n.d.). Investigation of the structural, magnetic, impedance properties in samarium-doped yttrium iron garnet. Ceramics International.

[2] Sadhana, K., Murthy, S. R., & Praveena, K. (2014). Effect of Sm3+ on dielectric and magnetic properties of Y3Fe5O12 nanoparticles. Journal of Materials Science: Materials in Electronics, Springer Science+Business Media. doi:10.1007/s10854-014-2194-9

Keywords: *Structural properties, Solid-state reaction, Magnetic properties, Ferromagnetic Resonance, Yttrium Iron Garnet.*

EXCITING ELECTRONIC PHENOMENA IN NOVEL CHIRALLY MAGNETIC ANTIPEROVSKITES

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In the condensed matter field, perovskites (i.e. ABX_3) have stood as one of the most reliable families of materials where multifunctional properties converge. A forgotten associated family of compounds, the antiperovskites (i.e. A_3BX), have been recently gaining considerable interest thanks to their remarkable and intertwined magnetic and topological features. Magnetically active antiperovskites, having chiral noncollinear antiferromagnetic ordering, have shown negative thermal expansion, superconductivity, and anomalous Hall effects, among other properties. Nevertheless, in-depth details on the electronic structure, vibrational features, and topological response are still scarce. Here, we show a theoretical study, based on first-principles calculations in the framework of density-functional theory (DFT), on the electronic, phononic, and topological properties associated with the spin-phonon coupling, strain effects, topological response, and in-depth electronic understanding of the multifunctional properties. We demonstrate and explain the enormous spin-phonon coupling and the effect of the Coulomb exchange correlations in the magnetic exchange interactions at the Mn_3NiN, considered as a prototype among the family [1]. With the latter in mind, we explored the origin behind the potential enhancement and control of their magnetic and topological properties by means, for example, of an external epitaxial strain. With this strategy, we achieved an enhancement of the conductivity by compression in the [111] crystallographic plane. Furthermore, we explained the observed coupling between the Weyl nodes, electronic structure, chiral magnetism, and symmetry considerations as a function of this external control parameter [2]. We also revealed, based on the Bader charges and the electronic structure analysis, the negative and positive oxidation states of the Ni- and Mn-sites, respectively. This agrees with the expected $A_3^{a+}B^{b-}X^{c-}$ oxidation states to satisfy the charge neutrality in antiperovskites. Therefore, we extrapolated our findings on the oxidation states to several Mn_3BN compounds, showing that the antiperovskite structure is an ideal platform to encounter negative oxidation states for metals sitting at the corner B-sites [3]. Finally, by employing the acquired knowledge on antiperovskites, we predicted the novel crystal V_3AuN in which, the chiral magnetism prevails and the topological features result in an enhanced AHC value. It is worth noticing that the latter is the largest theoretically reported in these compounds [4].

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References:

[1] L. Flórez-Gómez, W. Ibarra-Hernández, A. C. Garcia-Castro, Lattice dynamics and spin–phonon coupling in the noncollinear antiferromagnetic antiperovskite Mn3NiN, Journal of Magnetism and Magnetic Materials 562 (2022) 169813. doi:https://doi.org/10.1016/j.jmmm.2022.169813.

[2] D. Torres-Amaris, A. Bautista-Hernandez, R. Gonzalez-Hernandez, A. H. Romero, A. C. Garcia-Castro, Anomalous hall conductivity control in Mn3NiN antiperovskite by epitaxial strain along the kagome plane, Phys. Rev. B 106 (2022) 195113. doi:10.1103/PhysRevB.106.195113.

[3] E. Triana-Ramirez, W. Ibarra-Hernandez, A. C. Garcia-Castro, Anionic nickel and nitrogen effects in the chiral antiferromagnetic antiperovskite Mn3NiN, Phys. Chem. Chem. Phys. 25 (2023) 14992–14999. doi:10.1039/D3CP00183K.

[4] J. M. Duran-Pinilla, A. H. Romero, A. C. Garcia-Castro, Chiral magnetism, lattice dynamics, and anomalous hall conductivity in V3AuN antiferromagnetic antiperovskite, Phys. Rev. Mater. 6 (2022) 125003. doi:10.1103/PhysRevMaterials.6.125003.

Keywords: *Chiral magnetism, Antiperovskites, Kagome lattices, Topology, Density-functional theory*

FERROIC ORDERS ANALYSIS FOR MOSE2 AND MOTE2 SOLID SOLUTIONS

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Ferroic orders are a group of phenomena characterized by the spontaneous alignment of magnetic, electric, or crystalline domains on a material, even in the absence of their conjugate field (for example, magnetic field for the case of ferromagnets). The coexistence of at least two of these orders is denominated multiferroicity but its observation in materials is scarce. Most of the multiferroics known to date belong to the 3-dimensional transition metal oxides, which suffer from depolarization and other effects detrimental to the observation of multiferroicity in the nanoscale. In this sense, the fabrication of nanostructured multiferroic devices based in these compounds is highly challenging. The recent observation of multiferroicity at room temperature in the intrinsically 2-dimensional van der Waals compound represents a great advancement in the field, [4] and calls for the study of multiferroicity in alternative solid solutions of similar van der Waals compounds. One promising candidate in this search is the solid solution between and , provided that they are reported to be ferromagnetic or ferroelectric, respectively. Here we will present the recent advances in our study of the chemical, structural, magnetic and electronic properties of single crystals of . In light of our results, we will discuss about their potential for the presence of multiferroic states in this 2-dimensional compound.

References:

[1] Cardenas-Chirivi, G. et al. Room temperature multiferroicity in a transition metal dichalcogenide. npj 2D Materials and Applications 7, 54 (2023).

Keywords: *Transition metal dichalcogenides, Ferroelectric, Ferromagnetic, Multiferroic, Vacancies, Doping.*

GROSS-PITAEVSKII EQUATION: REVEALING THE BEHAVIOR OF BOSE-EINSTEIN CONDENSATES

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In this work we will study the behavior of Bose-Einstein condensates, in particular their behavior upon change of the confining trap. Bose-Einstein condensates are a state of matter formed by bosons, which are elementary particles with integer spin. Bosons can occupy the same quantum state, unlike fermions, which are subject to the Pauli exclusion principle [1].

Bose-Einstein condensates arise when a group of bosonic atoms experience temperatures close to absolute zero and all are in their fundamental state, behaving as a single physical entity with quantum properties. The Bose-Einstein Condensate was proposed by Nath Bose and Albert Einstein in the 1920s, and achieved the first experimental observation with Rubidium-87 atoms in 1995 [2].

In a Bose-Einstein condensate, the atoms are superfluid, which means that they can flow frictionlessly through the system and to show the formation of vortex states. In addition, an important physical property of the system is that they is a dilute gas, which means that the density of the atoms is low enough to facilitate control of the necessary experimental properties. A key feature of these condensates is the repulsive atomic interaction, which is characterized by the scattering length of the atoms. This repulsion prevents the collapse of the condensate and plays a crucial role in determining the density and stability of the system [3].

The dynamics and steady states of the Bose-Einstein condensate can be described by the Gross-Pitaevskii equation which considers the atomic interaction under an external potential that for a harmonic oscillator trap takes the form [1]:

$$i\hbar\frac{\partial\Psi(r,t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2) + g|\psi(r,t)|^2\right]\Psi(r,t)$$

With normalization condition $\int_{-\infty}^{\infty}|\Psi(r,t)|^2 dr = 1$; and atomic interaction constant $g = 4\pi\hbar^2 aN/m$ where $\hbar$ is the reduced Planck constant, a is the scattering length (this parameter characterizes the interaction between the atoms), ω_x; ω_y; ω_z are the angular frequencies of the trap in x, y and z-direction respectively, m is the mass of each atom and N represents the number of particles in the condensate. The Gross-Pitaevskii equation is solved numerically and to facilitate these calculations it is modified in its different symmetries and expressed in a dimensionless form as explained in the article [3]. It is solved using the programs provided by [4] where parameters of the physical system can be specified in order to simulate different experimental situations and study the behavior of the condensate.

We will approach the study of the Bose-Einstein condensate in different dimensions: one, two and three dimensions, using as a reference system an alkali atom with parameters of experimental interest. In this context, the trap frequency parameters will be adjusted to observe and analyze how as the trap frequency value changes in one direction the condensate tends to "compress" in that direction because the potential energy of the trap in that direction is higher and it will have less freedom of movement.

References:

[1] Pethick, C. J., & Smith, H. (2008). Bose–Einstein condensation in dilute gases. Cambridge university press.

[2] Cornell, E. A., & Wieman, C. E. (1995). Bose-Einstein condensation in a dilute gas: The first 70 years and some recent experiments. Reviews of Modern Physics, 74(3), 875–893.

[3] Muruganandam, P., & Adhikari, S. K. (2009). Fortran programs for the time-dependent Gross–Pitaevskii equation in a fully anisotropic trap. Computer Physics Communications, 180(10), 1888-1912.

[4] L. E. Young-S., P. Muruganandam, S. K. Adhikari, V. Lončar, D. Vudragović y A.Balaž, (2017). «OpenMP GNU and Intel Fortran programs for solving the time-dependent Gross–Pitaevskii equation», Computer Physics Communications, vol. 220, págs. 503-506, issn: 0010-4655. doi: https://doi.org/10.1016/j.cpc.2017.07.013.

Keywords: *Bose-Einstein condensate, Gross-Pitaevskii equation, numerical results.*

LUTTINGER/FERMI LIQUID MIXING IN ONE-DIMENSIONAL QUANTUM FLUIDS

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By resorting to tensor network techniques in the thermodynamic limit, we identify a new universality class of one-dimensional, interacting fermions beyond the low-energy regime, termed the "quasi-Fermi liquid." This fermionic liquid exhibits traits of both Luttinger and Fermi liquids, depending on the probing energy scale. We characterize the ground state and dynamic properties by computing the momentum distribution, spectral function and dynamic structure factor. The momentum distribution displays a finite jump at the Fermi momentum. The spectral function, in contrast, shows both power-law and quasiparticle excitations, depending on whether particle-hole symmetry is broken or not. The dynamic structure factor shows similarities to that for weakly-interacting fermions with a finite, effective mass. These results indicate that the quasi-Fermi liquid paradigm goes beyond the Luttinger and Fermi liquids models, establishing it as a distinct framework for interacting fermions in one spatial dimension.

References:

[1] Joshua D. Baktay, Alexander V. Rozhkov, Adrian E. Feiguin, and Julián Rincón, "Quasi-Fermi liquid behavior in a one-dimensional system of interacting spinless fermions." Phys. Rev. B 108, 245134 (2023).

[2] Joshua D. Baktay, Adrian E. Feiguin, and Julián Rincón, "Universal quasi-Fermi liquid physics of one-dimensional interacting fermions." arXiv:2406.10063 [cond-mat.str-el].

Keywords: *Luttinger liquid, Fermi liquids, tensor networks, matrix product states, density matrix renormalization group, universality classes, quantum liquids.*

PEARSON CORRELATION COEFFICIENT AS A TOOL TO IDENTIFY THE NON-COMPOSITE VORTEX STATES IN A TWO-BAND SUPERCONDUCTING SLAB

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For the identification of non-composite vortex states in a two-band superconducting slab, we employed the Pearson product-moment correlation coefficient, r [1]. This coefficient is calculated in terms of the square modulus of the order parameters of the two condensates. In statistics, the values of r oscillate between -1 and 1. For composite vortices, this coefficient tends to 1, while for non-composite vortices, it tends to 0. Negative values of r have no relevant meaning in this context. This tool allowed us to identify the degree of decoupling of the vortex network, facilitating the task of identifying fields and currents for which the uncoupled vortex states are present in the superconducting sample. This is important for controlling energy dissipation in the multiband superconducting materials used in the industry.

Keywords: *Pearson Correlation Coefficient, Non Composite Vortex, Multiband Superconductor*

SINGLE AND TWO-PARTICLES DYNAMICS OF SPIN-1 LATTICE BOSONS IN PRESENCE OF EXTERNAL PERIODIC MAGNETIC FIELDS

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In this work, we analyze the temporal dynamics of one and two bosons (alkaline atoms) with the lowest internal spin degree of freedom, i.e., spin 1, confined in a one-dimensional optical lattice [1]. The optical lattice simulates the crystalline structure of a solid, and in this this work the kinetic energy dominates over the bosonic interaction so this leads to the superfluid regime [2]. The interactions are limited only to bosons in the same potential well and the chemical potential regulates the addition or subtraction of particles. We uses the Spin-1 Bose-Hubbard Hamiltonian, commonly represented in the basis of S_z. However, it is proposed to use the spin coherent basis and the quadrupolar basis [3], taking advantage of the SU(3) symmetry present in the system, in addition to being relevant to study the properties of the system in the presence of external magnetic fields. Temporal dynamics are modeled using Floquet's theory [4], establishing parallels with Bloch's spatial analysis but in a temporal context.

References:

[1] A. M. Rey, "Ultra-cold bosonic atoms in optical lattices: An Overview", en, Revista de la Academia Colombiana de Ciencias Exactas, F´ısicas y Naturales 45, 666 (2021).

[2] M. Greiner, O. Mandel, T. Esslinger, T. W. H ̈ansch, and I. Bloch, "Quantum phase transition from a superfluid to a mott insulator in a gas of ultracold atoms", Nature Physics 415, 39 (2002).

[3] F. Reyes Osorio and K. Rodrıguez Ramırez, "Separation of quadrupole, spin, and charge across the magnetic phases of a one-dimensional interacting spin-1 gas", Phys. Rev. B 107, 085424 (2023).

[4] T. Oka and S. Kitamura, "Floquet engineering of quantum materials", Annual Review of Condensed Matter Physics 10, 387 (2019).

Keywords: *Optical lattices, Spin-1 Bose-Hubbard model, Superfluid regime, Floquet theory.*

SIZE-DEPENDENT SUPERCONDUCTING STATE IN PB ISLAND NANOSTRUCTURES GROWN ON SI (111)

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Superconductivity of nanosized Pb-island structures whose hole radius and deepness was modified to study through theoretical calculations in order to reveal the evolution of the superconducting condensate under the effect of a strong applied magnetic field. The results of this study provide an insight about the emergent superconducting properties under such conditions, using the Ginzburg-Landau numerical simulations and offer a new path to tune superconducting circuits by nanoengineered size of the Pb islands. Critical magnetic fields for vortex penetration, free energy and vortex configuration were the results obtained for each designed Pb island.

References:

[1] Roditchev, D.; Brun, C.; Sierrer-Garcia, L.; Cuevas, J.; Liola, V.; Miloševic, M.; Debontridder, F.; Stolyarov, V.; Cren, T. Direct observation of Josephson vortex cores. Nature 2015, 11, 332–337.

[2] Orús, P.; Sigloch, F.; Sangiao, S.; De Teresa, J.M. Superconducting Materials and Devices Grown by Focused Ion and Electron Beam Induced Deposition. Nanomaterials 2022, 12, 1367

Keywords: *Vortex, Superconductivity, Ginzburg-Landau Equations, Superconducting island.*

SRFEMOO THIN SLABS, PROPERTIES AND APPLICATION AREAS

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The Sr_2FeMoO_6 perovskite is widely used in the solid oxide fuel cells; however, other physical properties than their conductivities make it attractive for different applications, as in the development of spintronic devices or ion batteries [1-3]. Among the mechanisms to modify the physical properties, doping and confinement are the most relevant; then, for this work, were modelled thin slabs to explore the free surfaces reactivity, looking for applications in the energy storage or spintronic devices areas. It was found a strong dependence of the electronic conduction behavior on the exposed surface, keeping different behavior for each spin channel. Also, the elastic properties for these slabs were calculated.

References:

[1] Eman Abdul Rahman Assirey, Saudi Pharmaceutical Journal, 27 (2019) 817

[2] K. I. Kobayashi, et al., Nature, 395 (1998) 677.

[3] Akihiro Kojima, et al., Journal of the American Chemical Society, 131 (2009) 6050.

Keywords: *Perovskites, thin films, spintronics, fuel cells.*

STUDY VIA EPR AND HEAT CAPACITY (HC) OF A ZN0.95CR0.05O SAMPLE PREPARED BY THE SOL-GEL METHOD

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Samples of zinc oxide doped with 5% chromium ($Zn_{0.95}Cr_{0.05}O$) were studied via EPR and prepared using the sol-gel method at three calcination temperatures (500 °C, 550 °C, and 600 °C). EPR spectra of the samples were taken using the Bruker 300 equipment belonging to the Department of Physics at the Universidad Nacional de Colombia, varying the temperature between 90 K and 300 K.

It was determined that at a calcination temperature of 600 °C, there was a complete replacement of zinc atoms by magnetic chromium ions in the wurtzite-type structure. Simulations of the experimental spectra allowed the determination of the symmetry in which these ions were housed and the transitions between energy levels that produced the EPR lines of the spectra.

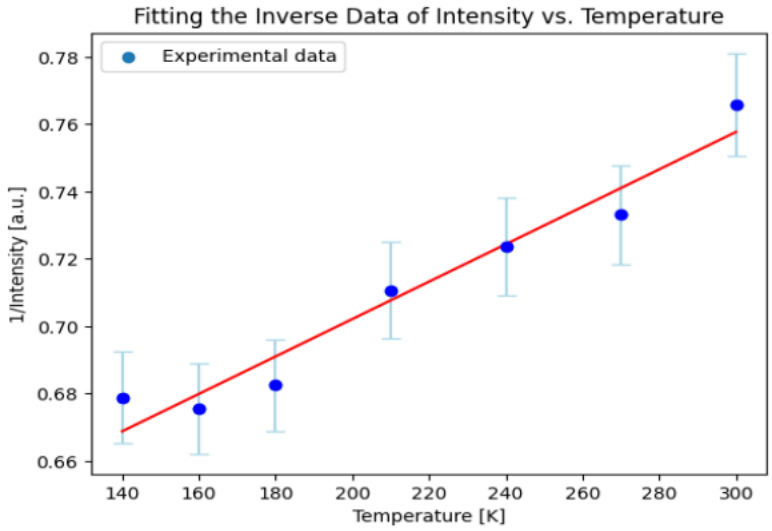

Fig. 1. Fitting on the inverse data of intensity versus temperature to determine the Néel temperature TN.

At this calcination temperature (600 °C), the nature of the interaction of chromium ions in the structure was determined to be antiferromagnetic, with a Néel temperature of 929 ± 14 K. A ferrimagnetic behavior was ruled out due to the trend of the points beyond the linear part.

This sample was also subjected to a specific heat study using the HC module of the PPMS equipment from the Electromagnetic and Thermometric Measurements Laboratory of the Department of Physics, within the temperature range of 1.8 K to 300 K. The obtained data were subtracted from the specific heat data of an undoped zinc oxide (ZnO) sample, measured over the same range and

with the same sequence, to estimate the contribution of chromium ions to the specific heat in the wurtzite structure. The result was then fitted to the Debye and Einstein models, as shown in Figure 2.

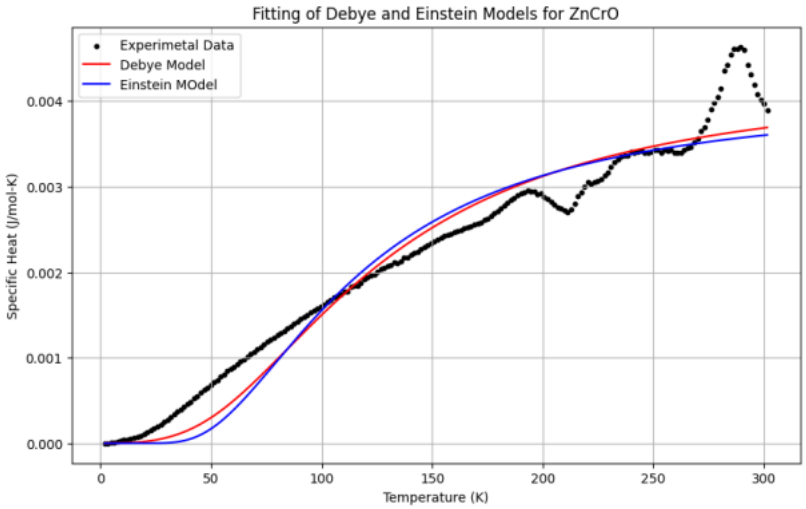

Fig. 2. Experimental data on the contribution of chromium ions to the specific heat in the ZnO structure and its fit to the Debye and Einstein models.

References:

[1] Manuel Acosta-Humánez, Luis Montes-Vides, and Ovidio Almanza-Montero. Sol-gel synthesis of zinc oxide nanoparticle at three different temperatures and its characterization via XRD, IR and EPR. DYNA, 83:224–228, 2016.

[2] John E. Wertz and James R. Bolton. Electron Spin Resonance Theory and Practical Applications, volume 1 of 1. Chapman and Hall, 29 West 35th St. New York, N.Y. 10001, 1 edition, 3 1986. Aplicaciones de EPR.

Keywords: *EPR, Calcination temperature, Antiferromagnetic interaction, Specific heat.*

SUBSTRATE DEPENDENCE IN THE STRUCTURAL AND MAGNETIC PROPERTIES OF COO THIN FILMS

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In this work, the influence of different substrates on CoO thin film samples was studied by means of structural and magnetic characterization as a first approximation to the analysis of the spin transport in Co/Pt bilayers. CoO thin films were deposited on $LaAlO_3$ (LAO – (100)), $MgAl_2O_4$ (MAO – (100)) and MgO (100) single crystal substrates by using a DC magnetron sputtering system. The films were grown using a power of 20 W, under an Ar atmosphere at 400°C and 800°C, in order to observe the phase change on the electronic structure. For the MAO/CoO and MgO/CoO thin films, a growth pressure of $2.9x10^{-1}$ Torr was used, while for LAO/CoO thin film, a growth pressure of $3.5x10^{-1}$ Torr was applied. For all the substrates CoO thin films with a thicknesses near 60 nm were achieved. X-ray diffraction (XRD) structural characterization showed the presence of CoO in all samples with a lattice parameter of approx. 4.27 Å, without the presence of secondary phases, and slight distortions in the lattice due to the influence of the substrate [1]. These results were related to the magnetic properties of the samples, which were analized via vibrating sample magnetometry (VSM).

References:

[1] J. Phys. Chem. B 2006, 110, 43, 21588–21592

Keywords: *Thin films, Sputtering, Ferromagnetic resonance.*

SUPERCONDUCTING DIODE EFFECT VIA RATCHET EFFECT

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A superconducting diode is an electronic device that conducts supercurrent and exhibits zero resistance primarily for one direction of applied current. Such a dissipationless diode is a desirable unit for constructing electronic circuits with ultralow power consumption. We demonstrate a superconducting diode achieved in a conventional superconducting film including the ratchet effect. We showcase the superconducting diode effect by using the curve of current density when the current is applied in one specific direction through ratchets with different shapes. The introduction of ratchet for creating a superconducting diode is thereby proven as a convenient, tunable, yet vastly advantageous tool for superconducting electronics. This could be readily applicable to any superconducting materials, including cuprates and iron-based superconductors that have higher transition temperatures and are desirable in device applications.

References:

[1] Jin, B. B. et al. High-frequency vortex ratchet effect in a superconducting film with a nanoengineered array of asymmetric pinning sites. Phys. Rev. B 81, 174505 (2010).

[2] Villegas, J. E. et al. A superconducting reversible rectifier that controls the motion of magnetic flux quanta. Science 302, 1188–1191 (2003).

Keywords: *Vortex, Superconductivity, Ginzburg-Landau Equations, Ratchet effect.*

SUPERCONDUCTIVITY IN TRIGONAL γ -PTBI2

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We present electrical transport experiments on high quality γ − $PtBi_2$ single crystals. The results show a superconducting transition at TC = 1.1 K and a critical field $\mu_0 HC_2$ (0) ≳ 1.5 T with a low critical current density Jc(0) ≈ 40 A cm^2/at H = 0. The critical temperature and field are the highest reported so far at ambient pressure. An anisotropy Γ = Hc_2^{ab} Hc_2^c/< 1 was found, which is unusual among superconductors. Under magnetic field, the transition becomes broader, asymmetric and dependent of the sample. Together with the low critical current, the results are consistent with an inhomogeneous superconducting state. Differential scanning calorimetry experiments suggest that inhomogeneities could arise from a thermal decomposition of the metastable γ -phase.

References:

[1] Zabala, J., Correa, V. F., Castro, J., & Pedrazzini, P. (2024). Enhanced weak superconductivity in trigonal γ -PtBi2. Journal of physics. Condensed Matter: an Institute of Physics Journal.

Keywords: *Semimetal, Superconductivity, Magnetoresistance.*

VORTEX MATTER OF HYBRID SUPERCONDUCTING-MESOSCOPIC HETEROSTRUCTURES

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We propose a study of vortex matter in a hybrid superconductor made of two superconductors where each side of a sample offer the possibility to tune their fundamental parameters, such as temperature, penetration depth l, coherence length, electron mass, and the order parameter, that help to improve the superconducting properties. Thus, in this work, we used Ginzburg–Landau theory to investigate a hybrid superconductor (HS), as well as to find a highly tunable and adjustable theoretical tool for theoretically explaining the experimental results involving the HS in order to study the vortex behavior in superconductors of mesoscopic dimensions with extreme differences among their fundamental parameters. Therefore, we analized the effect of HS on the vortex configuration and its effects on field-dependent magnetization. The results show that once the applied magnetic field H is increased, the diamagnetic response of the HS (Meissner effect) included additional jumps in magnetization, while diamagnetism continued to increase in the sample. In addition, the tenability of parameters created an interface between both components; two different magnitudes of supercurrent and vortex sizes that caused less degradation of the local superconductivity, which increased the upper critical field. Additionally, this type of HS with differences in parameters on both sides can be used to control the vortex movement in the selected sample of the superconducting region with high precision.

References:

[1] Miloševic, M.V.; Perali, A. Emergent phenomena in multicomponent superconductivity: An introduction to the focus issue. Supercond. Sci. Technol. 2015, 28, 060201.

[2] McNaughton, B.; Pinto, N.; Perali, A.; Miloševi´c, M.V. Complex Causes and Consequences of Ordering and Dynamic Phases of Confined Vortex Rows in Superconducting Nanostripes. Nanomaterials 2022, 12, 4043.

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