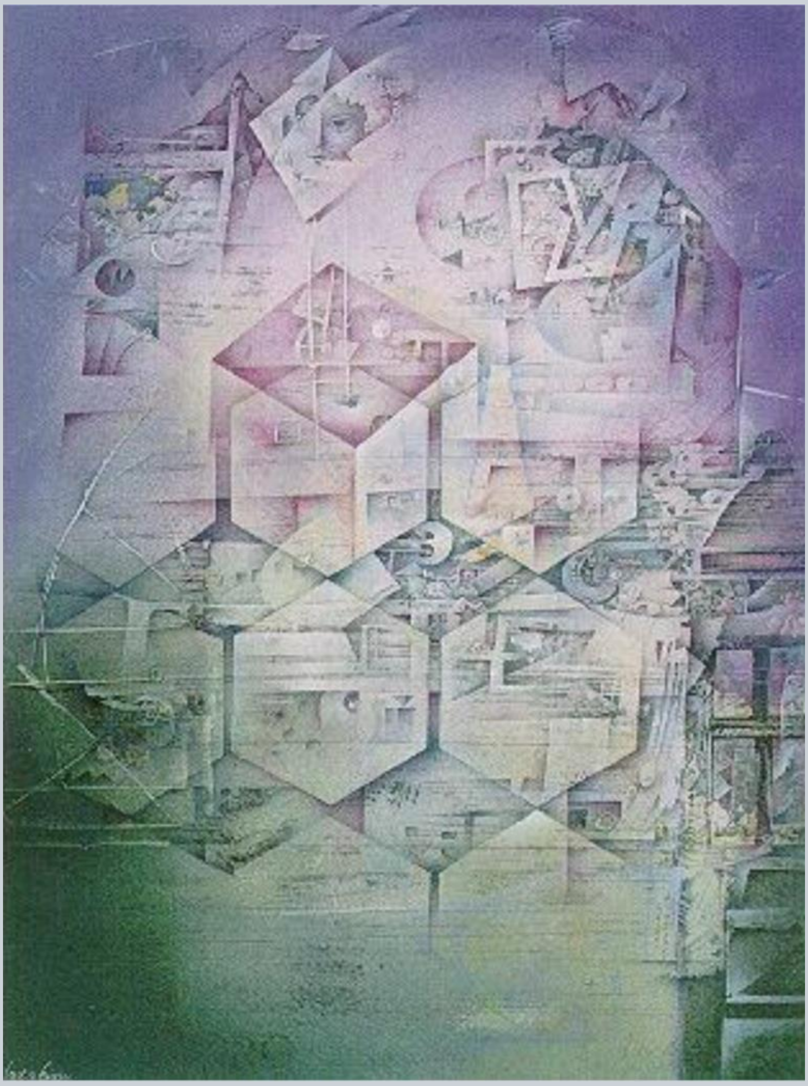
FCM 2024

At the Frontiers of Condensed Matter VII

Workshop dedicated to Ana María Llois

ABSTRACTS AND PROGRAM



Carlos Agüero. 1990.
La Herencia: gloriosos sueños - la gloria terrestre.
Water-based painting.

December 18-20, 2024 Buenos Aires, Argentina

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Full abstracts with all authors, references, and figures can be found at:
`https://www.argentina.gob.ar/cnea/frontiers-condensed-matter-vii`

The cover was designed by *Gustavo Murgida*

Contents

About

"At the Frontiers of Condensed Matter" workshop series, has been designed to encourage exchange, discussion, and future perspectives among researchers in the field. This event provides a unique platform for participants to share their latest findings and engage in meaningful dialogue.

This workshop continues a tradition that began with our inaugural meeting in 2002, held biennially in the same location. The last edition took place in 2012, and we are excited to revive this gathering.

FCM 2024

The VII workshop "At the Frontiers of Condensed matter" (FCM VII) aims to bring together theoretical and experimental researchers working on the state of the art in the field of material science.

The scope of the meeting is twofold. On the one hand, we aim to bring together researchers working on Condensed Matter to share and discuss their most recent results and future perspectives of the area. On the other hand, we take the chance to celebrate the research and academic career of Prof. Ana María Llois.

Scope

We expect to generate an appropriate climate for discussions and new collaborations in topics of current interest such as:

- New physical properties of materials with technological applications: sensors, memories, electronic devices, spintronics, etc.
- Topological materials and quantum technologies.
- Magnetism: fundamental properties, surface effects, interfaces and dimensionality.
- Materials for energy and environment: fuel cells, lithium and catalysis.

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- **Paula Bercoff** IFEG, CONICET - Córdoba - Argentina
- **Rubén Weht** DFMC, GIyA-CNEA; CONICET - Buenos Aires - Argentina

Invited Speakers

Mebarek Alouani	IPCMS - Strasbourg - FRANCE
Myriam Aguirre	UNIZAR - Zaragoza - SPAIN
Liliana Arrachea	UNSAM - Buenos Aires - ARGENTINA
Carlos Balseiro	CAB-CNEA - Bariloche - ARGENTINA
H. Fabio Busnengo	IFIR - Rosario - ARGENTINA
Ricardo Faccio	U.Rep. - Montevideo - URUGUAY
Santiago Figueroa	LNLS-CNPEM - Campinas - BRAZIL
Luis Foa Torres	FCFM - UCh - CHILE
Verónica Ganduglia Pirovano	ICP-CSIC - Madrid - SPAIN
Gastón Garbarino	ESRF - Grenoble - FRANCE
Alejandro Goñi	ICMAB-CSIC - Barcelona - SPAIN
Alfredo Levy Yeyati	UAM - Madrid - SPAIN
Pablo Piaggi	CIC nanoGUNE - Donostia - SPAIN
Patricia de la Presa	UCM - Madrid - SPAIN
Susana Ramos	PROBIEN - Neuquén - ARGENTINA
Claudia Rodriguez Torres	IFLP - UNLP- La Plata - ARGENTINA
Andres Saul	CINM - Marseille - FRANCE
Laura Steren	CAC-CNEA - Buenos Aires - ARGENTINA
Sergio Valenzuela	ICN2, CSIC, BIST - Barcelona - SPAIN
Elin Winkler	CAB-CNEA - Bariloche - ARGENTINA
Christof Wöll	KIT - Karlsruhe - GERMANY
Roberto Zysler	CAB-CNEA - Bariloche - ARGENTINA

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Timetable

Wednesday-morning, 18 of December

8:30–9:00	**CHECK IN TO ATOMIC CENTER**	
9:00–9:20	**Registration-Opening**	
9:20–9:30	**Welcome remarks**	
9:30–10:00	**Claudia Rodriguez Torres** UNLP, Argentina	From Basic Science to Technological Innovation: Magnetic Nanoparticles for Biomolecule Purification and Diagnostic Applications
10:00–10:30	**Patricia de la Presa** Madrid, Spain	Nano-Localized Heat Delivery: Magnetic Nanoparticles for Plastic Waste Upcycling.
10:30–11:00	**Roberto Zysler** INN-Bariloche,Argentina	Improved specific power absorption in magnetic hyperthermia experiments: linear chain arrangements of interacting nanoparticles with low anisotropy
11:00–11:30	**Coffee break**	
11:30–12:00	**Mebarek Alouani** Université de Strasbourg, France	Tailored spin-crossover in Fephen molecules adsorbed on metallic surfaces
12:00–12:20	**Julián Sereni** Centro Atómico Bariloche, Argentina	Hyperfine electro-nuclear coupling at the quantum criticality of YbCu$_4$Zn
12:20–12:40	**R. Severino** Universidad de Buenos Aires, Argentina	Phenomenological Ginzburg-Landau theory of unconventional superconductors with nematic order
12:40–13:00	**Luis Avilés** INN-Bariloche, Argentina	Spin transport and magnetization dynamics in ultra-low damping Co$_{100-x}$Fe$_x$/Ta bilayers
13:00–14:30	**Lunch**	

Wednesday-afternoon, 18 of December

14:30–15:00	**Andrés Saul** CNRS, France	Magnetoelastic interactions in CrOCl, a frustrated van der Waals magnet
15:00-15:30	**Ignacio Hamad** Instituto de Física Rosario, Argentina	Singlet polaron theory of low-energy optical excitations in NiPS$_3$
15:30–15:50	**Rodrigo Arias** Universidad de Chile, Chile	Scattering of magnetostatic surface modes of ferromagnetic films by geometric defects
15:50–16:10	**Fabiana Morales** Centro Atómico Constituyentes, Argentina	Magnetocaloric effect in nanostructures of La$_{0.6}$Sr$_{0.4}$CoO$_{3-\delta}$ and La$_{0.6}$Sr$_{0.4}$FeO$_{3-\delta}$
16:10–16:40	**Ricardo Faccio** Universidad de la República, Uruguay	Structural and Physical Study of Titanate-based Nanostructures
16:40–17:00	**Coffee break**	
17:00–19:00	**Poster Session***	

(*) Posters will be exhibited during the 3 days of the conference

Thursday-morning, 19 of December

8:30–9:00	**CHECK IN TO ATOMIC CENTER**	
9:00–9:30	**Carlos Balseiro** INN-Bariloche, Argentina	Topological phases of induced superconductivity in two-dimensional heterostructures with strong Spin-Orbit coupling
9:30–10:00	**Liliana Arrachea** INN-Bariloche, Argentina	Transport properties of superconducting heterostructures with spin-orbit coupling
10:00–10:30	**Luis Foa Torres** Universidad de Chile, Chile	What’s the hype about non-Hermitian systems? A personal tour from the search for topological states to the soul of quantum mechanics
10:30–11:00	**Coffe break**	
11:00–11:30	**Alfredo Levy Yeyati** Universidad Autónoma de Madrid, Spain	Photonic heat transport and the Schmid transition in Josephson junctions
11:30–12:00	**Gonzalo Usaj** INN-Bariloche, Argentina	A synchronized dance between exciton-polaritons and cavity phonons
12:00–12:20	**Graciana Puentes** Universidad de Buenos Aires, Argentina	2D Zak Phase Landscape in Photonic Discrete-Time Q
12:20–12:40	**Federico Escudero** Universidad Nacional del Sur, Argentina	Designing moiré patterns by strain
12:40–13:00	**Lucia Peralta Gavensky** Université Libre de Bruxelles, Belgium	The Stȓeda Formula for Floquet systems: Topological invariants and quantized anomalies from Cesàro summation
13:00–14:30	**Lunch**	

Thursday-afternoon, 19 of December

14:30-15:00	**Sergio Valenzuela** ICN2-Barcelona, Spain	Spin-Orbit Torques with Two-Dimensional Materials
15:00–15:30	**Victor Correa** Centro Atómico Bariloche, Argentina	Quantum oscillations evidence of sixfold fermions in the cubic Dirac semimetal β-PtBi$_2$
15:30–16:00	**Flavia Gómez Albarracín** Universidad Nacional de La Plata, Argentina	Machine learning techniques to explore skyrmion phase diagrams
16:00–16:30	**Coffe break**	
17:00–18:30	**Round Table* (Mesa Redonda)**	

(*) The Round Table will be in spanish

Mesa Redonda

Vinculación tecnológica: de la ciencia a la sociedad

Los participantes de la mesa son:

Ana María Llois (*moderadora*)	DFCM-INN, UNSAM
Diego Comerci	Subsecretario de desarrollo e innovación UNSAM-CONICET, CHEMTEST
Daniel de Florian	Director ICIFI UNSAM-CONICET
Verónica Garea	Presidente Fundación INVAP
Silvia Goyanes	Departamento de Física FCEN-UBA, IFIBA-UBA/CONICET
Mónica Martinez Bogado	Departamento Energía Solar CNEA - INN-CNEA-CONICET

Friday-morning, 20 of December

8:30–9:00	**CHECK IN TO ATOMIC CENTER**	
9:00-9:30	**Christof Wöll** Institute of Functional Interfaces, Germany	Unveiling the Dielectric Response of Oxides in the Infrared: Surprises from Experimental and Theoretical Insights
9:30-10:00	**Verónica Ganduglia-Pirovano** Institute of Catalysis and Petrochemistry, Spain	Challenges in Describing CO Vibrational Frequencies on Oxide Surfaces: Insights from Density Functional Theory
10:00–10:30	**Fabio Busnengo** Instituto de Física Rosario, Argentina	Understanding various elementary physical-chemistry processes involving greenhouse gases on surfaces using first principles atomistic simulations
10:30–11:00	**Coffee break**	
11:00–11:30	**Alejandro Goñi** Institut de Ciència de Materials de Barcelona	The ferroelectric-ferroelastic debate of metal halide perovskites
11:30–12:00	**María Dolores Perez** INN-Constituyentes, Argentina	Hybrid halide perovskite solar cells, unraveling the heat and photo-induced degradation under Raman spectroscopy
12:00–12:30	**Gastón Garbarino** The European Synchrotron, France	Pressure-Dependent Electronic Superlaticce in the Kagome Superconductor CsV$_3$Sb$_5$
12:30–13:00	**Santiago Figueroa** Brazilian Synchrotron Light Laboratory, Brazil	QUick x-ray Absorption spectroscopy for TIme and space-resolved experiments: Research opportunities in energy materials
13:00–14:30	**Lunch**	

Friday-afternoon, 20 of December

8:00–8:30	**CHECK IN TO ATOMIC CENTER**	
14:30–15:00	**Pablo Piaggi** CIC nanoGUNE, Spain	Machine learning as a tool for understanding crystallization from first principles
15:00–15:30	**Elin Winkler** INN-Bariloche, Argentina	Magnetic nanocatalyzers for environmental remediation
15:30–16:00	**Myriam Aguirre** CSIC -Universidad de Zaragoza, Spain	Study of the spin-to-charge conversion in Ir based-compounds/YIG
16:00–16:30	**Laura Steren** INN-Constituyentes, Argentina	Emergent phenomena at oxides surface and interfaces
16:30–18:30	**Brindis - Show**	

List of Abstracts – Talks

Wednesday 18th

Topic : *Magnetism*

From Basic Science to Technological Innovation: Magnetic Nanoparticles for Biomolecule Purification and Diagnostic Applications

Claudia E. Rodríguez Torres

Instituto de Física La Plata (IFLP), CONICET, CCT, La Plata, 1900 La Plata, Argentina
Departamento de Física - Facultad de Ciencias Exactas, UNLP, C.C. 67, 1900, La Plata, Argentina

The process of extracting (purifying and/or concentrating) biomolecules from complex mixtures constitutes one of the fundamental steps in biotechnology processes and plays a crucial role in human and veterinary disease diagnostic methods. Most purification procedures are based on the interaction between a solid phase and the biomolecule to be purified (RNA, DNA, proteins, antibodies, etc.) and involve several steps depending on the method employed. Among the different approaches, the use of functionalized magnetic nanoparticles (MNPs) has become increasingly interesting due to their efficiency, practicality, and potential for automation. In response to the need for high-performance molecular diagnostic technologies arising from the COVID-19 pandemic, an interdisciplinary group was formed to develop an extraction method using magnetic microparticles with high efficiency and sensitivity for nucleic acid extraction. Protocols for nanoparticle synthesis and nucleic acid purification from various matrices, including tissues and cultured cells, were optimized. The method was validated using nasopharyngeal swab samples from the COVID-19 diagnostic network in the Province of Buenos Aires. The synthesized nanoparticles demonstrated similar efficiency to the purification methods currently in use, with advantages in terms of costs and/or processability [1]. Subsequently, we have initiated development for the purification of recombinant proteins and made advances in the purification of antibodies using nanoparticles covalently bound to functional proteins [2]. The results can have a significant impact on reducing import dependence for molecular diagnostic supplies and other biomolecule purification applications. In this talk, I will present results on the use of MNPs applied to nucleic acid and protein purification.

[1] Capriotti, N., Morales, L.C.A., de Sousa, E., Juncal, L., Pidre, M.L., Traverso, L., et al. "Silica-coated magnetic particles for efficient RNA extraction for SARS-CoV-2 detection." Heliyon, 10(3), 2021.
[2] Rodríguez Torres, C.E., Juncal, L., De Sousa, E., Robaina, O.V., Capriotti, N., Rodríguez, K.S., et al. "Magnetic nanoparticles for purification of biomolecules: challenges and opportunities." Science Reviews - from the End of the World, 2(3), 39-51, 2020.

Topic : *Materials for Energy*

Nano-Localized Heat Delivery: Magnetic Nanoparticles for Plastic Waste Upcycling.

Patricia de la Presa

Insituto de Magnetismo Aplicado, Universidad Complutense de Madrid

High-temperature oil refining processes such as fluid catalytic cracking, hydrocracking, incur in significant energy costs due to the high temperatures required. Induction heating mediated by magnetic nanoparticles under radio frequency fields, offers a potential solution by delivering supplementary heat in a nano-localized manner, precisely at the active center where the catalytic process occurs. This process could reduce the energy normally required by standard processes. The challenge is to provide magnetic nanoparticles with the proper physical and chemical properties to reach the hydrocracking temperatures at optimal field conditions. This presentation demonstrates a proof of concept for achieving high temperatures using magnetic nanoparticles, radiofrequency fields, and a catalyst. Magnetic materials like FeNi and CoNi compositions are selected because their proper magnetic properties. The presentation will cover the synthesis methods and chemical and physical properties of the materials, emphasizing their magnetic characteristics. Additionally, the heating efficiencies of the materials are discussed, showcasing their potential to improve energy efficiency in high-temperature catalytic processes.

Topic : ***Magnetism***

Improved specific power absorption in magnetic hyperthermia experiments: linear chain arrangements of interacting nanoparticles with low anisotropy

Daniela Paola Valdés [1,2], Enio Lima Jr. [1], Roberto Daniel Zysler [1,2], Emilio De Biasi [1,2]

[1] Instituto de Nanociencia y Nanotecnología, CNEA-CONICET – Laboratorio Resonancias Magnéticas, Centro Atómico Bariloche, S. C. de Bariloche, Río Negro, R8402AGP, Argentina.
[2] Instituto Balseiro, Universidad Nacional de Cuyo, S. C. de Bariloche, Río Negro, R8402AGP, Argentina.

Magnetic fluid hyperthermia (MFH), the procedure of raising the temperature of tumor cells using magnetic nanoparticles (MNPs) as heating agents, has proven successful in treating some types of cancer. However, the low heating power generated under physiological conditions makes necessary a high local concentration of MNPs at tumor sites. Considerable effort is being invested to develop more efficient nanoheaters to minimize the administered dose while preserving therapeutic efficacy. The effect of magnetic interactions is a key issue for the performance of nanoparticles MFH.

There are results reporting benefic or detrimental effects on the performance of a magnetic fluid, thinking in terms of the Specific Power Absorption (SPA), depending on the intrinsic magnetic properties and the spatial arrangement of the nanoparticles. To understand this effect in depth, we have modeled an array of identical nanoparticles arranged in an ideal chain with the easy axis of the effective uniaxial anisotropy of each particle aligned to the chain, with the possibility of different orientations of the chain with respect to the applied field.

Furthermore, thermographic images will be used to obtain two-dimensional temperature maps that allow the determination of the power absorption and other relevant thermodynamic parameters in MHF experiments in a noninvasive way. This procedure and analysis are convenient to determine the heating performance of MNPs under the viscous conditions of in vitro and in vivo assays and to follow the time evolution of the temperature spatial distribution in the sample simultaneously. For this purpose, iron-oxide MNPs with 25-nm average diameter are coated with glucose and dispersed into different 8% polyacrylamide gels, which serve as phantoms that emulate intracellular viscosity. Power absorption experiments are performed under ac magnetic fields (H = 32 kA/m; f = 350 kHz) and the temperature evolution of the sample is monitored through a commercial thermographic camera.

Topic : *New Physical Properties of Materials*

Tailored spin-crossover in Fephen molecules adsorbed on metallic surfaces

R. Pasquier and M. Alouani

Université de Strasbourg, IPCMS, CNRS-UNISTRA, France

In this talk, we present the behavior of spin-crossover molecules adsorbed on metal surfaces using ab initio methods based on density functional theory. First, we describe the spin states of an FePhen molecule and its interaction with a Cu(001) metal surface, comparing it to a fluorine-doped FePhen molecule[1]. We observe an inversion of the spin states after fluorination, analyzed in detail using Bader analysis to determine intramolecular charge transfers, and the Nudged Elastic Band method to study the transition path between high spin (HS) and low spin (LS) states.

We then discuss the phonon spectra in these systems within the harmonic approximation, highlighting significant differences between the modes of the undoped and doped molecules. We explore their influence on the temperature evolution of thermodynamic quantities such as free energy, using the Slichter-Drickamer model to calculate the temperature-dependent evolution of the HS state fraction. Additionally, we introduce our preliminary results for a post-harmonic calculation of the phonon spectrum in molecular dynamics using the velocity autocorrelation function, to study the temperature-dependent evolution of the main spectral modes.

Secondly, we discuss our implementation of x-ray absorption and circular magnetic dichroism (XAS and XMCD) in VASP to theoretically obtain the $L_{2,3}$ spectra at the iron site of the FePhen molecule, both with and without the substrate. We show that the contribution of plane waves to these spectra is negligible, simplifying and accelerating the calculations, and that adding a static core hole does not improve the results. We also demonstrate the relatively small impact of the substrate on these spectra. Furthermore, we show that deviations from perfect octahedral geometry in the complexes induce noticeable effects on the spectrum and the magnetic anisotropy of the molecule. We emphasize the importance of the magnetic dipole tensor contribution in evaluating the XMCD sum rules [2].

Finally, we discuss our implementation of scanning tunneling microscopy (STM) images beyond the Tersoff-Hamann approximation (THA), using Chen's differential rule in ideal cases and with realistic tips, and with the full Bardeen formula. We compare these results with images obtained previously using the simple THA method, as well as with the few experimentally available images. We demonstrate that, despite apparent similarities among the methods, each approach reveals distinct fine details that could be experimentally observed with higher precision than currently available results.

[1] Inverse spin crossover in fluorinated Fe(1,10-phenanthroline)2 (NCS)2 adsorbed on Cu (001) surface, R. Pasquier, K. Rassoul, and M. Alouani Computational Condensed Matter **32**, e00735(2022)
[2] Calculated iron L2,3 x-ray absorption and x-ray magnetic circular dichroism of spin-crossover Fe(phen)2 (NCS)2 molecules adsorbed on a Cu(001) surface, R. Pasquier and M. Alouani, Phys. Rev. B **108**, 094423 (2023).

Topic : ***Magnetism***

Hyperfine electro-nuclear coupling at the quantum criticality of YbCu$_4$Zn

Julian G. Sereni [1], Slavo Gabani [2], Ivn Čurlík [3], Mauro Giovannini [4]

[1] Low Temperature Division, CAB-CNEA, CONICET, 8400 S.C. de Bariloche, Argentina.
[2] Institute of Experimental Physics, SAS, Watsonova 47 Košice, Slovakia.
[3] Faculty of Sciences, University of Prešov, 17. novembra 1, SK - 080 78 Prešov, Slovakia; [4] Department of Chemistry, University of Genova, Via Dodecaneso 31, Genova, Italy

Hyperfine electro-nuclear coupling effects are observed only under restricted conditions, among which are: the lack of magnetic order down to the mili-kelvin range, in systems with robust localized electronic moments and significant nuclear magnetism. An increasing number of Yb-based compounds fulfill these conditions because of the presence of magnetic 171-Yb and 173-Yb isotopes, while geometric frustration inhibits the formation of ordered ground states (GS). Nevertheless, reminiscences of short range magnetic interactions may be observed below 1K in those cases. An alternative to avoid such perturbation is provided by a compound tuned at the 'quantum critical point' (QCP [1]) where quantum fluctuations prevent magnetic correlations to develop.

Within the family of cubic YbCu$_4$M compounds (M = Ni [2], Au [3], Zn), we have investigated YbCu$_4$Zn that shows a logarithmic T dependence: CP/T α ln(T/TQ) in specific heat, as predicted for a QCP [4]. Simultaneously, no signs of RKKY interactions are detected down to 0.03K. Due to the low Kondo temperature of its doublet ground state, the localized '4f' electrons weakly couple with conduction electrons, allowing the coupling between nuclear and '4f' electron moments to become relevant. However, the reminder Kondo interaction acts on the electronic hyperfine field producing a small deviation from the standard CN(1/T2) dependence into a n <2 power law. The expected n =2 dependence is progressively recovered under applied magnetic field

[1] J. Custers et al., Nature 424 (2003) 524
[2] J. Sereni et al., Phys Rev. B 98 (2018) 094420
[3] J. Banda et al., arXiv:2308.15294 [cond-mat.str-el] 29 Aug 2023
[4] G. R. Stewart, Rev. Mod. Phys. 73 (2001) 797

Topic : *Magnetism*

Magnetocaloric effect in nanostructures of La$_{0.6}$Sr$_{0.4}$CoO$_{3-\delta}$ and La$_{0.6}$Sr$_{0.4}$FeO$_{3-\delta}$

Fabiana Morales[1,2], ***Mariano Quintero***[1,2], ***Joaquin Sacanell***[1,2]

[1]Laboratorio de Propiedades Eléctricas y Magnéticas de Óxidos Multifuncionales (LPEMOM), Centro Atómico Constituyentes, CNEA, Argentina.
[2]Instituto de Nanociencia y Nanotecnología, CNEA-CONICET, Argentina.

The magnetocaloric effect (MCE) is the change in temperature or entropy in a material when exposed to an external magnetic field, directly tied to its magnetic properties$\sim$[1]. This study investigated the MCE in ABO$_3$-type perovskites, focusing on the effects of La and Sr in A-sites and transition metals (Fe, Co) in B-sites. La$_{0.6}$Sr$_{0.4}$FeO$_{3-\delta}$ (LSFO) and La$_{0.6}$Sr$_{0.4}$CoO$_{3-\delta}$ (LSCO) were synthesized using the pore wetting method with polycarbonate membranes of 200 nm and 800 nm pore sizes, followed by heat treatments at 800°C and 1000°C. The samples exhibited nanotube and nanowire morphologies. Structural, morphological, and magnetic characterizations revealed that LSCO samples displayed magnetic saturation over 11.5 emu/g and coercive fields below 2500 Oe. In contrast, LSFO showed no magnetic saturation or transition in the studied range. The MCE study indicated that LSCO samples had a maximum entropy change (ΔS) of 1.13 J/(kg·K), while LSFO showed no significant ΔS.

Thanks to the GIYA, INN, and CONICET for the doctoral scholarship, and to ANPCyT for grants PICT 858/2017 and PICT 2397/2018.

[1] J. I. V. Franco, J. S. Blázquez et al., Progress in Materials Science, vol. 93, 2018. `https://doi.org/10.1016/j.pmatsci.2017.10.005`.

Topic : *Magnetism*

Spin transport and magnetization dynamics in ultra-low damping Co$_{100-x}$Fe$_x$/Ta bilayers

D. Velázquez Rodriguez, L. Saba, J. E. Gómez, J. L. Ampuero, A. Perez Martinez, T. Torres, M. H. Aguirre, J. Milano, P. Costanzo, A. Butera, L. Avilés-Félix

Instituto de Nanociencia y Nanotecnología (CNEA-CONICET), Bariloche (RN), Argentina.
Laboratorio Resonancias Magnéticas, Centro Atómico Bariloche, Bariloche (RN), Argentina.
Instituto Balseiro, Univ. Nacional de Cuyo, Comisión Nacional de Energía Atómica, Rio Negro, Argentina.

The manipulation of the electron charge and the spin for the development of more efficient spintronic devices has been a topic of increasing interest in recent years. In particular, systems based on metallic ferromagnets with very low damping, a parameter that determines the speed and energy consumption during the operation of modern electronic devices, are excellent candidates for spin current injection. Recently, it has been reported that the Co$_{25}$Fe$_{75}$ alloy exhibits low magnetic damping, due to the features of the band structure in Co$_{100-x}$Fe$_x$ alloys.

In this seminar I will discuss the magnetic and spin transport characterization in Co$_{100\text{-}x}$Fe$_x$ (20 nm)/Ta (10 nm) bilayer systems, with x = 65, 70, 75, 80, 85, grown on MgO (100) single crystal substrates. Characterization by Kerr magnetometry, transmission electron microscopy and ferromagnetic resonance allowed to determine that the Co$_{100\text{-}x}$Fe$_x$ films grow epitaxially with a cubic structure rotated 45° with respect to the (100) direction of the MgO substrate plane, determining the easy and hard magnetization axes. On the other hand, spin transport characterization using spin pumping and inverse spin Hall effect allowed the detection of induced voltages associated to the conversion of spin current to charge current, of the order of 100 μV (Fe$_{80}$Co$_{20}$), demonstrating efficient conversion of spin current to charge current in Ta layers.

Topic : *Magnetism*

Magnetoelastic interactions in CrOCl, a frustrated van der Waals magnet

***Amit Pawbake*[1], *Florian Le Mardele*[1], *Milan Orlita*[1], *Clement Faugeras*[1], *Benoit Greamud*[2], *Florian Petot*[3], *Julien Leveque*[3], *Andres Saul*[3]**

[1]LNCMI, CNRS & Université Grenoble Alpes, Grenoble (France),
[2]CPT (CNRS & Université Aix-Marseille, Marseille (France),
[3]CINaM, CNRS & Université Aix-Marseille, Marseille (France)

In this work we present a combined experimental and theoretical study of the magnetic properties of bulk CrOCl, a frustrated van der Waals system. The magnetic frustration gives rise to a rich magnetic phase diagram with magnetic phases having unit cells much larger than the crystallographic one. This additional periodicity imposed by the magnetic order changes both the phonon Raman scattering and the infrared responses by folding the phonon Brillouin zone onto the Γ point. By increasing the magnetic field up to 60 Tesla at low temperature, we observe that zone folded phonons (ZFP) appear and disappear giving information on the periodicity of the field induced magnetic order. Using density functional theory based methods, we show that the superstructure imposed by the magnetic order under magnetic field induces small atomic distortions through magnetoelastic interactions that make the zone-folded phonons Raman active.

Topic : *Magnetism*

Singlet polaron theory of low-energy optical excitations in NiPS$_3$

I. J. Hamad [1], C. S. Helman [2] , L. O. Manuel [1], A. E. Feiguin [3] , and A. A. Aligia [2]

[1] Instituto de Física Rosario (CONICET) and Facultad de Ciencias Exactas, Ingeniería y Agrimensura, Universidad Nacional de Rosario, 2000 Rosario, Argentina.
[2] Instituto de Nanociencia y Nanotecnología CNEA-CONICET, Centro Atómico Bariloche and Instituto Balseiro, 8400 Bariloche, Argentina.
[3] Physics Department, Northeastern University, Boston, MA 02115, USA

We develop a theory that explains the low-energy optical excitations near 1.5 eV observed by optical experiments in NiPS$_3$. Using ab initio methods, we construct a two-band Hubbard model for two effective Ni orbitals. The dominant effective hopping corresponds to third-nearest neighbours. This model exhibits triplet-singlet excitations of energy near two times the Hund exchange. We derive an effective model for the movement of two singlets in an antiferromagnetic background, that we solve using a generalized self-consistent Born approximation, disentangling the nature of these novel excitations, which move coherently as "singlet polarons" [1].

[1] I.J. Hamad, C.S. Helman, L.O. Manuel, A.E. Feiguin and A.A. Aligia. Phys. Rev. Lett. **133**, 146502 (2024).

Topic : ***Magnetism***

Scattering of magnetostatic surface modes of ferromagnetic films by geometric defects

Rodrigo E. Arias

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A problem of interest in the area of Magnonics is the propagation of spin waves in thin ferromagnetic films or stripes. Presently this interest is related with the possibility of using spin waves as a practical mechanism of transferring information within nano-devices, either coded in their amplitudes or phases. In particular, to elucidate the effect of geometric obstacles or simply roughness in their propagation is of relevance for practical applications.

The present study focuses on the scattering of particular spin wave modes in a particular geometry of interest: the propagation of magnetostatic Damon-Eshbach surface waves [1] in ferromagnetic films, these are modes that propagate perpendicularly to the magnetization and that may have high group velocities. We consider that the surfaces of the films have localized geometric modulations perpendicular to the direction of propagation of the waves, that may be of arbitrary shape, but in particular we consider in this study bumps and depressions. The analysis of the effect of the obstacles in the spin wave flow of energy allows to define transmission and reflection coefficients of the scattering process. These coefficients may be simply obtained in terms of phase shifts of even and odd modes that describe the scattering solutions of the same frequency. We determine these spin wave modes with symmetry properties through the Green-Extinction theorem [2,3], that renders sets of integral equations for the modes evaluated on the geometrically modified surfaces: at the end a standard matrix eigenvalue problem renders the frequencies, shape of the modes and their phase shifts. Depending on the shape of the obstacles, from the band of surface modes we do see emerging localized modes: these emerge from the highest frequency of the band, that corresponds to the frequency of surface modes in semi-infinite media. Also, depending on the shape of the obstacles the transmission coefficient presents frequency dependent regions of high transmission, that are associated with resonant modes of the geometry [4].

Acknowledgments: Fondecyt Project 1240310

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Topic : *New Physical Properties of Materials*

Phenomenological Ginzburg-Landau theory of unconventional superconductors with nematic order

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Over the last four decades, most research on superconductors has been directed towards the study of non-conventional materials, which cannot be described by the standard BCS theory. In 2008, a new family of superconducting materials based on iron was discovered and has since been extensively studied, both experimentally and theoretically. One of their most notable properties is the appearance of large transport and optical anisotropies, which are typically associated with the existence of an electronic nematic phase.

Due to the lack of consensus on the microscopic origin of superconductivity in these compounds, it seems appropriate to approach the problem from a Ginzburg-Landau (GL) phenomenological perspective. We present the simplest theory of a superconducting complex s-wave order parameter with the addition of an Ising-type real parameter for electronic nematicity. Using spectral methods, adapted from the study of the dynamics of Bose-Einstein condensates, we study two types of coupling: a biquadratic coupling and one that explicitly breaks the symmetry in a particular crystalline direction.

We present results of numerical simulations of the dynamics of vortices and nematic domain walls and characterize their interaction. We show that despite the simplicity of the model, many experimental findings—such as the pinning or anti-pinning of vortices on twin boundaries, the ellipticity of vortices, and the symmetries of the vortex lattice—can be explained within our model. We finally show how vortices move under the influence of a transport current and show how the ellipticity of the vortices affects the Bardeen-Stephen dissipation constant.

Topic : *Materials for Energy*

Structural and Physical Study of Titanate-based Nanostructures

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Titanate nanostructures hold promise as electrodes in dye-sensitized solar cells (DSSCs) and as electrolytes in lithium and sodium-ion batteries, making it crucial to study their electrical and ionic transport properties. This work presents experimental and computational results on the synthesis and characterization of titanate nanotubes (NTs). Structural characterization was performed using X-ray diffraction, small-angle X-ray scattering (SAXS), transmission electron microscopy (TEM), atomic force microscopy (AFM), and confocal Raman microscopy [1]. These techniques were complemented by computational simulations [5-6], which provided deeper insights into the NTs' superstructure, morphology, and electronic properties [2, 7,9].

DSSC prototypes were constructed and tested, with NTs used as photoelectrodes. Their performance was evaluated via I-V curves, revealing an efficiency of 8%, outperforming anatase-based standards (6%) [4, 7, 9]. Impedance spectroscopy was conducted to study charge transfer mechanisms. Furthermore, NTs were electronically characterized for their potential application as electrolytes in lithium and sodium-ion batteries [2, 4, 7, 8].

This research highlights the synthesis and multi-technique characterization of titanate nanotubes, demonstrating their promising performance in energy-related applications. The role of computational simulations in understanding the NTs' key structural and physical properties at the nanoscale is emphasized.

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Thursday 19th

Topic : *Topological Materials*

Topological phases of induced superconductivity in two-dimensional heterostructures with strong Spin-Orbit coupling

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Induced superconductivity in 2D electron gases offers new opportunities for devise applications at the nanoscale. In particular 2D systems with strong spin-orbit interaction in the presence of external magnetic fields show non-reciprocal responses: the superconducting diode effect. However, the physics of these systems turned out to be much richer than originally thought. Different groups presented a series of experimental studies on 2D Al-InAs heterojunctions analyzing the nature of the superconductivity induced in the semiconductor and its evolution in the presence of a magnetic field. When the in-plane magnetic field exceeds a critical value it creates the so-called Bogoliubov-Fermi surfaces and generates an anisotropic suppression of the superfluid density together with the occurrence of p-wave pairing. We have shown that in this regime and in the low electron density limit, the magnetic field induces a topological phase with edge states. We interpret these edge states as particular analog of Fermi-strings, the two dimensional version of the Fermi-arcs in topological semimetals.

Topic : *Topological Materials*

Transport properties of superconducting heterostructures with spin-orbit coupling

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Superconducting quantum wires have garnered significant attention in various research fields, such as materials science, quantum physics, and condensed matter physics. The appealing features of these systems rely on three crucial ingredients: resilient induced superconductivity, strong spin-orbit coupling (SOC) and large gyromagnetic factor. The goal of achieving a topological phase featuring Majorana zero modes was the driving force for numerous theoretical and experimental studies into superconducting InAs wires. An equally fascinating phenomenon is the emergence of Bogoliubov-Fermi surfaces, whose signatures have been recently observed in InAs two-dimensional systems with an applied in-plane magnetic field proximitized by superconductors.

We have shown that the emergence of Bogoliubov Fermi points in a superconducting wire with SOC and magnetic field can lead to a strong nonlocal thermoelectric signature [1]. These wires exhibit a topological phase across a range of chemical potentials (μ), pairing amplitudes (Δ) and Zeeman energies (ΔB) subject to the condition that the angle (θ) between the directions of the SOC and the magnetic field satisfies $|\cos(\theta)| < \Delta/\Delta B < 1$. Bogoliubov Fermi points emerge as the gap in the spectrum of the topological phase is partially closed by a twist beyond the critical angles defined by this condition. We are now extending our study to two-dimensional heretostructures with the same ingredients.

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Topic : *Topological Materials*

What’s the hype about non-Hermitian systems? A personal tour from the search for topological states to the soul of quantum mechanics

Luis E. F. Foa Torres

Universidad de Chile

In the last few years there has been a revived hype around non-Hermitian lattices [1,2,3], systems where non Hermiticity is used to model gains and losses (as in photonic or acoustic systems), non-reciprocal couplings or the effect of interactions, and, in particular the search for topological states in these systems. In this talk I will provide a personal overview on this topic with a focus on how a macroscopic fraction of the states become localized at a boundary [4], now called the non-hermitian skin effect [5], and our recent research aimed at bringing quantum measurements to "classical emulators" [6,7].

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Topic : *New Physical Properties of Materials*

Photonic heat transport and the Schmid transition in Josephson junctions

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The Josephson junction is a building block of quantum circuits. Its behavior, well understood when treated as an isolated entity, is strongly affected by coupling to an electromagnetic environment. In 1983 Schmid [1] predicted that a Josephson junction shunted by a resistance exceeding the resistance quantum RQ = h/4e$^2 \approx$ 6.45 kΩ for Cooper pairs would become insulating since the phase fluctuations would destroy the coherent Josephson coupling. Such transition is nowadays a matter of big experimental and theoretical debate [2,3].

In spite of this intense activity little is known regarding this system properties beyond dc charge transport. Motivated by recent experiments [4] in this work we analyze photonic heat transport through a Josephson junction in a dissipative environment. For this purpose we derive the general expressions for the heat current in terms of non-equilibrium Green functions for the junction coupled in series or in parallel with two environmental impedances at different temperatures. We show that even on the insulating side of the Schmid transition the heat current is sensitive to the Josephson coupling exhibiting an opposite behavior for the series and parallel connection and in qualitative agreement with experiments. We also predict that this device should exhibit heat rectification properties and provide simple expressions to account for them in terms of the system parameters.

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Topic : *New Physical Properties of Materials*

A synchronized dance between exciton-polaritons and cavity phonons

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In this talk I will describe how the complex nonlinear dynamics of an exciton-polariton condensate in a semiconducting microcavity leads to the generation of cavity phonons via the development of limit cycles. Such limit cycles are intrinsic to the polariton+reservoir dynamics and occur despite the fact that the excitation leading to the creation of the condensate is non-resonant and has a time independent amplitude. The self-induced cavity phonons, which have a very well defined frequency Ω, back-react on the polariton system leading to a synchronized dance at the frequency Ω (or half of it). The relation with continuous and discrete time crystals will also be discussed.

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Topic : *New Physical Properties of Materials*

2D Zak Phase Landscape in Photonic Discrete-Time Quantum Walks

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We present a study of the 2D Zak phase landscape in photonic discrete-time quantum walk (DTQW) protocols[1]. In particular, we report numerical results for three different DTQW scenarios which preserve spatial inversion symmetry (SIS) and time-reversal symmetry (TRS), while presenting a non-trivial Zak phase structure, as a consequence of a non-vanishing Berry connection. Additionally, we propose a novel approach to break TRS in photonic systems, while preserving a vanishing Berry curvature[1, 2, 3, 4].

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Topic : *New Physical Properties of Materials*

Designing Moiré patterns by strain

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Over the last years, many experiments have reported the observation of unconventional superconductivity and strongly correlated phases of matter in superlattices formed by the stacking of two dimensional materials. A prominent example is twisted bilayer graphene, where strong correlations have been observed around the so-called "magic angle". These unique electronic properties depend critically on the Moiré pattern of the superlattices. Although for two rotated graphene layers one only expects to see hexagonal Moiré patterns, experiments have yet reported a plethora of Moiré patterns geometries, usually attributed to the presence of small strain in the samples.

Here, we show that the Moiré patterns of such systems actually depends crucially on the interplay between twist and strain. We find that under the right twist and strain combinations one can practically obtain any Moiré pattern, even if the underlying layers are barely distorted. We identify the conditions for the formation of special Moiré patterns, such as square patterns, one-dimensional patterns, and hexagonal Moiré patterns arising solely from strain. We further note that the strain reshapes the Moiré Brillouin zone into a cell that reflects the new geometry of the superlattice. The modification of the Moiré patterns leads to significant changes in the electronic properties of the system. In particular, we find that the strain tends to suppress the formation of flat bands around the magic angle, even in the hexagonal patterns formed solely by strain. Finally, we discuss how these implications are reflected in the continuum model and in the possible role of electrostatic interactions. Our results give a general description of the plethora of Moiré patterns observed in experiments, and provide a solid theoretical foundation from which one can design Moiré patterns with novel electronic properties.

Topic : *Topological Materials*

The Stȓeda Formula for Floquet systems: Topological invariants and quantized anomalies from Cesàro summation

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I will discuss our recent findings on the generalization of the Streda formula to out-of-equilibrium Floquet systems [1], in which effective topological properties are generated by means of a time-periodic external field. Such phases can host "anomalous" edge channels, which elude the conventional topological classification of static systems. Building on fundamental notions of spectral flow, which underpin the Středa relation, we are able to derive the abstract winding numbers used to classify Floquet topological phases from physical principles and to connect them to tractable response functions. Interestingly, this formalism unveils a fundamental mechanism that lies at the heart of Floquet phases bearing anomalous edge states: the emergence of a magnetic-field-induced energy-pump that operates between the system and the external drive, encoding a genuine anomaly in the effective description of the particles dressed by the driving field. The results emanating from this work suggest that there should be a deep connection between the anomaly that arises in the semiclassical theory of Floquet systems and the measurable physical properties of cavity quantum materials, where the driving field is treated quantum mechanically.

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Topic : *Topological materials*

Spin-Orbit Torques with Two-Dimensional Materials

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Van der Waals (vdW) heterostructures, including those comprising topological insulators (TIs) of the Bi_2Te_3 family of materials, have disruptive potential for magnetic random-access memory applications [1]. The boundary states of a TI can generate a non-equilibrium spin density to control the magnetization of a ferromagnet (FM) by means of the spin-orbit torques (SOTs). Recent reports have demonstrated large SOT efficiencies with TIs, however, to identify the microscopic mechanisms at play, as well as to maximize the SOT, a deep understanding and control of the properties of the TI/FM interface is needed. In this talk, I will first introduce the potential advantages of vdW heterostructures and of TIs for non-volatile spintronics memories. I will then describe the relevance of their boundary states and of preserving the quality of the TI/FM interface. I will show that the introduction of a (non-magnetic) metallic [2] or graphene [3] interlayer between the TI and the FM, when FM is a transition metal, can notably suppress Te diffusion into the FM and change the nature of the SOT and its efficiency [2]. Finally, I will argue that the discovery of vdW FMs, which can be grown as high-quality thin films [4,5], can further improve the TI/FM interface, as the weak vdW interaction between the TI and the vdW FM can limit chemical reactions, intermixing and electronic hybridization. Our recent results using Fe_3GeTe_2 demonstrate large SOTs and magnetization switching with currents densities about 10^{10} Å/m^2 [6].

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Topic : *Topological Materials*

Quantum oscillations evidence of sixfold fermions in the cubic Dirac semimetal β-PtBi$_2$

V. F. Correa[1], E. Bavaro[1], J. Castro[2,3], V. Vildosola[2,3], J. I. Facio[1,4]

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The exploration of materials exhibiting multiple band crossings near the Fermi energy is a very active area of research [1]. Here we report an experimental study of de Haas-van Alphen oscillations in high-quality single crystals of cubic β-PtBi$_2$. Combined with density functional theoretical calculations, we identify quantum oscillations from all the calculated Fermi surfaces in the system. Our results reveal three small double-degenerate electron pockets centered at a sixfold band touching point which occurs ~ 25 meV below the Fermi level at the R point of the Brillouin zone. Our work is in line with recent ARPES results [2] and firmly establish the existence of sixfold fermions in close proximity to the Fermi energy of β-PtBi$_2$.

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Topic : ***Magnetism***

Machine learning techniques to explore skyrmion phase diagrams

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In less than a decade, machine learning (ML) techniques have gained significant interest and relevance, being applied to a wide variety of situations and physical systems. In particular, ML has been applied to explore several aspects of magnetic skyrmions systems, spin textures with topological characteristics and potential technological interest. Here, we first present a supervised ML approach, resorting to a convolutional neural network, to classify the phases that arise with temperature and magnetic field in a typical skyrmion model, taking spin configurations obtained from Monte Carlo simulation. We pay particular attention to the intermediate phases induced by thermal fluctuations, which are not easily distinguished with parameters such as the structure factor or the scalar chirality (the discrete order parameter associated with the skyrmion topological charge). Then, we utilize an unsupervised ML technique (anomaly detection), comparing the error of magnetic textures encoded and decoded by a convolutional autoencoder, to search for possible exotic phases in skyrmion models. In both cases, we compare the chosen ML algorithms with simpler ML techniques, and discuss future work.

Friday 20th

Topic : *New Physical Properties of Materials*

Unveiling the Dielectric Response of Oxides in the Infrared: Surprises from Experimental and Theoretical Insights

Christof Wöll

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Infrared Reflection-Absorption Spectroscopy (IRRAS), a well-established technique for studying metallic surfaces, has recently emerged as a powerful tool for probing the dielectric response of oxide materials, despite the challenges posed by their unique optical properties. This presentation uses ceria (CeO_2) as a case study to highlight the stark optical contrasts between metals and oxides. While IR-active vibrations parallel to metal substrates are screened by free electrons, this constraint is lifted on oxide surfaces. However, oxides exhibit reduced reflectivity in the infrared regime, resulting in vibrational band intensities approximately two orders of magnitude weaker than on metals. This limitation delayed systematic investigations into the dielectric response of oxides until recent experimental advances. With these breakthroughs, unexpected phenomena such as polarization-dependent shifts and the appearance of both positive and negative vibrational bands have been uncovered. These experimental findings will be compared with recent theoretical models, offering fresh insights into the dielectric behavior of oxides in the IR spectrum and their implications for surface studies under real-world conditions.

Topic : *Materials for energy*

Challenges in Describing CO Vibrational Frequencies on Oxide Surfaces: Insights from Density Functional Theory

M. Veronica Ganduglia-Pirovano, Alexander Contreras Payares, and Pablo G. Lustemberg

Institute of Catalysis and Petrochemistry-CSIC, Madrid, Spain

Describing the vibrational frequencies of adsorbed molecules like CO on metal oxide surfaces such as cerium oxide (CeO_2) is essential for understanding surface interactions and catalysis. Density Functional Theory (DFT) has become a popular tool for investigating these interactions due to its ability to handle complex materials and reaction pathways. However, accurately capturing the vibrational frequencies of CO on CeO_2 presents significant challenges [1,2]. This talk discusses the sources of these challenges and explores the limitations and strengths of various DFT functionals in describing the CO vibrational modes on CeO_2.

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Topic : *New Physical Properties of Materials*

Understanding various elementary physical-chemistry processes involving greenhouse gases on surfaces using first principles atomistic simulations

H.Fabio Busnengo

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In this talk I will present results of combined Density Functional Theory (DFT) and classical trajectory (CT) calculations intended to understand the main mechanisms behind various Physical-Chemistry processes involving molecules of greenhouse gases like CH_4 and CO_2, and their products of dissociation (i.e. H, CH_x, CO, O) on transition metal surfaces. In particular, I will focus on the dissociative and molecular adsorption processes, stability and mobility of adsorbates, and stimulated desorption. In connection with the CT calculations, I will briefly comment on the use of Artificial Neural Networks (ANN) to generate computationally efficient gas-surface potentials from DFT calculations.

Topic : *New Physical Properties of Materials*

The ferroelectric-ferroelastic debate of metal halide perovskites

Alejandro R. Goñi

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Metal halide perovskites (MHPs) are solution-processed semiconductor materials with exceptional photo-conversion efficiencies that have brought a paradigm shift in photovoltaics. The nature of the peculiar optoelectronic properties underlying such astounding performance is still controversial. The existence of ferroelectricity in MHPs and its alleged impact on photovoltaic activity has fueled an intense debate, in which unanimous consensus is still far from being reached. In this talk, I will critically review recent experimental and theoretical results with a two-fold objective: to argue that the occurrence of ferroelectric domains is incompatible with the A-site cation dynamics in MHPs and to propose an alternative interpretation of the experiments based on the concept of ferroelasticity. I will further underline that ferroic behavior in MHPs would not be relevant at room temperature or higher for the physics of photo-generated charge carriers, since it would be overshadowed by competing effects like polaron formation and ion migration.

Topic : *Materials for energy*

Hybrid halide perovskite solar cells, unraveling the heat and photo-induced degradation under Raman spectroscopy

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Solar cells based on perovskite materials have emerged as a promising technology for thin-film photovoltaic conversion due to their high efficiencies and ease of processing, which promise reduced manufacturing costs. Perovskites crystallize easily, forming an ionic solid with optimal optical properties for solar energy harvesting (high extinction coefficient in the visible range) and excellent electrical properties (high diffusion length and carrier lifetime). It has been well established that Raman measurements can cause alterations on the perovskite crystalline environment due to the laser incidence. The degradation pathway reactions of the material give rise to different Raman signal depending on the laser time exposure, power and wavelength. While environmental degradation mechanisms mediated by water or via UV light have been well established in the literature, the decomposition upon the Raman laser incidence is still a question that demands further study since the distinction between photoactivation versus the thermal activation degradation pathways is still a subject of discussion.

In this work, we perform Raman measurements with a 633nm laser incidence to establish a few common grounds of the laser degradation pathway and to further investigate the different signals obtained from the “burnt” laser zone on the perovskite film. We can visually observe two different zones that behave differently upon further light incidence and time of exposure. While the center zone evolves irreversibly into a degraded material with a weak Raman signal, the peripheral zone shows an intense signal that has been often described as the $MAPbI_3$ Raman spectra, that can further degrade by exposure to the laser light. We carefully and systematically studied the behavior of both zones by Raman signal and observed the photoluminescence at different temperatures. We were able to determine that the center shows a photoactivated degradation, while the periphery is thermally activated.

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Topic : *Large Facilities*

Pressure-Dependent Electronic Superlattice in the Kagome Superconductor CsV3Sb5

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The EBS-ESRF light source allowed a great improvement of our fundamental understanding of materials under high compression due to the unprecedented characteristics of the generated X ray beams. The array of techniques, in the early days restricted to structural measurements using X-Ray diffraction, is now extended and includes many others such as Inelastic X-ray Scattering, Nuclear Inelastic Scattering, X ray absorption and emission spectroscopy, X ray magnetic circular dichroism, X-ray Compton scattering and X-ray magnetic scattering. As a direct consequence, many scientific breakthroughs have been achieved across fields ranging from Earth and planetary sciences to fundamental physics, chemistry and materials research, and extending into biophysics and biochemistry including questions concerning life and biological function under extreme conditions. The investigation of matter under extreme conditions is one of the pilar scientific cases to exploit the new fourth generation EBS-ESRF. In this presentation, we will show the status of the two extreme conditions XRD beamlines and we will discuss future opportunities available on the beamlines. Finally, we will present very recent results on the kagome superconductor CsV3Sb5 using high-resolution single crystal x-ray diffraction under extreme hydrostatic pressure. We discovered that at low temperatures, the structural modulations of the electronic superlattice, commonly associated with charge-density-wave order, undergo a transformation around $p \approx 0.7$ GPa from the familiar 2 × 2 pattern to a long-range-ordered modulation at wave vector $q=(0, 3/8, 1/2)$. Our observations align with inferred changes in the charge-density-wave pattern from prior transport and nuclear-magnetic-resonance studies, providing new insights into these transitions. Interestingly, the pressure-induced variations in the electronic superlattice correlate with two peaks in the superconducting transition temperature as pressure changes, hinting that fluctuations within the electronic superlattice could be key to stabilizing superconductivity. However, our findings contrast with the minimal pressure dependency anticipated by ab initio calculations of the electronic structure.

Topic : *Large Facilities*

QUick x-ray Absorption spectroscopy for TIme and space-resolved experiments: Research opportunities in energy materials

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In this talk, we will present the opportunities offered by QUATI beamline (QUick x-ray Absorption spectroscopy for TIme and space-resolved experiments) to research energy materials. The beamline is under construction at the 4th generation Brazilian synchrotron source Sirius [1]. QUATI [2] will be dedicated to high-quality hard X-ray absorption spectroscopy for time and space resolved experiments under in situ/operando conditions. Thanks to the high intensity of photons and low emittance obtained from 4th generation facilities of synchrotron, fast acquisitions are expected, which are crucial for the study of dynamic processes.

The beamline's design has focused on a high flux of photons in a wide energy range, 4.5–35 keV (i.e. allows XAS from Ti to Xe in K edges; other higher Z elements in L edges), with flexibility in beam size (10's μm to mm) and with focus towards a combination of multi-techniques. Taking advantage of the high flux of hard X-rays, it will be possible to perform not only conventional XAS measurements, but also spectro-tomography, high resolution XAS and X-ray emission spectroscopy with dedicated instrumentations. Besides, a complete samples infrastructure is proposed to perform true operando characterizations with the combination of techniques, such as Raman, Infrared and X-ray diffraction. Finally, special attention has been dedicated to the new opportunities for research in energy materials.

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Topic : *Materials for energy*

Machine learning as a tool for understanding crystallization from first principles

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Crystallization is a process of key importance for many modern technologies, such as the manufacturing of pharmaceuticals, and it also plays a central role in geological, planetary, and climate sciences. Over the years, molecular dynamics simulations have provided key insights into the microscopic mechanisms underlying crystal nucleation and growth processes. However, classical molecular dynamics simulations based on semi-empirical force fields are limited in accuracy and cannot describe important physical phenomena such as bond forming and breaking. On the other hand, ab initio molecular dynamics overcome some of these limitations, yet are limited to very small system sizes and short total simulation times. These shortcomings of classical and ab initio molecular dynamics have resulted in a significant knowledge gap in the microscopic mechanisms of crystallization.

In this talk, I will discuss a new approach to this problem based on using machine learning to train interatomic potentials on large datasets of ab initio calculations. Such potentials can be used to drive large-scale, highly-accurate and reactive molecular dynamics simulations of crystallization phenomena. I will illustrate this approach with several examples. First, I will show that we can leverage this tool to compute homogeneous ice nucleation rates from first principles which are in remarkable agreement with experiment [1]. Furthermore, I will discuss some results about the formation of ice on feldspar, the most important ice nucleating particle in the atmosphere [2] . Finally, I will discuss the application of this technique to study the crystallization of calcium carbonate from aqueous solution, a process where reactivity plays an essential yet poorly understood role [3]. Taken together, these results show the great promise of machine learning as a tool to bridge time and length scales, and to provide insight into complex phenomena which were thought to be out of reach for molecular simulation.

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Topic : *Magnetism*

Magnetic nanocatalyzers for environmental remediation

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Magnetic nanoparticles (MNPs) are used in a wide range of applications and hold great promise for providing solutions for actual challenges in environmental remediation, energy, and medicine. What distinguishes this family of materials is the remarkable versatility to tune their properties by adjusting factors such as size, shape, composition, crystallinity, and interactions. Furthermore, materials with different functionalities can be combined in a single nanoparticle, allowing the design of multifunctional materials. In this context we present the strategies followed to develop magnetic nanocatalyzers for environmental remediation. Our approach involves designing MNPs with core/shell architecture, optimizing the shell properties to catalyze the decomposition of organic contaminants while adjusting the magnetic response of the core to enable magnetic harvesting and reuse of the nanocatalysts.

The composition of the shell was tailored to enhance the production of reactive oxygen species (ROS), via Fenton-like reactions, which are highly effective in degrading organic pollutants. With this aim copper-doped iron oxide MNPs were fabricated and their ROS production and ability to degrade organic compounds was analyzed. We found that while Fe^{2+} is the most active ion at room temperature, it rapidly oxidizes to Fe^{3+}, diminishing its efficacy. In contrast, copper exhibits lower activity than Fe^{2+} at room temperature but demonstrates improved performance at higher temperatures. Furthermore, the magnetic anisotropy of the MNPs core can be precisely controlled to induce magnetic hyperthermia. This effect increases the reaction kinetics through temperature elevation, enhancing the catalytic performance. The synergistic combination of magnetic and catalytic properties improves the overall kinetics and efficacy, making these nanostructures highly promising for treating high-temperature industrial wastewater and offering compelling solutions for environmental remediation.

Topic : *New Physical Properties of Materials*

Study of the spin-to-charge conversion in Ir based-compounds/YIG

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Ir-based compounds are promising materials for spin-current detection applications due to the high spin–orbit coupling (SOC), which makes possible an efficient conversion of pure spin-currents on charge-currents via the so-called inverse spin Hall effect (ISHE) [1,2]. The performance of IrO_2 as spin detector is found to be even better in the amorphous state. In the thermoelectric generation via spin Seebeck effect (SSE) in ferromagnets(FM)/heavy metals (HM) bilayers, spin currents caused by a temperature gradient across the interface generate an electric voltage via the inverse SHE (ISHE) in the conductive HM layer. In IrO_2, like in any other heavy metal layer, the sign of θSH is typically thought to be fixed, thus limiting both the magnetization switching and the thermoelectric voltage. However, our recent works show that it can be tuned via textured growth effects. The spin pumping effect and the spin Seebeck effect (SSE) approaches have been used to generate spin current-driven electric voltages in several IrO_2/FM heterostructures by the ISHE. Si/YIG/IrO_2, GGG/YIG/IrO_2, TiO_2/IrO_2/YIG and Si/Co/IrO_2 with different IrO_2 crystal orientation and degree of crystallinity have been studied. Consistent signs of the VISHE are found in all the cases indicating a change of sign for the (110) texture relative to (100) and non-textured IrO_2 samples. In addition, the comparison of Si/YIG/IrO_2, GGG(111)/YIG/IrO_2 and GGG(100)/YIG/IrO_2 reveals a reduced magnitude of the VISHE for YIG(111) relative to other orientations suggesting a poorer spin mixing conductance likely associated to a lower magnetic density at the interface. These results bring the possibility of tuning the desired functionality of IrO_2-based spintronic and caloritronic devices.

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List of Posters

Topic : *Magnetism* **Poster Number:** 1

Effect of Ir growth pressure on the magnetic domain wall dynamics in Ta/Pt/Co/Ir/Ta stacks

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The dynamical response of magnetic domain walls in ultrathin magnetic films to external magnetic fields is determined not only by the composition and thickness of the layers but also by the growth conditions. Growth conditions can induce significant structural changes to the layers and at the interfaces between them, affecting in particular the dynamics of domain walls, their mobility, elastic tension, and the pinning forces acting on them.

In this work, we focus specifically on the effect of Ir layer growth pressure in Ta/Pt/Co/Ir/Ta ultrathin multilayered films. Measurements of the DC magnetic properties, domain wall velocity, and domain morphology in the creep regime for both constant and alternating field pulses were performed for a batch of samples where the Ir layer was grown at different pressures. We find that the saturation magnetization, the effective anisotropy constant, and the domain wall surface tension grow with increasing pressure and saturate at a threshold pressure, while the Dzyaloshinskii-Moriya field and the strength of the disorder remain practically unaltered over the range of pressures considered.

Topic : *Magnetism* **Poster Number:** 2

Stability of magnon edge states in disordered skyrmion arrays

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Skyrmions are topological quasiparticles, of great interest for data storage applications due to their ultra-small sizes, no transverse deflection, and efficient manipulation. When these quasiparticles are arranged periodically, they support magnonic bands with topologically protected edge states. Here we investigate the interplay between local disorder and topology in the magnonic excitations of skyrmion systems. Our findings show that topologically protected edge states persist even when the crystalline order of skyrmions is disrupted by localized magnetic impurities. This robustness is quantified by the Bott index computed in real space, which remains quantized even for significant impurity strengths ($K_{imp} \sim J$) and an impurity concentration of 20%, indicating the presence of a topological phase. However, the introduction of disorder impacts the system in two primary ways: first, it leads to the closing of topological gaps, and second, it causes the topological edge states to progressively delocalize into the bulk as the disorder strength increases.

Topic : *Magnetism* **Poster Number:** 3

Modelling the magnetic properties of 1D arrays of FePc molecules

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We investigate the magnetic properties of Fe Phthalocyanines (FePc) that are experimentally arranged in quasi one-dimensional chains when they are grown in thin films or powders. By means of DFT calculations we reproduce the structural parameters found in experiments, and then we build a generalized Heisenberg magnetic model with single ion anisotropy, and calculate its parameters. The results show a anisotropic exchange interaction J between FePc molecules, and an easy plane single ion anisotropy D. By means of Monte Carlo simulations, with this model, we found an explanation to the non-saturation of the magnetization found at high fields, which we interpret is due to the anisotropic exchange interaction J. Finally, we also investigate the presence of magnetic solitons versus temperature and magnetic field. This results provide additional evidence that FePc is a soliton bearing molecular compound, with solitons easily excited mainly in the molecular xy plane.

Topic : *Magnetism* **Poster Number:** 4

Magnetic interactions in ZnFe$_2$O$_4$ with structural defects: An approach using first-principles models

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Zinc ferrite (ZnFe$_2$O$_4$, ZFO) has a normal spinel-like structure, it is characterized as a paramagnetic semiconductor at room temperature but depending on the sample growth conditions and induced structural defects, its electronic and magnetic properties can change, altering its resistivity, increasing the magnetic moment or favoring ferrimagnetism. Neutron diffraction experiments allow interpreting ZFO as an intrinsically frustrated system with antiferromagnetic first-neighbor interactions. However, the reported Curie-Weiss (CW) temperature is positive (of the order of 120 K). This discrepancy has its explanation in a previous study we performed of the pristine structure by ab-initio and Monte Carlo calculations, where the interaction between Fe extends to third neighbors (of the order of meV), resulting in all cases antiferromagnetic and from the calculations of the magnetization curves a negative Curie temperature was obtained [1]. Based on these results, new adjustments were made to the experiments, proposing extrinsic contributions, where the Curie temperature is negative, in perfect agreement between calculation and experiment.

To better understand what these extrinsic contributions would be, we studied magnetic models for ZFO with structural defects (oxygen vacancies, cation inversion). We know that the presence of vacancies favors inversion and inversion favors ferrimagnetic response. For this study we calculated the energies of different magnetic configurations by first-principles calculations based on density functional theory (DFT) using the linearized augmented plane wave method (FP-LAPW). These energies were mapped into a Heisenberg-type model by which we calculated equilibrium constants up to fifth neighbors. In this work we show how the presence of oxygen vacancies and cation inversion, even at very low concentration, can have a significant impact on magnetic interactions, favoring ferrimagnetic coupling and hence an increase in CW temperature.

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Topic : *Magnetism* **Poster Number:** 5

Tailoring the magnetic anisotropy of segmented Co-Pt nanowire arrays

Martina Arce(1), M. del Carmen Aguirre(2), Julieta S. Riva(3), and Paula G. Bercoff(1,2)

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Multilayered nanowire (NW) arrays are interesting nanoarchitectures which can have easily tuned magnetic properties, when compared to uniform wires of single-element or single-alloy compositions. Phase-alternating segments can provide additional functionalities, since introducing several interfaces along the wires' axis may lead to anisotropy and coercivity enhancement through magnetostatic coupling among the segments. Co-Pt alloys are known for their exceptional magnetic stability, high coercivity, and resistance to demagnetization as a result of a high anisotropy, which is attributed to the crystal structure formed during the solidification process, allowing a well-defined orientation of magnetic moments. In this work we prepared arrays of segmented NWs composed of alternating segments of a Co-rich and a Pt-rich phase each, by the pulse electrodeposition technique, using nanoporous alumina templates with 55 nm diameter pores. Two samples were obtained, with segments of different lengths by changing the pulse duration, and adjusting the total time to obtain NWs of similar total length. Sample 1 is composed of 66 nm Co-rich segments and 100 nm Pt-rich segments, while Sample 2 alternates 23 nm Co-rich and 70 nm length Pt-rich segments. The arrays were characterized using SEM, EDS, XRD and magnetometry. Hysteresis loops were measured at different temperatures from 5 K to 300 K applying the field parallel (PA) and perpendicular (PE) to the NW axis. The area method was used to calculate the effective magnetic anisotropy K_{eff}. Both samples have an easy axis in PA direction. Sample 1 is rather isotropic ($K_{eff} \sim 0$) at almost all temperatures while Sample 2 is very anisotropic in the whole temperature range. It is remarkable how the effective magnetic anisotropy of Sample 2 is greatly enhanced with respect to Sample 1 by only increasing the number of interfaces along the NW (shorter segments led to more interfaces).

Topic : *Magnetism* **Poster Number:** 6

The role of exchange parameters on the spin resistivity

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A strong impurity potential affects in a significant way the resistivity associated to a local moment. However, the potential acting only in a single-band model excludes the possibility of discussing transition metal-like hosts. In fact, the existence of two bands (s and d) and consequently, two exchange couplings, may change the standard results. It is well known that the phase shifts associated to the spin-independent impurity potential appear multiplying only by the square of the exchange parameter. In the transition-metal case the situation is very different include cross exchange products, among the usual J^2. In the case of impurities like cerium, $J^{(s)} \leq 0$, one has cross products, which may strongly affect the magnitude of the derived effective exchange parameter. These results suggest that one should take into account, in the detailed comparison, of the calculated bare exchange parameters, the characteristic of the impurity with respect to the host.

In this work, we present a two band model in order to study the resistivity of rare-earth impurities like Gd, Tb, Dy and Lu in transition 5d-metal hosts. From the model is clear that the rare-earth impurity introduced in the transition host acts in two ways: (i) The simplest effect is that the f level (supposed to lie below the conduction s-d bands) provides only a source of one-electron spin-dependent potential via the exchange interactions J^s and J^d. (ii) The valence state of the usual rare earths (trivalent in general) introduces a source of scattering. In the case discussed here, primary importance is given to the nature of the host, namely, the existence of $s-d$ bands. Our calculation may explore a typical feature of narrow d bands. In fact, besides providing the limit, it is known that the behavior of phase shifts depends strongly on the details of the d density of states, which in our case may assume in two ways: a parabolic like Moriya and another more realistic one from DFT calculations with VASP. We study the role of the band structure in resonant scattering (virtual bound states) to adopt a realistic band structure and calculate the susceptibilities involved. By changing in the band structure the position of the Fermi level, in order to scan the neighborhood of the top of the band, the regions of narrow peaks, etc. As far as the experimental situation is concerned, we would like to point out some possible uses of our calculations. Besides the determination of the residual resistivity of transition alloys with nonmagnetic rare earths, which could provide a way of estimating the hybridization $s-d$ matrix term by measuring of indirect phase-shift could be of interest. This class of experiments would measure the indirect g shifts, keeping fixed the “resonant” (e.g., Gd) and “nonresonant” (e.g., Tb) rare-earth impurity but changing the transition host, in order to vary the nature of the host band structure.

Finally, we want to point out that we present a the general equation being valid to any order in perturbation theory may serve as a starting point for a calculation of the effect of the impurity potential in the logarithmic Kondo term. In a future work, we also include the electronic transport calculations as implemented in the semiclasical python module, which uses our present results of the Band structure calculations with VASP. In this way we compare our numerical results when there are not available experimental data.

Topic : *Magnetism* **Poster Number:** 7

Intrinsic contribution of the Berry curvature in anomalous Hall effect

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We present an experimental and theoretical study of the anomalous Hall effect (AHE) in MnAs epilayers grown over GaAs. With the aim to identify the intrinsic contribution to the AHE, we accurately calculate ab initio electronic structure calculations along with Berry phase formalism. Our magnetotransport measurements show a quadratic behavior of the Hall resistivity with longitudinal resistivity, characteristic of scattering-independent processes, thus enabling the comparison with our calculations. The Berry phase contribution to the AHE is in quantitative agreement with the measured AHE in these epilayers. Moreover, the predicted anisotropic dependence of the experimental AHE on the magnetization is well reproduced.

Topic : *Magnetism* **Poster Number:** 8

Spin torque ferromagnetic resonance in Co/Pt

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The manipulation of electron charge and spin for the development of more efficient spintronic devices has been a topic of much interest in recent years. In particular, controlling the magnetization of thin magnetic layers using spin currents is key in the information storage industry because it allows the design of faster and more energy-efficient memories for writing information.

In this work we discuss the progress and first results of a new line of research focused on studying spin transport phenomena using high-frequency rf currents (1 – 20 GHz) to excite the magnetization of a magnetic layer using the Spin Hall effect in a thin layer with strong spin-orbit coupling. The mechanisms that allow controlling the magnetization with spin currents will be discussed as well as the first spin-torque ferromagnetic resonance experiments in the Co/Pt system.

Topic : *Magnetism* **Poster Number:** 9

Magnetization process in single crystal Fe$_{85}$Co$_{15}$ films via anisotropic magnetoresistance measurements

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Magnetotransport measurements were performed on Hall bar structures on epitaxial thin films of Fe$_{85}$Co$_{15}$. Kerr effect measurements on samples fabricated using the same procedure allowed the identification of uniaxial and cubic magnetocrystalline anisotropies. It was determined that when a current of 10^6 A/cm^2 is applied in the direction of a hard magnetization axis due to magnetocrystalline anisotropy, an AMR value of 0.21 % is obtained. This experiment was carried out for fields between 150 and 800 mT and temperatures between 80 and 150 K, without observing any dependence on these variables. Similarly, it was determined that when the current is applied in the direction of an easy axis, an AMR value of 0.17 % is obtained. Additionally, transport measurements were performed by varying the magnitude of the magnetic field at a constant temperature of 150 K. This was repeated for different directions of the field in the plane of the sample. Furthermore, the magnetocrystalline and uniaxial anisotropy constants were fitted to the experimental points, resulting in $K_c = 21(5)$ kJ/cm^3 and $K_u = 11(5)$ kJ/cm^3, respectively.

Topic : *Magnetism* **Poster Number:** 10

Non-collinear magnetism d^0 in TiO_2 (anatase) induced by structural defects

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In recent years, d^0 magnetism in different oxide metals induced by structural defects has been reported. In the present work, we have studied the influence of the structural defects on the magnetic behavior of the TiO_2 (anatase), we have considered vacancies of Ti and O atoms, and the substitution of these vacancies by H atom. The structural and magnetic ground state was explored, where spin-orbital coupling and full relativistic effects were considered. This allowed us to analyze the non-collinear magnetism and the magnetic anisotropy.

All calculations have been performed in the framework of the Density Functional Theory (DFT), using the pseudopotential and plane-wave method (Quantum Espresso code). The exchange-correlation part was described by the Perdew-Burke-Ernzerhof parametrization of the General Gradient Approximation (PBE-GGA).

Topic : *Magnetism* **Poster Number:** 11

Ab Initio study of structural, electronic, and hyperfine properties at and near pure and Cd-doped (110) Cu surface

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In this work, we present a complete *ab initio*/DFT study of structural, electronic, and hyperfine properties of pure and Cd-doped (110) Cu surface, with Cd localized at different depths from the surface. We studied the structural and electronic changes produced by the generation of the surface itself and by the inclusion of the Cd impurity. As a first step we performed a complete optimization of all atomic positions in the supercell of the pure system. For the doped ones, a Cd atom replaced a Cu atom at the different inequivalent Cu sites (depths) of this pure optimized surface, followed by a new complete optimization. The magnitude, symmetry, and orientation of the electric-field gradient (EFG) tensor were studied as a function of the depth from the surface. The predicted EFG are compared with those observed in Time-Differential Perturbed $\gamma-\gamma$ Angular Correlation (PAC) experiments with ^{111}In(EC$\rightarrow$^{111}Cd) ions deposited layer-by-layer onto the (110) Cu surface [1]. This combined approach enables us to understand the behavior of the EFG, and therefore of the electronic environment (i.e., the electron density) of the Cd probe atom as it moves away from the surface, until the recovery of the EFG value measured in both the bulk of Cu and also when 7 Cu monolayers were deposited above the ^{111}Cd probes localized onto the (110) Cu surface.

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Topic : *Magnetism* **Poster Number:** 12

Comprehensive analysis of magnetic $CoFe_2O_4$ nanoparticles: experimental reaction-time dependence, phonons and electronic structure studies

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A comparative study of experimentally synthesized magnetic $CoFe_2O_4$ nanoparticles and *ab initio* calculations of their electronic structure and phonon behavior has been conducted. The nanoparticles were synthesized using the co-precipitation method with varying reaction times of 0, 15, 30, and 45 minutes and characterized through X-ray diffraction (XRD), confocal Raman microscopy, vibrating-sample magnetometry (VSM), diffuse reflectance spectroscopy, and Mössbauer spectroscopy. The electronic and phononic band structures obtained from theoretical calculations based on Density Functional Theory (DFT) were compared with experimental results to provide a comprehensive understanding of the material's behavior. Finally, the key physical properties of $CoFe_2O_4$ were studied, revealing that the relationship between reaction time and nanoparticle size played a crucial role. A reaction time of 30 minutes was identified as optimal for achieving the best nanoparticle formation and exhibiting superparamagnetic effects.

Magneto-transport and anomalous Hall effect in ferromagnet/superconductor heterostructures

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Ferromagnetism and superconductivity attract a lot of attention in the condensed matter physics community not only due to the rich physical phenomena they embrace but also due to their great potential in different applications (memories, sensors, quantum devices…). Although they are considered antagonist effects, the interplay between them can lead to a wide variety of exotic phenomena. Some examples are superconducting vortex pinning induced by magnetic nanostructures [1], domain wall superconductivity [2], triplet superconductivity [3] and superconducting vortex – magnetic skyrmions interactions [4,5].

In this work, we investigate magneto-transport properties of a ferromagnetic (FM) multilayer with perpendicular magnetic anisotropy (PMA) in contact with a superconductor (SC). The SC is either a plain or nanostructured Nb film or an exfoliated flake of NbSe2. We observe clear changes in the magneto-resistance and Hall resistance of the FM at temperatures below the transition temperature of the SC. The symmetry of the Hall response indicates that these changes are likely not due to topological effects but possibly caused by modifications in FM multilayer domains or due to proximity effects.

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Topic : *Magnetism* **Poster Number:** 14

A tight-binding approach to impurity adsorption on 2D Xenes

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In this work, a tight-binding Anderson model was used to theoretically study the formation of local magnetic moments when an impurity is adsorbed at either a hollow or top site in two-dimensional group-IV Xenes—namely, silicene, germanene and stanene—and the results were compared with graphene. The real and imaginary parts of the self-energy of the impurity were analytically calculated in the low-energy approximation in order to derive expressions for the spin-polarized density of states. With the aim of calculating the local magnetic moments at the impurity, a self-consistent numerical calculation was implemented, taking into account the effect of an applied external electric field. For each of the Xenes considered, a magnetic domain was identified in terms of the hybridization strength of the impurity with the sublattices, the Fermi energy and the Hubbard parameter for different electric field intensities. The effect of the electric field was studied for negative and positive on-site impurity energies, generalizing the results found in the literature for graphene. The results obtained have potential applications in nanoelectronics and spintronics, particularly where tunability of local magnetic moments is required and can be achieved through an electric field.

Topic : *Magnetism* **Poster Number:** 15

Structural and magnetic ground state of the Ni_2MnGa Heuler alloys: A DFT study

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Ni_2MnGa is a Heusler alloy known for its remarkable mechanical, thermal, and magnetic properties, making it an ideal candidate for exploring phenomena such as the magnetocaloric effect and magnetic shape memory effects. Its importance primarily stems from its martensitic phase transformation (transitioning from a cubic phase at high temperatures to a tetragonal phase at low temperatures) coupled with a magnetic phase transition (paramagnetic at high temperatures and ferromagnetic at low temperatures). A deeper understanding of these coupled phases could enable precise control over these effects, potentially leading to advancements in technologies like magnetic refrigeration.

In this study, the structural and magnetic properties of Ni_2MnGa are investigated using Density Functional Theory (DFT) with the Quantum ESPRESSO code, employing PBE-GGA functional for the exchange-correlation part. First, the focus is on determining the most stable crystal structure, particularly the lowest-energy tetragonal phase. Then, the magnetic ground state is analyzed, followed by the calculation of J-exchange coupling parameters. In future work, these parameters will be used in an effective-like Hamiltonian model to further investigate thermal properties and the magnetocaloric effect.

Topic : *Magnetism* **Poster Number:** 16

Magnetic and magneto transport properties in Tb/Co multilayers

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Rare earth - transition metal multilayers have been extensively studied due to their potential application in several fields of magnetism, being of particular importance in the field of spintronics and optoelectronic devices such as magnetic memories, high-frequency oscillators, etc. In particular, multilayer systems based on Tb and Co have gain attention in the last years due to its ability to present field-free all-optical switching and readout when being part of a magnetic tunnel junction.

In this work, we present the structural, magnetic and transport characterization of a series of ferrimagnetic multilayers based on Tb/Co. All the samples have a constant Co thickness of 1.7 nm and the Tb thickness ranging from 0.5 nm to 1.2 nm. This family of samples exhibit a dominant perpendicular magnetic anisotropy and a strong dependence of the compensation temperature and saturation magnetization on the Tb relative concentration. The DC magnetic characterization with a SQUID and a vibrating sample magnetometer allowed to identify that the magnetic anisotropy is not fully perpendicular to the plane of the multilayers but tilted a few degrees. To describe the magnetic behavior of the Tb/Co multilayers we proposed a model which minimizes the magnetic free energy and reproduce qualitatively and quantitatively the experimental magnetic hysteresis loops. The proposed model is modified a Stoner-Wohlfarth one that takes into account that the magnetization reversal is given by domain nucleation instead of coherent rotation; and its strengths and limitations are analyzed and discussed. We also present the first results of the magnetotransport characterization of the [Tb(0.91 nm)/Co(1.7 nm)]5 focusing on the anisotropic magnetoresistance and anomalous Hall effect in detail as a function of temperature and the angle of the applied magnetic field.

Topic : *Magnetism* **Poster Number:** 17

Comparative study of Ni nanoparticles synthetized using electroless Ni plating waste and an analytical Ni reagent, a haracterization and possible application in magnetic fluids

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Wastewater from the electroless industry poses environmental and health risks due to its heavy metal content. In this study, nickel nanoparticles (NPs) were synthesized through chemical reduction using electroless nickel plating waste and hydrazine as a reducing agent. The goals are to extract nickel, lowering its concentration to levels allowed by regulations, and to valorize the residue by recovering nickel to be applied in magnetic fluids (MF). The synthesis method used here let us reduce the Ni concentration in the waste by 97.49%. The properties of the recovered Ni (Ni-R) were compared with NPs synthesized from analytical-grade nickel sulfate (Ni-A). Both Ni-R and Ni-A precipitates produced spherical NPs of 8-10 nm, with bimodal size distribution for Ni-R (174.6 and 383.4 nm) and monomodal for Ni-A (63.6 nm). Both samples are ferromagnetic, though Ni-R has a higher magnetic saturation, likely due to less surface oxidation from its larger average particle size. Magnetic fluids were prepared using the NPs from both waste and reagent sources, with silicone oils as the continuous phase. Magnetorheological (MR) properties, measured through viscosity and shear stress tests, showed an interesting MR behaviour in the fluid made from waste. In summary, this study demonstrates the potential to valorize Ni-based industrial waste by producing Ni precipitates that yield superior results in magnetic fluids, even outperforming those made under more controlled experimental conditions where precursor quality is typically critical.

Topic : *Magnetism* **Poster Number:** 18

Monte Carlo Approach of the Magnetic Behavior in Strongly Anisotropic Multilayer Films

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The heterostructures formed by ferromagnetic layers antiferromagnetically coupled via non-magnetic spacers (called metamagnets) have caught the attention of the scientific community by its applicability. In particular, the metamagnets that exhibit a strong anisotropy perpendicular to the layers have been described by an Ising metamagnet, where each layer consists of n bidimensional ferromagnetic sublayers. When an external magnetic field h is applied perpendicularly to the multilayer plane, its behavior depends on if the number of layers C is odd or even. On the one hand, if C is odd, the ground state for low values of h is composed of ferromagnetic ordered layers that are coupled antiferromagnetically (AF phase). If h=2J/n, where J is the coupling exchange constant, a phase transition occurs to a paramagnetic phase, PM, where the spins are directed along the field axis. On the other hand, if C is even, an intermediate phase (IP) appears. In the IP the top and bottom layers are aligned with h. As consequence two transitions are produced: AF-IP and IP-PM.

This system has been extensively studied, and it has been demonstrated for T>0 that the AF-IP transition is of first-order and the IP-PM changes from first-order to continuous in a tricritical point. Furthermore, the transitions lines depend on n for fixed C. Nevertheless, research on the phase behavior of anisotropic metamagnets with odd C is limited. Consequently, the characteristics of the AF-PM transition, the existence of a multicritical point, and the influence of C and n on the transition line in the (h,T) phase diagram remain unresolved. This work is devoted to study the phase diagram of anisotropic metamagnets with C=3, 5, 7, 9 and 11 for fixed n=2.

Monte Carlo simulations were performed with periodic boundary conditions in the layer planes and open in the field direction. The dynamic evolution to the equilibrium state was registered and analyzed, and it is observed how the interfaces affect the coupling with the external field. By employing the short-time dynamics technique, the AF-PM transition line was obtained. The results show that the transition line is independent of C, and changes its character at a tricritical point from first-order to continuous. Furthermore, the last transition was characterized by estimating the critical exponents.

Topic : *Magnetism* **Poster Number:** 19

Spherical Clusters of Magnetic Monodomain Nanoparticles: Effects of Dipolar Interactions on Hysteresis Loops

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The use of magnetic nanoparticles (MNPs) in hyperthermia, where they locally increase temperature under the application of oscillating (AC) magnetic fields, has become a significant topic in nanomedicine. The heating performance of MNPs and their assemblies is closely related to the area of the hysteresis loops they produce. This work presents a theoretical study of nanoclusters composed of spherical, uniaxial, monodisperse MNPs that exhibit single magnetic domains and rotate coherently with the applied field. The systems are modeled using the Stoner-Wohlfarth model, accounting for dipolar interactions, and the magnetic moments of the nanoparticles are treated under the macrospin approximation. Additionally, Néel relaxation is considered, assuming that the MNPs are immobilized in a solid gel, thus forming a ferrogel. The relevance of these basic theoretical investigations lies in their assistance in interpreting experimental data, including the effects of MNP spatial distribution and the orientation of their anisotropy axes. The nanoclusters are generated by randomly distributing the MNPs within a compact spherical region, with the anisotropy axes considered either parallel or random, mimicking clusters of MNPs known as nanoflowers with either crystallographically oriented or random axes, respectively. These nanoflowers are isotropically expanded to reduce their density—and therefore the strength of dipolar interactions—without affecting the geometrical distributions. The results demonstrate a strong dependence of coercive field, remanence, and hysteresis loop area on the MNP distributions. Moreover, the dispersion of the data decreases with increasing temperature. This behavior is discussed in terms of the interplay between dipolar interactions, anisotropy, the applied magnetic field, and thermal fluctuations, highlighting the differences between individual and collective behaviors.

Topic : *Magnetism* **Poster Number:** 20

Study of phase diagram for the two-dimensional anisotropic Heisenberg model with dipolar interactions

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The phase behavior of ferromagnetic thin films is studied by Monte Carlo simulations, modeling it as a classical two-dimensional anisotropic Heisenberg model with dipolar interactions. The phase diagram of the model reveals a rich phenomenology that includes low-temperature phases characterized by stripe-ordered domains (SO), oriented along the anisotropy axis, perpendicular to the film, and planar ferromagnetic domains (PFM). The apparition of these phases depends on the magnitude of anisotropy. Furthermore, a PM phase is present at high temperatures. The stripe width (h) in the SO phase depends on the relation between the exchange (J) and dipolar (g) constants δ. The considered value of $\delta = 1$ corresponds to h=1. For this value, the phase diagram presents a reorientation transition line SO-PFM, and transition lines PFM-PM and SO-PM. The former has been determined as first order while the last continuous. However, the critical behavior of the last lines has not yet been fully characterized, and there is still an ongoing controversy regarding the nature of the transitions near the triple point, including the existence of a reentrant region and a possible tricritical point. Appropriate order parameters are selected and their dynamic evolution within the short-time regime are studied with the aim of determining the transition lines between the above-mentioned phases, their character, and estimate the critical exponents in the case of continuous transitions.

Topic : *Magnetism* **Poster Number:** 21

Spike-timing-dependent-plasticity learning in a planar magnetic domain wall artificial synapse

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The ability to learn in a biologically inspired artificial synapse relies on its capacity to reconfigure in response to a stimulus, weakening or strengthening its synaptic weight. Future neuromorphic architectures will require millions of artificial synapses, making understanding the physical mechanisms behind their plasticity functionalities mandatory. In this work, we propose a simplified spin memristor, where the resistance can be controlled by magnetic field pulses, based on a Co/Pt multilayer with perpendicular magnetic anisotropy as a synapsis emulator. We demonstrate plasticity and spike time dependence plasticity (STDP) in this device and explored the underlying magnetic mechanisms using Kerr microscopy imaging and Hall magneto-transport measurements. A well-defined threshold for magnetization reversal and the continuous resistance states associated with the micromagnetic configuration are the basic properties allowing plasticity and STDP learning mechanisms [1-4] in this device.

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Topic : *Magnetism* **Poster Number:** 22

Synthesis and characterization of mesoporous nanostructured magnetic hematite and maghemite

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Interest in nanotechnologies and magnetic nanoscale materials is continuously increasing, and their applications have attracted the attention of scientific and industrial communities in the chemical, environmental, and medical sectors. In particular, nanoparticles based on iron species also have interesting redox properties that can lead to the degradation of a wide range of organic and inorganic contaminants present in contaminated water sources. In this sense, synthesis methodologies for materials with mesoporous structural order emerge as attractive alternatives for obtaining porous iron materials with specific structural, catalytic, and magnetic properties.

In this article, mesoporous iron oxides were synthesized by a hard template method using a silica matrix (SBA-15) as a template. The SBA-15 matrix was divided into two aliquots, which were impregnated with an ethanolic solution of $Fe(NO_3)_3 9H_2O$ and $Fe(C_5H_7O_2)_3$, respectively. Finally, the silica template was then removed in an alkaline medium. The materials have been exhaustively characterized through different instrumental techniques, including the analysis of physicochemical properties by N_2 adsorption, TEM, SEM, XRD, and XPS. Magnetic properties have been tested by means of magnetization curves at room temperature and 5 K, ZFC-FC curves, and Mössbauer spectroscopy at room temperature and 13 K. Both samples showed good specific surface area and structural order, as well as high magnetization and negligible magnetic hysteresis and remanence. The sample impregnated with $Fe(NO_3)_3 9H_2O$ exhibited higher structural order resulting in a higher specific surface area, while the sample impregnated with $Fe(C_5H_7O_2)_3$ showed the highest magnetic saturation moment due to the presence of mesoporous maghemite. These features are very relevant for future applications as heterogeneous catalysis systems, among other uses.

Topic : *Magnetism* **Poster Number:** 23

Magnetic Domain Transitions in Wedged Ni Thin Films: From Stripes to Labyrinths

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In recent years, ferromagnetic thin films have attracted significant attention due to their potential applications in magnetic recording, logic, and memory devices. Depending on the thickness and fabrication technique, these materials can exhibit out-of-plane magnetization components, originating from magnetocrystalline, magnetoelastic, and interfacial contributions. Nickel (Ni) thin films develop a self-organized magnetic domain structure known as stripe domain, which exhibit an out-of-plane magnetization component when the thickness exceeds a critical value.

In this work, Ni films with a thickness gradient were deposited on Si substrates using DC magnetron sputtering. We investigated the evolution of the magnetic domain structure along the thickness wedge. MFM observations revealed that stripe domains are formed in the film's thicker regions. These domains evolve into different patterns, including branched stripes, bubbles, and labyrinths, which coexist along the direction of decreasing thickness. The critical thickness for stripe domain formation was observed at approximately 80 nm, with distinct transitions in domain morphology occurring below this threshold. Magnetic hysteresis loops at different thicknesses were obtained using the Magneto-Optical Kerr Effect (MOKE). The relationship between the magnetic anisotropy and the thickness gradient leading to the formation of stripe magnetic domains below critical thickness is discussed. This study provides valuable insights for designing Ni-based thin film systems.

Topic : *Magnetism* **Poster Number:** 24

Linear model of magnetic entropy difference in manganite composites for the study of the magnetocaloric effect

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The magnetocaloric effect (MCE) is the adiabatic temperature change or the isothermal change of magnetic entropy of a material due to the application of an external magnetic field. This phenomenon constitutes a fundamental part of magnetic refrigeration cycles, a more environmentally friendly alternative to traditional methods [1].

This work explores the characteristics of the MCE in mixed-valence manganese oxide systems, known as “manganites”, and the potential advantages of combining powders of different compositions and magnetic phases. This results in a variety of combined systems that present magnetic properties of all of their constituent parts.

Magnetic characterization was performed on two powder samples of the compounds ($La_{0.305}Pr_{0.32}Ca_{0.375}MnO_3$) “LPCMO” and ($La_{0.75}Sr_{0.25}MnO_3$) LSMO. By measuring their magnetization in a vacuum with a vibrating sample magnetometer, the change of magnetic entropy as a function of temperature was calculated for external magnetic field variations of up to 3 Teslas.

An extension in the temperature range of the observed magnetocaloric effect was obtained for one of the magnetic transitions of LPCMO (180 K - 225 K) by incorporating the LSMO compound into the same system, achieving a broad range of (180 K - 400 K). A simple model was proposed to predict the change of magnetic entropy in composite systems consisting of a mixture of two powders of different manganites. It was observed how the model predicts the general shape of the changes in magnetic entropy, and its limitations were discussed.

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Topic : *Magnetism* **Poster Number:** 25

Influence of nanoprecipitates distribution on the magnetic properties of irradiated steel in reactor pressure vessels

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During the operation of a nuclear reactor, the reactor pressure vessel (RPV) is subjected to significant irradiation, which gradually leads to its degradation by altering its mechanical properties. This deterioration is primarily associated with the formation of nanoscale copper-rich precipitates, which act as obstacles to the movement of magnetic domain walls. These nanoprecipitates (NPs) hinder domain wall motion, resulting in observable changes in the magnetic properties of the steel. Consequently, there is a strong correlation between the mechanical degradation of the steel and variations in its magnetization, providing a potential pathway for non-destructive monitoring of material integrity.

In this study, we aim to investigate how the distribution of these NPs, specifically their size, density, and spacing, affects the magnetic properties of the steel used in RPVs. We utilize several magnetic characterization techniques to analyze samples with distinct NP distributions, created through exposure to different irradiation fluxes (resulting in different lead factors). Additionally, we perform micromagnetic simulations to model the interaction between magnetic domain walls and the NP, providing a deeper understanding of the mechanisms governing the observed changes in coercivity and other magnetic properties. By comparing these simulation results with experimental data, we offer a comprehensive interpretation of how NP distributions influence the magnetic behavior of irradiated steel.

Topic : *Magnetism* **Poster Number:** 26

Photocatalytic degradation of methylene blue using magnesium ferrite: a low-cost, magnetically recyclable catalyst for wastewater treatment

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Magnesium ferrite is a spinel-structured material that facilitates electron transfer, with a band gap around 2.2 eV, stability in aqueous environments, and magnetic properties that make it an ideal candidate for use as a photocatalyst in water-based systems [1]. Its magnetic nature also allows for easy removal after the catalytic process using external magnets. Additionally, its low-cost and straightforward synthesis, along with its low toxicity, make it an environmentally friendly and economically viable material for large-scale wastewater treatment applications.

This work explored the use of magnesium ferrite for the catalysis of methylene blue in aqueous media under various conditions [2]. The degradation process was studied both with and without light, with different concentrations of hydrogen peroxide, and under different mixing conditions: mechanical stirring, ultrasound, and static conditions. The effects of varying the ratio of ferrite to methylene blue concentration, exposure times, and the reusability of the ferrite after use were also tested. The results show that for a certain ratio the addition of hydrogen peroxide significantly accelerates and enhances the degradation of methylene blue, allowing complete degradation to occur in less than an hour under static conditions and natural light. In all experiments, magnesium ferrite proved to be an effective catalyst, achieving up to 100 % efficiency in some cases.

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Topic : *Magnetism* **Poster Number:** 27

Magnetic characterization of $Fe_{40}Co_{40}B_{20}$/Ta bilayers

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In this study, a series of $Fe_{40}Co_{40}B_{20}$/Ta bilayers with different thicknesses deposited on MgO [100] and Si substrates were grown, using the magnetron sputtering technique. Magnetic characterization of the samples was performed by means of vibrating sample (VSM) and magneto-optical Kerr effect magnetometries (MOKE). VSM studies show similar results than MOKE, revealing a coercive field ranging from 40-50 Oe to 3-7 Oe as the thickness is increased. The hysteresis loops show different shapes, depending on the direction of the applied field. To determine the thickness of the bilayers, X-ray reflectometry and atomic force microscopy studies were carried out. In plane and out of plane measures were made using ferromagnetic resonance (FMR) in X-Band (9.78 GHz). The obtained results were analyzed by using the Smit and Beljers model. The in plane measures show the existence of a uniaxial axis of magnetization of $\sim$60 Oe. By performing out of plane studies, the Keff values were obtained, and saturation magnetization (Ms) could be estimated. Ms obtained by FMR matches with the Ms calculated VSM. On the other hand, Magnetic Force Microscopy (MFM) studies do not reveal stripe domains in any of the samples.

Topic : *New Physical Properties of Materials* **Poster Number:** 28

Size and shape dependence of the vibrational properties and specific heat of small metal clusters: a systematic ab initio approach

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While the cohesive and electronic properties of small metallic clusters are well-studied, their vibrational and thermal behaviours remain less understood. Anomalies in thermal properties, such as specific heat, Debye temperature, and melting point, have been observed in small clusters, linked to peculiarities in their vibrational density of states (vDOS) [1]. Deviations from the Debye T^3 law and excess heat capacity at low temperatures have been reported. Vibrational properties are crucial to understand thermodynamic properties and, as they are sensitive to nanoparticle morphology, low-temperature measurements can reveal structural configurations.

This talk presents *ab initio* spin-polarized density functional theory (DFT) calculations on the vibrational and thermal properties of Ni_n (n = 13, 55) [2] and Pt_n (n=13, 19 ,55, 79, 85) [3] clusters, focusing on size and geometry effects. We compare the stabilities of symmetric octahedral (O_h), icosahedral (I_h), and cuboid structures recently observed experimentally for Pt_{13}. By performing *ab initio* DFT molecular dynamics simulations we explore transitions to lower-energy isomers. We calculate the vDOS and heat capacities using equilibrium geometries, comparing them with bulk counterparts. Results show clusters have enhanced low- and high-frequency modes, including super-bulk frequencies. All clusters exhibit a low-frequency confinement gap (CG), varying with size and geometry. For Ni, I_h clusters have higher super-bulk frequencies due to strain, while O_h clusters display a smaller low frequency CG. Regarding heat capacity, clusters show an excess at low temperatures, approaching a value lower than the Dulong-Petit limit at high temperatures.

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Topic : *New Physical Properties of Materials* **Poster Number:** 29

Determining excited-state properties using the Hermitian operator method and Hellmann–Feynman theorem within the doubly occupied configuration interaction space

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The Hermitian operator method (1) within the doubly occupied configuration interaction space (2) was formulated (3) to accurately determine excitation energies in systems with strong electronic correlations. By employing low-order reduced density matrices obtained from a reference state, the method provides a robust framework for exploring excited-state energies. Additionally, the Hellmann–Feynman theorem was recently extended within this space (4), enhancing the method's capability for computing more properties of excited states. The approach is evaluated against the reduced Bardeen–Cooper–Schrieffer and Richardson–Gaudin–Kitaev integrable models, demonstrating its potential as a practical and cost-effective tool for determining excited-state properties.

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Topic : *New Physical Properties of Materials* **Poster Number:** 30

Influence of magnetic nanoparticles in the morphology, structure and electrical conductivity of PEDOT

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Conducting polymers have unique chemical, physical and mechanical properties which are tunable through the synthesis. Hybrid materials (composites) formed by inorganic nanoparticles (NP) embedded in a polymer matrix are of interest due to the possibility of combining and improving the properties of both materials. In this work, it is shown that the inclusion of magnetic NP in the synthesis of PEDOT has a non-trivial effect, affecting the morphology, electrical conductivity and chemical structure of the polymer in different ways than a simple mixture would suggest.

Composites based on PEDOT and $CoFe_2O_4$ NP (mean diameter 14 nm) were prepared via chemical oxidative polymerization, by varying the concentrations of DBSA (the surfactant and dopant) and EDOT. The composites were compared to pure PEDOT synthesized without NP. The conductivity of the samples resulted in between 10^{-5} and 10^{-2} S/cm, with those with a higher DBSA concentration being more conductive, demonstrating its doping ability. The composites, that include non conducting NP, are unexpectedly more conductive than their respective pure PEDOT samples, and this effect is more notable in samples where the polymer has a lower conductivity by itself.

Microscopy studies showed that PEDOT tends to grow around the NP, indicating that they guide and favor the polymerization. Spectroscopy studies (UV-Vis, FTIR, Raman) agreed that samples with NP present a higher doping and oxidation level, greater conjugation length, and higher proportion of quinoid structures, all which generally improve electrical conductivity. The conductivity results were discussed with the aid of a general effective medium model. The composites were considered as being composed of two phases: a low conductivity pristine polymer and a high conductivity polymer closely associated to NP. It was estimated that the NP improved the conductivity of the latter phase in over two orders of magnitude respective to that of pure PEDOT.

Topic : *New Physical Properties of Materials* **Poster Number:** 31

Interplay between bonding, magnetism and superconductivity in Sr(Ni$_{1-x}$Co$_x$)$_2$P$_2$ and Sr(Ni$_{1-x}$Rh$_x$)$_2$P$_2$ single crystals

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Bond formation and bond breaking in crystalline intermetallic solids can strongly impact other properties associated to delocalized electrons, such as itinerant magnetism and superconductivity. This has been observed on numerous occasions in materials with collapsed tetragonal transitions [1,2,3]. Although SrNi$_2$P$_2$ adopts the common ThCr$_2$Si$_2$ structure for $T \geq 325$ K, being in an uncollapsed tetragonal (ucT) state, it is a special case for the ThCr$_2$Si$_2$ class: on cooling below 325 K it adopts a one-third collapsed orthorhombic (tcO) phase where one out of every three P-rows bond across the Sr layers [4,5]. It is also known for exhibiting bulk superconductivity at 1.4 K at ambient pressure, and no magnetic ordering down to 50 mK [4,6]. We find that both types of substitution cause a rapid decrease of the one-third collapse transition temperature, as well as alter either the magnetic or the superconducting properties of the pure compound. On one hand, Co substitution levels above 50% serve to stabilize antiferromagnetic and ferromagnetic orderings [5]. On the other hand, when substituting with Rh, an enhancement of the superconducting transition temperature is observed immediately after the suppression of the collapse transition.

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Topic : *New Physical Properties of Materials* **Poster Number:** 32

Investigating the role of graphene in the formation and stability of beta phase antimonene islands

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Two-dimensional materials have shown tremendous potential for various technological applications. Particularly, 2D antimony exhibits high applicability in electronics, sensors, and batteries. This 2D material, known as antimonene, presents two stable phases: alfa (rectangular lattice) and beta (honeycomb lattice), whose formation depends on the substrate where antimony is deposited.

In this study, we investigated the growth of antimonene islands on graphene, forming an antimonene/graphene heterostructure. To demonstrate the significance of graphene in the synthesis of antimonene, we also studied antimony deposited on a bare copper foil similar to the one used for the graphene substrate. Antimony deposition exhibits the beta phase antimonene structure when deposited on top of monolayer graphene, but not when deposited on a bare copper foil, nor on top of multilayer graphene. Additionally, we investigated the stability of the heterostructure after exposure to air. Pure antimony islands are formed when evaporated in high vacuum on top of graphene and copper substrates, and antimony atoms oxidize upon exposure to air. After annealing the sample in ultra-high-vacuum at temperatures lower than 200 °C, more than half of pure antimony is recovered and almost all oxidized antimony is desorbed from the graphene substrate. In contrast, almost none of the oxidized antimony is desorbed from the bare copper substrate, highlighting the key role of the heterostructure on the formation and preservation of the physical and chemical properties of the deposited 2D material.

Topic : *New Physical Properties of Materials* **Poster Number:** 33

On the origin of filamentary resistive switching in oxides-based memristive devices

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The control and manipulation of filamentary resistive switching (FRS), which relies on a the formation/disruption of conducting filaments due to the application of an external stimulus, is a key resource for potential applications of memristors in areas such as non-volatile memories and neuromorphic computing. Yet, central aspects such as filament formation and their impact on the device resistance as a whole, are still not properly assessed.

In this work, we employ a 2d model which combines the dynamics of oxygen vacancies (OV) and a resistor network to study the formation of conducting paths (CP) and the concomitant change in the resistance of oxide-based memristors. We analyze the stability of OV filaments (OVF) upon the application of the electrical stimulus, concluding that as a prerequisite for the formation of a low resistance CP connecting both electrodes of the device, the OV concentration along the filament must exceed a given threshold. In addition, in the case of applying voltage ramps with positive and negative polarities, we show that the FRS is ruled by the retraction and subsequent growth of the OVF/CP.

In the presence of static defects, we conclude that OV percolation between the top and bottom electrodes is a necessary but not sufficient condition for the formation of a CP. As a function of the concentration of defects, we identify different regimes and, in particular, a transition region for which the OV percolation probability is 1 but the CP probability is negligible.

Our results are promising for understanding the mechanisms behind FRS and designing novel memristive devices with better performance.

Topic : *New Physical Properties of Materials* **Poster Number:** 34

Structural, magnetic and nanoacoustic characterization of Co/Pt superlattices

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Semiconductor superlattices presenting a spatial modulation of the elastic properties appear as a main tool to reach the GHz-THz regime in nanoacoustic devices. The exploration of alternative materials with multifunctional properties remains a fertile domain of research.[1] In this work, we study the structural, magnetic, and acoustic characteristics of metallic superlattices made of Pt/Co.

Co/Pt superlattices (SLs) were deposited by magnetron sputtering on Si substrates. The [Pt(t_{Pt}) /Co(t_{Co})] period was repeated 10 times and a Pt(t_{Pt}) capping layer was deposited on top. The deposition time for Pt was kept constant to get $t_{Pt} = 4.2$ nm, while the deposition time for Co was varied throughout the series, with 0.18 nm$\leq t_{Co} \leq 0.72$ nm.

The SLs present a well-defined periodicity, as determined by X-ray reflectometry. Scanning transmission electron microscopy with local compositional analysis reveals that the SLs present a gradual modulation in composition rather than sharp interfaces between Co and Pt layers. Out-of-plane magnetization loops evidence strong perpendicular magnetic anisotropy for samples with $t_{Co} \geq 0.45$ nm, which increases with increasing Co thickness.

We study the phonon dynamics through coherent acoustic phonon generation experiments in a pump-probe scheme. The studied samples support short-lived acoustic modes up to 900 GHz, and up to 7 echoes at lower frequencies, revealing the periodic character of the spatial modulation of the elastic properties. These are promising results for the development of magnetoacoustic devices working at ultrahigh frequencies.

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Topic : *New Physical Properties of Materials* **Poster Number:** 35

Electronic structure and charge density analysis of arsenide-based semiconductor heterojunctions

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Arsenide-based semiconductor heterojunctions play a crucial role in various technological applications, including electronics, optoelectronics, and nanotechnology. In this study, we present a detailed analysis of the electronic structure, structural properties, and charge density of $(GaAs)_m/(AlAs)_n$ y $(GaAs)_m/(InAs)_n$ (m, n = 2, 3), using density functional theory, as implemented in the Quantum Espresso code to solve Kohn-Sham equations. The exchange-correlation described by the Perdew-Burke-Ernzerhof for solids (PBEsol-GGA) was applied. The energy of each heterojunction interface was minimized to determine the optimal lattice parameter and interface height. Formation energies and adhesion work were calculated to assess stability. A vacuum layer of 15 Åwas added between adjacent layers. Bandgap variations were studied through density of states and band structure calculations, alongside a charge density difference analysis to show electron redistribution at the heterojunctions. This study is relevant for explaining the stability and electronic properties of arsenide-based semiconductor heterojunctions, essential for designing and optimizing optoelectronic and nanotechnological devices.

Topic : *New Physical Properties of Materials* **Poster Number:** 36

Nuclear Quadrupole Moment of the ^{47,49}Ti, ^{63,65}Cu isotopes: A comparison between experimental data and DFT-based calculations

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The characterization of materials using nuclear properties is widely used, being Nuclear Magnetic Resonance (NMR), Nuclear Quadrupole Resonance (NQR) and Mössbauer spectroscopy some of the most applied. In this context, the electric field gradient tensor (EFG) and the nuclear quadrupole moment (Q_N) play a crucial rol in the study of these properties.

With the purpose to determinate the Q_N for ^{47}Ti (I=5/2), ^{49}Ti (I=7/2), ^{63}Cu (I=3/2) and ^{65}Cu (I=3/2) isotopes, we have correlated the quadrupolar coupling constant (Cq) obtained from the literature with the EFG determined by ab-initio calculations based on the Density Functional Theory (DFT). For each case, a vast set of Ti-based and Cu-based compounds has been considered. All DFT-based calculations were performed using two complemented frameworks, the Full-Potential Augmented Plane-Wave method (FP-LAPW, Wien2k code) and the Plane-Wave + Pseudopotential method with Gauge Including Projected Augmented (GIPAW, QuantumEspresso code) pseudopotentials. The exchange-correlation functional were described by the Perdew-Burke-Ernzenhof parametrization of the Generalized Gradient Approximation.

Topic : *New Physical Properties of Materials* **Poster Number:** 37

Multiple approach to study the electronic relaxations after an EC decay to probe electronic properties in materials

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The electron-capture *a*ftereffects (ECAE) phenomenon has been intensively studied in the last decades in semiconductors and insulators when doped with the most used ^{111}In (EC$\rightarrow$^{111}Cd) probe isotope in Perturbed γ-γ Angular Correlations (PAC) experiments. It consists in a strong electronic relaxation of the ^{111}Cd atom produced by Auger processes following the EC decay of the ^{111}In isotope. Since the experimental observation and behavior of this phenomenon as a function of temperature are related with the host electron availability, the effect of donor and acceptor impurities and other electric conductive properties may be studied in a large variety of materials.

In this work we demonstrate the complementarity of two very different approaches to analyze this phenomenon in PAC experiments, which in turn reinforce the validity of our *a*b initio/DFT analysis [1, 2] of the *a*ftereffects: 1) that developed by Lupascu *e*t al. [3], consisting in complete simulations of the PAC spectra based in a perturbation factor that consider very fast random fluctuations between different initial electronic states of the probe-atom, i.e., between different initial electric-field gradients (EFG), until the atom decays with a certain probability to a final stable electronic configuration (then, to a final EFG); 2) that proposed by Bäverstam *e*t al. [4], based in a simple but analytic perturbation factor, describing the same physical scenario, only having two free parameters. This last approach enables to fit perfectly the experimental spectra determining the final EFG, the probability to decay to this state (related to the lifetime of the electronic holes), and the strength of the loss of anisotropy originated in the electronic relaxation of ^{111}Cd produced after the EC process of its father ^{111}In. As an example, we show here the application of this multiple approach (experimental, *a*b initio, and two different perturbation factor analysis) to the case of α-Al_2O_3 single crystals implanted with ^{111}In ions [5].

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Topic : *New Physical Properties of Materials* **Poster Number:** 38

Nanotechnology in nature: The Band Gap Photonic Crystals and The Iridescent Effect

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This work presents the results of a research project that utilizes examples from nature with the objective to increase awareness of nanotechnology among students. According to Mallmann (MALLMANN, Matthias, 2008), although the word nanotechnology will be familiar to many students, the subject is not widely taught in European schools. The Iridescence effect is an example of nanotechnology in nature. This optical phenomenon occurs when light is reflected or refracted. The butterflies Morpho cypris and Greta oto (BARRERA-PATIÑO, Cláudia, et al., 2020), are examples of iridescent animals. The color that we see on the butterfly's wing is related to absorbed and reflected wavelengths. The composition of a butterfly's wing can be modeled similarly to the structure of one dimensional photonic crystals (BARRERA-PATIÑO, Cláudia, et al., 2020). This paper will investigate the band gap effect of one dimensional photonic crystals as an eigenvalue problem. For the purposes of this research, one dimensional photonic crystals were considered to have two dielectric layers in the primitive cell, with thicknesses A1=A2 or A1 $\neq$ A2 and with different refractive indexes (n1 and n2), permittivity (ϵ_1 and ϵ_2) and frequency (f1 and f2) per layer. Index 1 is related to information from layer 1 and index 2 refers to layer 2. The results obtained utilizing these parameters can be seen in table 1. It was observed that material and geometric parameters influence the band gap behavior. This range increases due to the difference between the value of the dielectric constants. By increasing the thickness of the layer with the lowest refractive index, the gap increases. From the results it is possible to verify the relationship between the color of the butterfly's wings and a band gap, since in multilayer materials such as photonic crystals, the band gap will determine the color of the absorbed or emitted light, and the energy of a photon will determine its color.

Table 1: Band Gap in a one dimensional photonic crystal with two layers

ϵ_1	n1	A1	ϵ_2	n2	A2	f1	f2	Band gap
12	3,4641	0,5L	13	3,6056	0,5L	0,1432	0,1397	0,0035
1	1	0,5L	13	3,6056	0,5L	0, 2566	0,1500	0,1066
1	1	0,6L	13	3,6056	0,4L	0, 3070	0,1600	0,1470
1	1	0,8L	13	3,6056	0,2L	0, 4536	0,2000	0,2536

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Topic : *New Physical Properties of Materials* **Poster Number:** 39

Understanding the interlayer coupling in 1T/1H-NbSe$_2$ heterobilayers

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The properties of 2D materials are strongly influenced by their substrate, leading to a variety of "proximity effects" like screening, charge transfer, and hybridization. Surprisingly, there is a dearth of theoretical studies on these effects. Particularly, previous theoretical research on the Star of David (SOD) structure in 1T-NbSe$_2$ has focused on single-layer configurations or stacking with the same 1T phase without any real substrate. Here, we depart from these approaches and explore how these proximity effects shape the electronic and magnetic properties of the 1T-NbSe$_2$ phase when it is grown on the metallic 1H-NbSe$_2$ substrate.

Using Density Functional Calculations, we establish a common framework to define the key characteristics of both free-standing 1T-NbSe$_2$ and 1H-NbSe$_2$. We then identify the optimal stacking arrangement for these two layers, revealing a transfer from the 1T to the 1H phase and a reorganization of charge within each layer. Our findings indicate that the magnetic moment of the SOD structure is still robust; however, is diminished due to a reduction in the on-site Coulomb interaction of the Hubbard bands. Additionally, the interlayer coupling induces metallicity in the 1T phase and increases the decoupling of the lower Hubbard band from the valence band.

Topic : *New Physical Properties of Materials* **Poster Number:** 40

Momentum entanglement in (1+2) QED in double-layer honeycomb lattice

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It is well-established that electrons in graphene behave as massless relativistic Dirac particles. This has led to the application of high-energy physics frameworks, such as quantum field theory (QFT) and quantum electrodynamics (QED), to better understand phenomena within condensed matter systems. However, there has been less exploration of related materials with honeycomb structures that exhibit spin-orbit interactions because of lattice corrugations. In these systems, spin-orbit coupling manifests itself as a second-neighbor interaction and contributes a term to the diagonal of the tight-binding Hamiltonian.

In these materials, such as silicene, germanene, among others, can be considered as massive Dirac fermions, where the spin-orbit coupling term serves as an effective mass. This analogy strengthens the connection with (1+3) dimensional QFT used to describe high-energy particles, with the Fermi velocity of electrons in these materials playing a role analogous to the speed of light.

We employ a (1+2) dimensional QFT formalism to investigate the momentum entanglement of electrons in two-dimensional double-layered honeycomb lattices. It is essential to note that this formalism is not meant to represent a true relativistic spacetime but serves as an effective tool within the appropriate energy regimes. Specifically, we explore the interactions between these electrons and an external electromagnetic field, mediated by a planar microcavity with well-defined boundary conditions. In this regime, the electron dynamics become non-separable from the behavior of the electromagnetic field.

To quantify this entanglement between the electrons, we employ the Bethe Salpeter equation:

$$\psi_{ab}(r_a, r_b) = \int d\sigma_\mu(r_1) d\sigma_\nu(r_2) \gamma_1^\mu \gamma_2^\nu S_{ab}(r_a, r_b; r_1, r_2) \psi_{ab}(r_1, r_2)$$

This formalism provides a means to compute the wave function in a perturbative manner, allowing the calculation of entanglement measures, such as entanglement entropy.

Topic : *New Physical Properties of Materials* **Poster Number:** 41

Transport measurements under controlled stress and strain in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ single crystals

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Nowadays, superconducting materials are widely used in different applications and postulated as key for novel developments, as qubits in quantum computing. However, whereas conventional superconductivity is explained from first principles in the framework of BCS theory, the mechanism responsible for unconventional superconductivity is still under discussion. In this context, several families of Fe-based superconductors evidence an interplay between the nematic order, i.e., symmetry breaking in the electronic properties, and the superconducting order [1]. It has been postulated that this coupling could be related to the origin of superconductivity in these compounds.

One of the observable postulated as proportional to the nematic order parameter is the resistivity anisotropy in the B$_{2g}$ channel. The approach of our work is mainly focused on low temperature transport experiments in single crystals under uniaxial stress, subjected to magnetic fields of variable direction, with the aim to find experimental evidence of the influence of the nematic order and nematic domains in the mixed superconducting state **[2]**.

Recently, by means of simultaneous high-resolution X-ray measurements and elasto-resistivity in Ba(Fe$_{0.96}$Co$_{0.04}$)$_2$As$_2$ compounds subjected to uniaxial stress, the formation and cleaning of nematic domain boundaries have been characterized. Authors also showed that, near the structural-nematic transition, the nominal deformation is not proportional to the real one [3]. Here we used a novel device that allows applying uniaxial stress to small samples by means of a compensated arrangement of piezoelectrics, measuring both the nominal deformation and the applied stress [4]. Our first goal is to find information comparable to that published in [3] without using such sophisticated technique.

We present and discuss preliminary results conducted in a Ba(Fe$_{0.941}$Co$_{0.059}$)$_2$As$_2$ single crystal. The free (no stress) resistivity is characterized and compared with the elasto-resisitivity under stress, focusing on both the region near the structural-nematic transition and the superconducting transition.

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Topic : *New Physical Properties of Materials* **Poster Number:** 42

Electric polarization control of magnetic interactions in van der Waals heterostructures

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Over the past decade, there has been significant interest within the scientific community in the search for robust low dimensional ferroelectric (FE) materials, with the aim of integrating them into multiferroic heterostructures that exhibit magnetoelectric coupling to control magnetic properties through electric fields. An alternative route for magnetoelectric coupling in low dimensions, currently beginning to be explored, involves two-dimensional layered materials. Structurally different from conventional ferroelectric oxides with rigid atomic structures, van der Waals (vdW) ferroelectrics have layered structures with a combination of strong intralayer and weak interlayer interactions. This atomic arrangement, coupled with ferroelectric order, gives rise to fundamentally new phenomena and functionalities not found in conventional materials. Recently, it has been experimentally found that In_2Se_3, a vdW material, exhibits robust ferroelectric properties in one of its most stable phases, the zinc-blende structure. In this work, we investigate, by means of first-principles calculations based on Density Functional Theory (DFT), the magnetic interaction between transition metal atoms embedded in different structures deposited on an In_2Se_3 monolayer, and analyse the role played by the Se atoms in the intermediation of the magnetic coupling. Additionally, we explore the effect of the polarization reversal of the FE layer on the magnetic properties, searching for sizable magnetoelectric coupling.

Topic : *New Physical Properties of Materials* **Poster Number:** 43

Fractal analysis of quantum transport properties in the universal regime

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Mesoscopic physics investigates systems that bridge the gap between microscopic and macroscopic scales, where quantum effects predominate. The "universal regime" refers to a behavior observed in mesoscopic systems, wherein certain physical properties become invariant to specific microscopic details and depend solely on symmetry and geometric dimensions. This study aims to explore universal properties of quantum transport in fractal structures, focusing on conductance fluctuations and shot noise. We examine the Sierpinski carpet, a fractal-shaped scattering region with a fractal dimension of approximately 1.89. By analyzing conductance and shot noise curves as functions of energy, we calculate the fractal dimension both within the universal regime and in the absence of disorder. Our results demonstrate that the fractal dimension of conductance curves in the universal regime exhibits a remarkable degree of universality, displaying consistent values with low standard deviation. Furthermore, we investigate the impact of geometric disorder introduced into the system. Notably, lower-order fractals necessitate larger disorder values (W) to characterize the universal regime compared to higher-order fractals. This observation implies that higher-order fractals inherently possess greater geometric disorder, which contributes significantly to the attainment of the universal regime. These findings present novel insights into the relationship between fractal dimension, geometric disorder, and the universal regime in mesoscopic physics. Our study contributes to the understanding of quantum transport phenomena in fractal structures and underscores the importance of considering universal properties in such systems.

Topic : *New Physical Properties of Materials* **Poster Number:** 44

Epitaxial growth of Sb on Ag(111): Pathway from Surface Alloy to α-Antimonene

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Antimonene is a 2D material that has received considerable attention because of its exceptional physical properties, which include chemical stability, strong spin-orbit coupling, tunable band gap, high carrier mobility, and topological properties. Many potential applications are foreseen for this material, which can be synthesized by mechanical and liquid-phase exfoliation or epitaxially grown on a substrate. An open debate exists about the crystalline structure formed by depositing sub- and monolayer-thickness layers of Sb on Ag(111), as different research groups have reported preparing several 2D Sb phases and antimonene allotropes in that system. Shao et al. [Nano Lett. 18, 2133 (2018)] reported the formation of a flat honeycomb antimonene monolayer on top of the Ag substrate. Mao and coworkers [Front. Phys. 13, 138106 (2018)] proposed that this phase corresponds to highly strained (honeycomb) antimonene on top of an $AgSb_2$ alloy, while Sun et al. [J. Phys. Chem. Lett. 11, 8976 (2020)] claimed instead that the underlying alloy is Ag_2Sb. In 2022, Zhang et al. [Phys. Rev. Mat, 6, 074002 (2022)] stated the absence of honeycomb antimonene formation and reported the growth of a different antimonene allotrope called α-antimonene. Very recently, Fuhr et al. [J. Phys. Chem. C (2024), in press] proposed pure Sb film formation after a dealloying transition. In this work, we will present results on the evaporation growth of antimony on Ag(111), from the sub-monolayer regime to several atomic layers, including studies of its crystalline and electronic structure using a wide variety of complementary analysis techniques and calculations (TOF-DRS, LEED, AES, UPS, XPS, Raman spectroscopy, DFT). Electronic band measurements and calculations confirm that the first growth stage is indeed an Ag_2Sb alloy followed by pure Sb film formation similar to that observed previously on Au(111). For larger thicknesses, the formation of α-antimonene is confirmed.

Topic : *Topological Materials* **Poster Number:** 45

Nonlocal thermoelectricity in quantum wires as a signature of Bogoliubov-Fermi points

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We study nonlocal thermoelectricity in a superconducting wire subject to spin-orbit coupling and a magnetic field with a relative orientation θ between them. We calculate the current flowing in a normal probe attached to the bulk of a superconducting wire, as a result of a temperature difference applied at the ends of the wire. We focus on the linear response regime, corresponding to a small temperature bias. We find that the nonlocal thermoelectric response is strongly dependent on the angle θ and occurs in ranges which correspond to the emergence of Bogoliubov Fermi points in the energy spectrum of the superconducting wire.

Topic : *Topological Materials* **Poster Number:** 46

Anisotropic entanglement in kondo clouds

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Since the theoretical explanation of the Kondo effect, the existence of the so-called Kondo cloud has captured the attention of the community. This electronic cloud forms a singlet with the impurity, leading to the screening of its spin. Entanglement plays a crucial role in this process, exhibiting unique behavior. In recent years, the distribution of entanglement within and beyond the Kondo cloud has become a topic of growing interest [1]. In the case of multichannel Kondo systems, the entanglement becomes more complex, as electrons from each channel compete to screen the impurity spin [2].

In this work, we study the entanglement distribution in a two-channel Anderson model with a $S = 1$ impurity, where the couplings to the channels are anisotropic. Using the density matrix renormalization group, we explore the spatial distribution of the Kondo cloud and its entanglement with the impurity and the rest of the conduction electrons. Additionally, we demonstrate how the composition of the cloud changes as the anisotropy between the couplings increases.

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Topic : *Topological Materials* **Poster Number:** 47

Binding zero modes in Josephson junctions

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We study the joint dynamics of the phase bias ϕ and the propagating Majorana fermions of the edge modes in Josephson junctions containing 2D time-reversal invariant topological superconductors (TRITOPS). We consider TRITOPS-TRITOPS junctions, as well as junctions between topological and non-topological superconductors (TRITOPS-S). Both types of junctions are described by effective Dirac Hamiltonians with a ϕ-dependent mass. We analyze the effect of the phase fluctuations in the junction, as well as solitonic solutions of ϕ generated by fluxons trapped in the junction. We show that these solitons generate a spatial-dependent mass with a sign change akin to the Jackiw-Rebbi model. This enables the formation of zero-energy fermionic states localized at the fluxon. For the TRITOPS-TRITOPS junction these consist of a Kramers pair of Majorana modes, while for the TRITOPS-S one, there is a single Majorana fermion. The localized bound states hybridize in soliton-antisoliton configurations. Depending on the occupation state, these modes generate an effective attraction or repulsion in the dynamics of the soliton-antisoliton collision.

Topic : *Topological Materials* **Poster Number:** 48

Topological surface states in interaction with dimer molecules

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Topological insulator bismuth selenide (Bi2Se3) has many potential applications due to its topological surface states (TSS). Here, TSS of Bi2Se3 in interaction with carbon monoxide and nitric oxide are studied using density functional theory (DFT). In the first case, the electronic structure of the system is calculated with the molecules set in different adsorption sites allowing for different orientations at the (0001) surface of the topological insulator. The dimer induces a structural change on the surface quintuple layer (QL), reducing the Van der Waals gap and total width of the QL. In turn, this affects the Dirac cone and the TSS effectively bend towards larger binding energies. Also, as the dimer gets closer to the surface, the energy of the SST at the gamma point and the binding energy of the system increase. In addition, charge density differences analysis show charge transfer between the dimer and the surface state indicating a weak chemical adsorption. Finally, the adsorbed magnetic NO molecule induces larger changes in the TSS.

Topic : *Materials for Energy* **Poster Number:** 49

Numerical and experimental study of the difussion of Fe in αZr%nSn alloys

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We study the impact of the αZrSn phase on Fe diffusion coefficient (D_{Fe}) within the αZrSn%nFe alloy in terms of the content of Sn. We present an improved phenomenological model for D_{Fe}, which enhances the ones existing in the literature. Furthermore, our investigation extends to the influence of Sn content on D_{Fe} on the hcp-phase of αZr. Our model employs the transition state theory incorporating ab-initio parameters calculated with VASP. In this context, we consider nine different ordered alloys, each having different content of Sn. In this way, we have computed the effective activation energies for every alloy using an Arrhenius fit. We compare our numerical results with experiments performed in our laboratory using the Libs technique. In parallel, we perform DICTRA calculations in order to obtain the Fe diffusion profiles and previously obtaining the thermodynamic parameters for the ZrSnFe system using the Thermocalc module. In summary, our work presents an improved model for Fe diffusion on ZrSn-based alloys, probing the Sn content's impact, and establishing connections between microstructural changes and diffusion behavior.

Topic : *Materials for Energy* **Poster Number:** 50

Molecular dynamics of methane sticking over Ni(111) with Atomistic Neural Network Potentials

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Production of syngas from methane is an important process, relevant to various industries and a potential tool for reducing greenhouse emissions in the energy sector [1].

The process is enhanced with metal catalysts, and its rate limiting step is the reaction of dissociative sticking of the molecule over the surface of the catalyst [2]

CH4(g) -> CH3*(ads) + H*(ads)

Understanding this mechanism is crucial for the development of new catalysts [1].

In this work, we present simulations of the reaction over a nickel (111) surface. Our method relies on classical molecular dynamics simulations based on an Atomistic Neural Networks Potential (ANNP) [3]. These potentials are built ad hoc for each system by training on high-quality electronic structure data, and can reproduce its energies with a computational cost several orders of magnitude smaller. This allows for the simulation of large numbers of trajectories required to build good statistics in different regimes, which is unfeasible with ab initio dynamics.

The main outcome of our studies are the dissociative sticking curves for CH4 and CHD3. We discuss the influence of surface deformations and impact site, incident translational and vibrational energy of the molecule, and isotopic exchange of hydrogen.

Our results align with previous theoretical [4-7] and experimental [7-8] works, though some discrepancies appear in the low kinetic energy regime of the molecule.

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Topic : *Materials for Energy* **Poster Number:** 51

Experimental $^{1}19$Mössbauer and density functional theory study of (Sb, Sn) co-doped Te-Ge material for thermoelectric applications

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Te-based chalcogenide materials have been found to exhibit very outstanding characteristics for use in thermoelectric and phase-change memories applications. For this reason, thermoelectric materials (TM) have attracted a lot of attention because of their capability to transform heat into electricity without the use of moving parts [1, 2].

Among the existing good TM materials, GeTe-based compounds in the cubic rock-salt structure are those with the highest ZT values in the medium temperature range [2, 3] but have a poor thermal stability and a high concentration of Ge vacancies [2]. Also, the presence of Ge vacancies reduces ZT. Counter doping (Pb, Bi, and Mn co-doping) is commonly employed to reduce the Ge-vacancy concentration [2, 3]. The intrinsic Ge-vacancy concentration in the rhombohedral phase is much lower than that in the cubic phase. With this recognition, the hole concentration of GeTe can be tuned simply by annealing below the phase transition temperature. As a result, compositional and phase planification can be realized in the high-performance GeTe-based thermoelectric with reduced amounts of counter dopants [2, 3].

In this work we present a Density Functional Theory (DFT) based ab initio study of the electronic, structural and hyperfine properties of (Sn, Sb) doped Te32Ge13Sn5Sb9). To determine the localization of the dopants, the obtain the hyperfine parameters (isomer shift, quadrupole splitting) at the Sn sites for both the cubic and rhombohedral phases as a function of the distribution of the Ge-vacancies and the Sb and Sn dopants. Our results are compared to those obtained in 119Sn Mossbaüer experiments.

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Topic : *Materials for Energy* **Poster Number:** 52

Synthesis of Li-ZnO by mechanical milling: Improvement of photoelectrochemical and optoelectronic properties

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Zinc oxide (ZnO) is a type II-VI semiconductor that has garnered significant interest due to its unique properties, including intrinsic defects that lead to diverse photoluminescence in the ultraviolet and blue-green regions. These characteristics make it a promising candidate for applications in white LEDs, displays, and photocatalysis. However, a major challenge in advancing these technologies is the difficulty in producing p-type ZnO, which is crucial for device functionality. Theoretical studies indicate that doping with group I elements, particularly lithium, may effectively facilitate the achievement of p-ZnO.

This study investigates the effects of lithium doping on various properties of ZnO, including photoelectrochemical, structural, morphological and optical characteristics. The methodology involves synthesizing ZnO from spent alkaline batteries. The process begins with dissolving the anodic paste using HNO_3 and HCl. Subsequently, ZnO is precipitated using NaOH, followed by drying and calcination. Lithium doping is accomplished by mixing the ZnO with Li_2CO_3 (lithium carbonate) at a 3% atomic ratio and mechanically milling the mixture for 10 hours. The obtained powders were used for fabricating electrodes using a spin-coating technique for application in dye sensitized solar cells (DSSC). The samples were characterized by scanning electron microscopy (SEM) for morphological assessment, X-ray diffraction (XRD) for structural analysis, Raman spectroscopy for vibrational modes, and UV-Vis spectroscopy to determine the energy gap (Eg). The photoelectrochemical performance of the electrodes was evaluated through current-voltage (I-V) curves under both dark conditions and simulated solar illumination.

The results reveal significant differences between undoped and Li-doped ZnO regarding morphology, lattice parameters, optical properties, and photoelectrochemical performance. In summary, this study highlights the advancements made in understanding the impact of Li doping on ZnO properties. These findings pave the way for improved optoelectronic and photoelectrochemical devices and address existing challenges in p-type ZnO fabrication. Furthermore, utilizing ZnO recovered from spent batteries contributes to sustainable practices within a circular economy framework.

Topic : *Materials for Energy* **Poster Number:** 53

Theoretical comparative study of the properties of titania nanoparticles on graphene or graphene oxide as electrode supports used in fuel cells

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Among the various technologies proposed for electrodes, carbon-based supports have garnered special attention due to their conductive and porous structure, which enhances catalyst dispersion. A commonly used catalyst in proton exchange membrane fuel cells (PEMFC) is platinum (Pt). However, the inclusion of titania (TiO_2) nanoparticles presents a more economical and abundant alternative [1]. Both graphene (G) and graphene oxide (GO) [2], when combined with TiO_2, exhibit promising properties that could enhance fuel cell performance by facilitating electron transfer in electrochemical and photocatalytic reactions.

In this study, we explore the interaction of $(TiO_2)N$ (N = 1 to 5) nanoparticles deposited on GO and G. Simulations were conducted using ab initio calculations with the VASP code [3], incorporating van der Waals corrections. The results indicate that varying N induces significant changes in the electronic and optical properties of the systems. Adsorption energies suggest that adsorption is more favorable on GO than on G, with an increase of 70% to 90%, decreasing as N increases. Notably, for N = 2, the lowest adsorption energy on GO (-2.7 eV) is observed, along with a maximum absorption shift into the visible region.

The presence of oxygen on the GO surface facilitates the formation of Ti-O-C bonds, promoting electron transfer, as revealed by Bader charge analysis, and confirms the presence of high-mobility states within the band gap. A comparative analysis of the optical properties shows that nanoparticles deposited on GO exhibit a slightly narrower band gap than those deposited on G. The study also includes the presence of Pt nanoparticles and the adsorption of oxygen molecules.

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Topic : *Materials for Energy* **Poster Number:** 54

DFT and Kinetic Montecarlo study of the H_2O adsorption on AgI surfaces

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The research of such systems is of significant interest, particularly in industries like viticulture, which includes the growing of grapes for wine production. In viticulture, the economic implications of both public and private “anti-hail” programs are substantial. This is especially relevant in the province of Mendoza- Argentina, where cloud seeding measures are employed to safeguard crops from being damaged by hail. Consequently, the study of systems like AgI-H_2O contributes to our understanding of high-impact materials relevant to these agricultural practices.

In the present study, we conducted a series of ab initio calculations within the framework of Density Functional Theory (DFT) to investigate the adsorption of H_2O molecules on the (001), (011) and (101) AgI surfaces. We solved the Kohn-Sham self-consistent equations using the plane-wave and pseudopotential method, implemented in the Quantum Espresso code. The exchange-correlation part was described using the PBE parametrization of the General Gradient Approximation (PBE-GGA). We determined the preferential site for adsorption, the most reactive surface as well as the adsorption energy and lateral interaction energy between H_2O molecules at different coverage levels. These parameters are essential for studying dynamic processes such as Thermal Programmed Desorption (TPD) using kinetic Monte Carlo simulations.

Topic : *Materials for Energy* **Poster Number:** 55

Hydrogen storage on silicene and germanene doped with X = (Sn, V, Ti, Zn, Cu) and decorated with M = (K, Li, Mg). A DFT study

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In this study, we investigated hydrogen adsorption on bidimensional materials (Germanene and Silicene). These materials were doped with X = (Sn, V, Ti, Zn, Cu) and decorated with M = (K, Li, Mg). All calculations were performed using density functional theory, as implemented in the Quantum ESPRESSO code to solve Kohn-Sham equations. The Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional within the generalized gradient approximation (GGA) was applied. Additionally, Van der Waals interactions were considered using DFT-D3 and RVV10 corrections. The kinetic energy cutoff (Ecutwfc) was set to 60 Ry, and a cutoff limit of 600 Ry was applied for the augmented density. A $4 \times 4 \times 1$ supercell containing 32 atoms, with a vacuum spacing of 20 between adjacent layers, was used. Host atom substitutions were made with 3.125% X doping. Decoration atoms were relaxed in four possible positions, and the lowest-energy configuration was selected. Then, hydrogen molecules were placed around the decoration atoms for further analysis. In conclusion, Lithium-decorated Silicene systems showed promising performance, with copper and vanadium doping being the most effective. Finally, the density of states is presented to understand the electronic behavior of the studied systems.

Topic : *Materials for Energy* **Poster Number:** 56

A DFT study of the Fe(110)/SiC(100) interface as a possible candidate for RPVs

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Reactor pressure vessels (RPVs) are a crucial part of fuel storage in a nuclear power plant. A useful coating for the iron substrate (the main component of these vessels) could provide an advancement in containing the fuel in this harsh environment. SiC, a lightweight ceramic with a high melting point (2970 °C) and resistance to corrosion [1], could be a good candidate for addressing this issue. In this work, we present a theoretical study at the atomistic level on the adhesion of a Fe(110)/SiC(100) surface. The presence of atomic oxygen at different coverage (M=0.25, 0.5 and 1.0) between the substrate and the coating was also analyzed.

The calculations were performed using the Vienna Ab initio Simulation Package (VASP), based on Density Functional Theory. The general gradient approximation (GGA) parametrized by the Perdew-Burke-Ernzerhof functional (PBE) was employed as an exchange-correlation term, along with the projector augmented wave (PAW) pseudopotential method. For the plane-wave basis set, a cut-off energy of 520 eV was established and a Monkhorst-Pack cell of 9x7x1 k-points was used for both the Fe(110)/SiC(100) and the FeO(110)/SiC(100) interfaces. To better simulate the iron substrate magnetic behavior, spin-polarization was considering.

To establish an optimal interface separation gap, a post-processing analysis was carried out by using the UBER method to compute. The ideal adhesion work of the Fe(110)/SiC(100) interface ($W_{ads} = 4.23\ J/m^2$) was obtained. This result suggests that the aforementioned interface is a suitable candidate for a harsh environment vessel, such as a nuclear power plant, by considering its good stability.

[1] D. F. Johnson, E. A. Carter, J. Phys. Chem. A, 113 (2009), 4367–4373

Topic : *Materials for Energy* **Poster Number:** 57

Exploring preferential orientation on electrodeposited ZnO thin films through ab-initio calculations

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ZnO films were obtained via electrodeposition using two different Zn^{2+} solutions with distinct counterions: Cl^- and NO_3^-. The morphological and crystallographic orientation differences, observed through X-ray diffraction (XRD) and high-resolution field emission scanning electron microscopy (HR-FESEM), demonstrate the influence of the precursor type on the ZnO synthesis process. Samples grown from commercial nitrate solutions exhibit nanocolumnar structures with preferential growth along the (002) direction. In contrast, random growth patterns (e.g., hexagonal plates, agglomerations, clusters) were observed in samples derived from chloride-based solutions. To better understand the role of both counterions in determining the resulting morphologies, an *ab-initio* approach using Density Functional Theory (DFT) was employed. Two film surfaces were simulated: the (001) and (100) planes. The adsorption energies of Cl^- and NO_3^- were evaluated to verify the conditions that favor preferential growth along the c-axis for both ions. It was demonstrated that Cl^- preferentially adsorbs onto the (001) planes, hindering crystal growth along the c-axis and leading to the formation of platelet-like crystals. Furthermore, the morphology evolved from hexagonal tapers to hexagonal rods and rhombohedral rods by altering the composition of the capping agents.

Topic : *Materials for Energy* **Poster Number:** 58

Nanocolumnar growth of Li-doped ZnO through electrodeposition

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This work presents the straightforward, one-step growth of Li-doped ZnO thin films using the electrodeposition technique from an aqueous solution of common salts. Lithium is a key dopant due to its unique properties, enhancing the optoelectronic characteristics of ZnO, thus increasing its application in advanced devices. The proposed method is cost-effective and potentially scalable, allowing one to predict whether the grown oxide will exhibit a nanocolumnar morphology by simply observing the chronoamperogram. Structural analysis through X-ray diffraction (XRD) showed no formation of secondary phases associated with lithium, confirming the homogeneous incorporation of the dopant into the ZnO structure. Additionally, a systematic shift in the (002) plane position was observed with increasing Li^+ concentration, resulting in a decrease in the diffraction angle, indicating an increase in the lattice parameter according to Bragg's law. To confirm the presence of lithium in the film structure, time-of-flight secondary ion mass spectrometry (TOF-SIMS) analysis was performed, verifying the effective incorporation of Li^+ into the ZnO nanocolumns. This study highlights the importance of electrodeposition as a versatile technique for the fabrication of lithium-doped ZnO thin films, which could have useful future applications in sensors, catalysis, energy, or electrocatalysis.

Topic : *Materials for Energy* **Poster Number:** 59

In situ X-ray powder diffraction study on the development of zeolite-templated carbons in FAU zeolite

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A time resolved in situ X-ray powder diffraction investigation using synchrotron radiation allowed for describing the time evolution of the FAU structure during the development of a zeolite-templated carbon (ZTC) in its porous voids. During the ZTC formation the intensity decrease of most zeolite reflections and the simultaneous rise in intensity of the 222 reflection (of null intensity in the pristine zeolite) were observed. Full pattern profile fitting by Rietveld refinement allowed for achieving a detailed description of the underlying chemistry, with coincident pore filling with carbon atoms in specific positions and framework distortion. Monitoring the intensity profiles of the 222 reflection allowed assessment of the energetics of the ZTC formation. Our results contribute to a better understanding of the phenomena involved on the atomic scale in ZTC synthesis.

Topic : *Materials for Energy* **Poster Number:** 60

Unraveling Iron Oxide Nanoparticle Reactivity via Integrated Experimental and Computational Approaches

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With the increasing contamination, the promotion of sustainable industrial processes is imperative. In this context, enzyme-mimicking nanomaterials, or nanozymes, have emerged as promising alternatives. Among these, iron oxide nanoparticles exhibit peroxidase-like catalytic activity, efficiently decomposing H_2O_2 and oxidizing organic compounds. Despite extensive research on their catalytic properties, the precise reaction mechanisms governing their activity remain unresolved.

This study focuses on nanozymes composed of Fe_3O_4 (magnetite) and Fe_2O_3 (hematite) nanoparticles. Using density functional theory (DFT) and classical molecular dynamics simulations (MD), we explore the chemical reactivity of these materials in both vacuum and under microsolvation by water. The climbing image nudged elastic band (CI-NEB) method is employed to locate transition state structures, enabling the determination of thermodynamic feasibility and kinetic barriers of the H_2O_2 decomposition reaction. We analyze the (001) surface of both materials and relate our findings to experimental data, including electron paramagnetic resonance (EPR) and transmission electron microscopy (TEM) results.

Our simulations reveal key insights into the differences in reactivity between Fe_3O_4 and Fe_2O_3, particularly in the production of OH and OOH radicals, as observed experimentally. While both surfaces predominantly expose Fe^{3+} ions, Fe_3O_4 nanozymes exhibit significantly higher OH radical production. We have analyzed possible H2O2 decomposition mechanisms in the surfaces. Then we performed classical MD simulations that allowed us to extract solvent conformations, that we used to include a few water molecules in the electronic structure calculations. By examining the electronic structure and charge transfer mechanisms, we elucidate the influence of water microsolvation and provide a comprehensive explanation for the experimentally observed catalytic differences between these materials.

Topic : *Materials for Energy* **Poster Number:** 61

MnO_2 film on nickel foam substrates: An electrodeposition route for supercapacitor applications

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We investigated the electrodeposition of manganese dioxide (MnO_2) on nickel foam substrates for potential supercapacitor applications. The nickel foam, with its high surface area, was used to enhance the electrochemical performance of the deposited material. The deposition process was conducted in a solution of $Mn(CH_3COO)_2$ and Na_2SO_4 at a concentration of 0.07 mol/L. Four samples were prepared using deposition potentials of 0.6 V and 0.8 V for durations of 60 s and 120 s. The deposition potential was determined by linear sweep voltammetry.

Mass changes before and after deposition were recorded, with the mass varying from 0.48 to 0.94 mg/cm^2. Initial SEM imaging suggests a uniform thin film distribution on the substrates. Energy-dispersive X-ray spectroscopy confirmed the presence of manganese. Cyclic voltammetry was used to calculate the specific capacitance of the material. Our results indicate that thinner films tend to result in higher specific capacitance. The 0.8 V, 60 s sample, with a mass deposition of 0.48 mg/cm^2, achieved a specific capacitance that was 66.8% higher compared to the 0.8 V, 120 s sample, which had a mass deposition of 0.94 mg/cm^2.

Topic : *Materials for Energy* **Poster Number:** 62

Electrochemical Impedance Spectroscopy on Mesoporous YSZ Thin Films for SOFC applications

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We fabricated dense and mesoporous thin films of Yttrium Stabilized Zirconia (ZrO_2 doped with Y_2O_3) for solid oxide fuel cell (SOFC) applications. Our proposal is to control the porosity as a tool to increase the specific area at the electrolyte-electrode interface, enhancing the oxygen ion exchange with the electrolyte. The films were prepared following the sol-gel route and deposited by dip-coating on a SiO_2/Si and single crystalline YSZ substrates. Pluronic F127 and Brij58 molding agents were incorporated into the sol to combine with the evaporation-induced self-assembly strategy, in order to obtain mesoporous thin films with two different pore diameters. Using Electronic Microscopy and X-Ray Reflectometry we determined the morphology, the accessible porosity and the thickness of the samples.

We study the electrochemical properties of the films as a function of temperature and O_2 partial pressure. In particular, in-plane electrochemical characterization was performed in a probe station designed in the lab to characterize thin films and devices from room temperature to 700 $^\circ$C. We present here the structural characterization and electrochemical impedance spectroscopy results, as a function of the temperature and the partial pressure of oxygen of these YSZ films. This work represent a preliminar step for symmetrical cells building.

Topic : *Materials for Energy* **Poster Number:** 63

Electronic properties dependence on oxygen content on Ti_nO_{2n-1} ($4 \leq n \leq 9$) Magnéli phases by DFT modeling

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In this study, we theoretically characterized Magnéli phases of titanium oxides with the general formula Ti_nO_{2n-1} (where $4 \leq n \leq 9$) using density functional theory. Our findings highlight the crucial role of structural shear planes -specifically, those corresponding to the rutile (121) Miller planes- in determining electronic properties. Within these planes, the highest concentration of Ti 3d electrons is observed. These electrons in the Ti 3d orbitals induce a splitting of the Ti 3d band, resulting in a bandgap (pseudogap) and the emergence of impurity states near the Fermi level. Antiparallel spin configurations were found to be the most stable across all studied phases. As n increases, the electronic gap monotonically decreases toward the rutile value. Notably, in Ti_9O_{17}, the presence of unpaired Ti^{+3} ions lead to local spin densities and less symmetric magnetic configurations. Additionally, 3d orbitals from Ti^{+3} add states at the edges of the valence and conduction bands, significantly reducing the electronic band gap. The main absorption edge, associated with O2p – Ti3d transitions, monotonically decreases as oxygen content increases to the rutile bandgap value. The reflectivity in the suboxides seems to increase according to n until rutile´s composition except for Ti_6O_{11}.

For calculations, VASP (Vienna ab initio Simulation Package) with GGA exchange-correlation functional and PBE parametrization was utilized. A Coulomb term (U_{eff}) was included, using the DFT+U methodology proposed by Dudarev et al [1], to obtain a better description of the electronic properties. The effective Coulomb repulsion in-situ U_{eff}=U-J=5 eV was selected for the Ti-d. In addition, we include Density Functional Perturbation Theory for phonon calculations complemented by Phonopy analysis to corroborate the local minimum character of each structure.

[1] S. Dudarev, G. Botton, S. Savrasov, C. Humphreys, A. Sutton, Phys. Rev. B 57 (1998) 1505.

Topic : *Materials for Energy* **Poster Number:** 64

Ionic Liquids as additives in hybrid perovskite solar cells

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In recent years, hybrid organic-inorganic perovskite solar cells have attracted significant attention due to their low manufacturing costs, high light absorption coefficients, tunable bandgap, and excellent charge transport properties. However, when these films are produced by spin coating, defects form at the grain boundaries that facilitate material degradation and, consequently, undesired recombination, reducing the performance of the fabricated solar cells. As a potential solution, several groups have developed strategies for fabricating perovskite films using ionic liquids (ILs) as passivating agents or additives. Ionic liquids are salts with a low melting point (below 100°C), consisting of organic cations formed by imidazolium, pyridinium, pyrrolidinium, among others, as well as anions that can be either organic or inorganic.

This work aims to demonstrate how the chemical modification of hybrid perovskites with these types of compounds improves their long-term stability and prevents perovskite decomposition due to environmental factors, thereby enhancing the stability of solar cells made from these materials. Different concentrations of 2-naphthalenesulfonate 1-butyl-3-methyl imidazolium (BmimNafS) were prepared as thin films and solar cells were fabricated. It was confirmed that the crystal structure of the perovskite is not modified by IL addition as analyzed by X-ray diffraction. The absorption spectrum did not change and steady-state photoluminescence studies showed an increase in fluorescence intensity. TRPL measurements showed significantly increased fluorescence lifetimes with IL as additive. Depending on the additive concentration, the solar cell efficiency is increased (from a PCE of 14.5% for pristine $MAPbI_3$ up to 18.2%) mostly due to the increased photocurrent. A substantial increase of the EQE is consistently observed in the high wavelength region of the solar spectrum.

Topic : *Materials for Energy* **Poster Number:** 65

Adsorption and effect of explicit microsolvation of lithium sulfide on Li-S battery cathodes: a DFT Study

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The specific storage capacity of current rechargeable lithium batteries poses a serious limitation for their use in applications such as electric vehicles. One of the most promising technologies for the next generation of Li batteries is rechargeable lithium-sulfur (Li-S) batteries. These are based on a sulfur composite cathode, an organic electrolyte and metallic lithium as the active material for the anode. However, its implementation in daily life applications still presents several drawbacks. A possible solution with great potential is the use of lithium sulfide as a cathode material since it is possible to couple it to Li-free anodes, such as graphite, Si or Sn. However, both lithium sulfide and sulfur are electronic and ionic insulators, with a high activation potential for their initial oxidation step. To overcome this problem, different strategies have been explored, such as the use of catalytic surfaces. To computationally model these reactions, it is crucial to consider the effect of the solvent. In the present work, the interaction of Dimethyl ether (DME) and Dimethylformamide (DMF) with Li_2S, both in vacuum and adsorbed on a graphene sheet in explicit form, was studied and characterized by DFT calculations, using the Quantum Espresso (QE) program. Using ab initio molecular dynamics, the optimal number of molecules for the first solvation sphere of Li_2S was determined for both solvents. Subsequently, the activation barriers for the decomposition of Li_2S in vacuum and adsorbed on different reactive surfaces, such as graphene, were determined.

Topic : *Materials for Energy* **Poster Number:** 66

Study of the electronic and local structure of SrCo$_{1-x}$Mo$_x$O$_{3-\delta}$ perovskites (x = 0.05, 0.45, and 0.50) using Synchrotron X-ray Absorption Spectroscopy

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The growing concern over harmful gas emissions and greenhouse effects has driven the search for sustainable solutions to mitigate environmental impact. In this context, fuel cells have gained significant attention due to their ability to efficiently convert chemical energy into electricity. Solid oxide fuel cells (SOFCs) stand out for their versatility, as they can operate on unpurified hydrogen and various hydrocarbons, including methane and biogas. Currently, research is focusing on intermediate-temperature SOFCs (IT-SOFCs) that function between 500 and 800°C. To enhance performance at these temperatures, electrode materials with mixed ionic-electronic conductivity are being developed. Additionally, a key area of research is the development of symmetric fuel cells (S-SOFCs), which use identical materials for both the anode and cathode electrodes, thereby simplifying the manufacturing process and reducing costs.

The present study evaluates promising materials for S-SOFCs, concentrating on mixed ionic-electronic conductors based on Sr(Co,Mo)O$_{3-\delta}$ perovskites. The electronic and local structure of SrCo$_{1-x}$Mo$_x$O$_{3-\delta}$ perovskites (with $x = 0.05$, 0.45, and 0.50) was investigated using advanced techniques such as XANES (X-ray Absorption Near Edge Structure) and EXAFS (Extended X-ray Absorption Fine Structure) at the K edges of Co and Mo.

The experiments were conducted *in situ* under various reducing and oxidizing atmospheres over a temperature range of 20 to 700°C, allowing for the identification of significant changes in the oxidation state speciation of cations and important modifications in their coordination environments. Additionally, simulations were performed to compare theoretical results with experimental findings, providing a more comprehensive understanding of the observed phenomena.

This study expands knowledge about the properties of perovskites under operational conditions and opens new perspectives for their application in fuel cells, contributing to the development of cleaner and more sustainable energy technologies.

Topic : *Materials for Energy* **Poster Number:** 67

Structural analysis of $SrTi_{1-x}Fe_xO_3$ solid oxide fuel cell electrodes synthesized via the Pechini method and pulsed laser deposition

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Solid oxide fuel cells (SOFCs) are highly attractive for energy conversion due to their fuel flexibility, environmental benefits, and high efficiency. However, their typical operating temperatures above 800°C present challenges such as stability, sealing integrity, and safety. As a result, research is increasingly focused on reducing the operating temperature to 600°C or below, with one effective approach being the reduction of electrolyte thickness while maintaining performance and stability.

Pulsed Laser Deposition (PLD) is a promising technique for thin-film fabrication due to its precise control over film thickness, composition, and crystallinity. In this study, epitaxial thin films of $SrTi_{1-x}Fe_xO_3$ (STF) (X = 0.2, 0.35, 0.5) and gadolinia-doped ceria (GDC) were deposited on (001)-oriented yttria-stabilized zirconia (YSZ) substrates using PLD at 850°C under controlled oxygen flow. The films were characterized by high-resolution X-ray diffraction (HRXRD), revealing that 5 nm films experienced in-plane compressive strain and out-of-plane expansion. Thicker films progressively relaxed this strain towards bulk values, with relaxation rates dependent on Fe content—higher Fe levels resulted in faster relaxation (smaller critical thickness). X-ray absorption near-edge structure (XANES) spectra at the Ti and Fe K-edges were also measured, showing no significant changes in oxidation states, despite variations in composition and thickness. Ongoing simulations using FEFF 9.7 are modeling the crystal structure, accounting for distortions in the octahedral geometry and the effects of in-plane strain and out-of-plane deformation. Additionally, the Pechini method is being investigated for fabricating thicker films with the same composition, allowing a direct comparison of electrochemical properties between the samples obtained by two methods. Parameters such as ionic conductivity, charge transfer kinetics, and electrochemical stability will be evaluated to provide deeper insights into the performance of these materials in SOFCs applications.

Topic : *Materials for Energy* **Poster Number:** 68

Analysis of the potential use of 2D phosphorus-doped graphitic carbon nitride in next-generation batteries

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Next-generation secondary batteries, including Li-Sulfur (Li-S), Li-air and ion batteries, are promising technologies for energy storage. Li-S/air batteries, whose active anode material is metallic Li, present several problems that need to be solved before being commercialized: One is the growth of dendrites during charge/discharge cycles and the other is the low Coulombic efficiency of the process due to an unstable solid-state electrolyte interface (SEI). While Na/Mg/K ion batteries, which use these ions as charge carriers, the main drawback they present is the adsorption and desorption of the ions in the charge and discharge processes, due to their larger size.

Our work is focused on analyzing, using the Density Functional Theory (DFT), the potential use of 2D sheets of graphitic carbon nitrides (g-C_3N_4) doped with phosphorus (g-C_3N_4P), in order to be used as a protective sheet for the anodic lithium metal or as an anode material by itself for use in Na-ion, Mg-ion and K-ion batteries. For this purpose, the doping energies at different sites of the sheet were calculated. Subsequently, the adsorption energies for a metal atom on the most energetically stable sheets were determined, in order to then simulate the diffusion processes between adjacent sites of the sheet and through it. Our results allow us to affirm that doping occurs by preferentially replacing C atoms in the g-C_3N_4 sheet. The ionic adsorption energies for Li, Na, K and Mg show greater stability in films in which the identity of carbon atoms has been changed to phosphorus with respect to the pristine structure, while doping considerably reduces the energy barriers in the diffusion processes.

Topic : *Large Facilities* **Poster Number:** 69

Resonant Inelastic X-ray Scattering (RIXS) of $CaMnO_3$ ultrathin films: influence of tensile strain on electronic and magnetic properties

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Manganites are highly correlated systems characterized by a complex interplay between structural, charge, orbital, and spin degrees of freedom. In the $La_xCa_{1-x}MnO_3$ family, doping agents alter the electron filling, thereby modifying the electric and magnetic properties. Additionally, the incorporation of cations with varying sizes induces changes in Mn-O distances and Mn-O-Mn angles, affecting superexchange and double exchange magnetic interactions. The perovskite $CaMnO_3$ (CMO) stands out as a promising material for spintronics devices.

In this study, we investigate the impact of tensile strain on the electronic and magnetic properties of ultrathin $CaMnO_3$ films (3 nm and 30 nm thick) epitaxially grown on $SrTiO_3$(100) substrates and $BaTiO_3$ underlayers. Strain is a consequence of the mismatch between lattice parameters of the perovskites, which causes changes in atomic positions and the formation of oxygen vacancies. Therefore strain can induce similar effects to those of doping but constrained to the interfacial regime. Thinner films experience significant tensile strain effects, whereas thicker films relax their crystal structure and exhibit bulk-like behavior.

We employed X-ray Photoelectron Spectroscopy (XPS), synchrotron radiation X-ray Absorption Spectroscopy (XAS), and Resonant Inelastic X-ray Scattering (RIXS) to elucidate the effects of strain. XPS and XAS measurements reveal that the surface of 30 nm films present the nominal composition of Mn^{4+}. However, 3 nm films contain a notable amount of Mn^{3+} indicating a concentration of oxygen vacancies near the interface. RIXS spectra display d-d excitations and O 2p-Mn 3d charge transfers. Concomitant with the reduction of Mn centers in thinner samples, we observe an attenuation of the crystal field strength due to the increased Mn^{3+}-O distances. In addition, we observe an intersite eg transition which can be related with an enhanced ferromagnetic order, consistent with magnetic measurements and theoretical predictions.

Useful Information

Talks will be held at the **Emma Perez Ferreira-Auditorium** of Centro Atómico Constituyentes. It is situated on the ground floor of the Tandar Lab building (N° 42).

Coffee breaks and lunches will be offered in front of the main entrance of the conference hall.

The **poster session** will be held on Wednesday night on the **ground floor** of the Tandar Lab, close to the auditorium. Also, poster will be exhibited until the end of conference.

Wi-Fi will be available during the conference.

The location of the Conference is at the Tandar Lab in the Constituyentes Atomic Center.


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