21st BWSP
Brazilian Workshop on Semiconductor Physics

September 2nd to 6th, 2024
CNPEM | Campinas - SP

ABSTRACT BOOK

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Foreword

The Brazilian Center for Research in Energy and Materials (CNPEM) organized the 21st Brazilian Workshop on Semiconductor Physics (BWSP) from September 2 to 6, 2024, in Campinas-SP, Brazil.

Initiated in 1983, the BWSP became a traditional event in the field of Semiconductor Physics in Brazil, taking place biennially. Its purpose is to expose Brazilian students to renowned researchers and international leaders in various semiconductor research fields while fostering interaction between national and international researchers.

Over the years, the BWSP has evolved into an extremely comprehensive event, encompassing topics at the forefront of knowledge in Condensed Matter Physics. The 21st edition aims to bring together the Brazilian semiconductor physics community for lectures on the most important and current topics in the field. The program will cover diverse themes, including Traditional and Emerging Topics in Semiconductors, Nanostructure Fabrication Techniques, Devices, and Quantum Technologies, among others. It will feature lectures, plenaries, tutorials, presentations of contributions on the discussed topics, panel sessions for all participants, as well as visits to Sirius and the Brazilian Nanotechnology National Laboratory (LNNano) facilities.

The workshop program included 205 presentations with 22 invited speakers, 30 contributed oral talks, 13 young researcher talks, and 140 posters. Moreover, tutorials on excitons in two-dimensional materials and probing quantum materials with ARPES and synchrotron radiation were also included.

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Language

English.

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CNPEM; CNPq; CAPES; FAPESP; FAPEMIG.

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INVITED SPEAKERS

CNPEM - Brazilian Center for Research in Energy and Materials

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The Brazilian Center for Research in Energy and Materials (CNPEM) is a cutting-edge, multi-user, multidisciplinary scientific environment that supports the Brazilian National Science, Technology and Innovation System. It has globally competitive laboratory infrastructures open to the scientific community, such as Sirius, one of the world´s most advanced synchrotron light sources. The Center combines a range of skills, with an emphasis on nanotechnology, biosciences, biotechnology, biorenewables, cutting-edge engineering and scientific instrumentation, carrying out research and development in strategic areas such as health, energy, renewable materials, and sustainability, including innovative projects in partnership with the productive sector and contributing to the training of researchers and students. CNPEM has recently began developing the Orion project, a laboratory complex for advanced research in pathogens, which will host facilities with advanced levels of biological containment (BSL-3 and BSL-4), planned to be the first in the world to be connected to a synchrotron light source. In this seminar, an overview of the CNPEM's activities will be presented.

Controlling electron pairing and charge density waves by uniaxial strain in kagome lattices

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Topological and correlated phases arise in kagome lattices associated with Dirac fermions and flat dispersions in the single-particle energy spectrum [1]. We have further studied the interplay of attractive electron interactions and topological states in strained kagome lattices via a Hubbard Hamiltonian at different band-filling factors. It has been shown before that the system is driven into a charge density wave state beyond a critical attractive interaction Uc. We study the tunability of Uc employing uniaxial strains and doping levels and find various interesting phases as these physical parameters change. As uniaxial strain breaks the C3 symmetry of the lattice, we see the onset of a charge density wave ground state even for weak attractive interaction. In the presence of spin-orbit interaction, the system changes from a quantum spin Hall state to a charge density wave at Uc. We moreover find a region of strain and interaction values where the two phases coexist, before increasing strain results in a pure charge density ground state. When pairing correlations are allowed, we find interesting competition between a superconducting gap and that related to the charge modulation. Our general aim is to explore how electronic correlations and single-particle topological structures compete to create fascinating correlated phases in kagome systems.

[1] M. A. Mojarro, and S. E. Ulloa. Strain-induced topological transitions and tilted Dirac cones in kagome lattices. 2024 2D Mater. **11** 011001

Correlated quantum phases of spatially indirect excitons in heterostructures

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Strongly correlated quantum phases are at the focal point of many-body physics. An important subgroup are those were fermionic pairing leads to effective Bose particles that are allowed to condense into a quantum fluid. The study of Bose condensation dates back more than half a century ago. I will present a short overview of the current status and discuss new directions.
Spatially indirect excitons are promising candidates for realizing superfluidity and Bose-Einstein condensation in solid state devices. Another exotic phase is a quantum supersolid where a rigid lattice of particles flows without resistance. Within a mean-field approach we have determined the phase diagram** for the occurrence of Wigner crystal, exciton superfluid and exciton supersolid in the case of spatially indirect excitons in a double layer semiconductor heterostructure.

*Work in collaboration with: S. Conti, D. Neilson, M. Milosevic, A. Perali, A. Hamilton
** S. Conti et al., Phys. Rev. Lett. 130, 057001 (2023).

Effects of atmospheres in the wavelength-dependent photoconductivity of Co_3O_4

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Nowadays, two phenomena in semiconductor oxides deserve attention of the scientific community concerning the wide scope of applications: the interaction between surface and molecules in the air and the conversion of light to electricity. Surface reactivity in semiconductor oxides is widely employed to fabricate gas sensors. In addition, photocatalysis is another kind of application of these materials, which are the front liners in environmental remediation, especially in the degradation of organic pollutants in wastewater. Regarding multifunctionality, one such interesting material is the spinel cobalt oxide (Co_3O_4), an abundant and non-toxic semiconductor oxide, in which the loss of its stoichiometry provides a p-type conductivity.

Here we present the strategy to grow Co_3O_4 by spray-pyrolysis technique on amorphous and crystalline substrates, such as silicon and sapphire, using cobalt acetate as a precursor. After annealing at 500 °C in some controlled atmospheres, samples present strong preferential orientation at (111) direction. The optical absorbance displays two absorption edges at 1.5 eV and 2.2 eV associated with Co3+ and Co2+ bands, respectively. By adding electrical contacts, the photoresponse of Co_3O_4 was evaluated considering excitations in these two edges. The annealing in an argon atmosphere provided the best results in terms of photoresponse and response and recovery times. In addition, photoconductivity measurements in controlled atmospheres (Ar, O_2, N_2, synthetic air, and vacuum) exhibited a photoreactive surface, which depends on excitation wavelengths, except for oxygen atmosphere. The results are analyzed qualitatively in terms of the relative position of adsorbed molecules in the Co_3O_4 band diagram.

Energy efficient Organic Light Emitting Diodes

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Organic Light Emitting Diodes (OLEDs) have revolutionized display technology and are now widely integrated into commercial products such as mobile phones, TVs, and virtual reality headsets. Given the current energy crises, there is a pressing need for OLEDs to deliver even greater energy efficiency. In this talk, I will commence by discussing molecular strategies aimed at converting dark excited states (triplets) into emissive states (singlets) [1]. This will spotlight the latest progress in molecules demonstrating triplet harvesting via the thermally activated delayed fluorescence (TADF) mechanism. I will then explore the optical spectroscopy characterization of various TADF emitters, such as donor-acceptor [2] and multi-resonance materials [3]. Moreover, I will discuss the utilization of these materials in the emissive layer of OLEDs and present device strategies to achieve internal quantum efficiency of up to 100%. Thus, I aim to highlight the cutting-edge research driving the advancement of OLED materials and devices toward higher energy efficiency and superior performance.

References:

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Exciton transport driven by spin excitations in an antiferromagnet

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Magnetic excitons have recently been discovered in magnetic van der Waals crystals. Akin to the highly effective strategies developed for electrons, the intimate coupling of these excitons to the spin degree of freedom could offer novel solutions for long-standing problems in optics, such as controlling the flow of charge-neutral optical excitations in solids. A particularly important material for fundamental research in this direction is the van der Waals antiferromagnetic semiconductor CrSBr. It supports tightly bound excitons that interact strongly with light [1], magnetic fields [2], and magnons [3].

In this talk, I will present our recent study on exciton transport in CrSBr. Key results of our experiments include ultrafast, nearly isotropic exciton propagation substantially enhanced at the Néel temperature, transient contraction and expansion of the exciton clouds at low temperatures, as well as superdiffusive exciton transport behavior in ultrathin layers. These signatures largely defy description by commonly known exciton transport mechanisms but can be related to interactions of excitons with optically excited spin currents in this material. More specifically, we propose that the drag forces exerted by such currents can effectively imprint characteristic properties of magnons and other spin excitations onto the motion of excitons. The universal nature of the underlying exciton-magnon scattering promises driving of excitons by spin currents not only in CrSBr, but also in other magnetic semiconductors and even non-magnetic materials by proximity in heterostructures, combining the rich physics of magneto-transport with optics and photonics.

[1] Dirnberger, F. et al. *Nature* **620**, 533-537 (2023).
[2] Wilson, N. P. et al. *Nature Materials* **20**, 1675 (2021).
[3] Bae, Y. J. et al. *Nature* **609**, 282-286 (2022).

Exploring spin and orbital pumping in magnetic heterostructures

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Over the past decade, spintronics mainly focused on injecting spin current into nanomagnets for memory applications using spin-orbit torque, limited to materials with strong spin orbit coupling (SOC). Recent results revealed that the orbital Hall effect (OHE) is regarded more fundamental than the spin Hall effect, as it does not rely on the existence of SOC. While heavy metals like Pt, Pd, W and Ta were conveniently used to investigate spin currents, lighter materials likes Ti, Cu and Al were overlooked. Recent work demonstrated the efficacy of these materials for enhanced spin-orbital torque transfer in heterostructures, thus broadening the repertoire of spintronics materials, allowing the use of more cost-effective alternatives. This presentation explores fundamental spin-orbitronics concepts and phenomena, with an experimental investigation into converting spin-orbital currents to charge currents using spin pumping techniques driven by both ferromagnetic resonance (SP-FMR) and the longitudinal spin Seebeck effect (LSSE) [1]. Focus is on the interaction between spin, orbital and charge degrees of freedom in YIG (100 nm)/HM/NM/CuOx structures, with NM as Ti, Ru, and Ge, and HM as Pt or W. Without the CuOx cover layer, we examine the volume conversion of orbital current to charge in YIG/Pt/NM structures. Notably, YIG/Ti bilayer shows negligible SP-FMR signal, while the YIG/Pt/Ti exhibits a stronger signal attributed to the OHE of Ti. Replacing Ti by Ru reveals similar phenomena, attributed to orbital and spin Hall effects combined. Surface conversion of spin-orbital into charge current is further investigated, particularly with NM layer covered by CuOx. Our measurements reveal substantial increases in SP-FMR and LSSE signals compared to the YIG/Pt(2) sample [2, 3].

[1] E. Santos, et al., Phys. Rev. Applied 19, 014069 (2023); [2] E. Santos, et al., Phys. Rev. B 109, 014420 (2024); [3] E. Santos, et al., ACS Appl. Nano. Mater. (2024), DOI: 10.1021/acsanm.4c00770.

Exploring the Frontier of Flat Band Materials: the case of Nb3SBr7

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Quantum materials, described by fundamental principles of quantum mechanics, are essential for advancements in various emerging technologies. In this context, flat band materials near the Fermi level represent a promising frontier due to their potential to exhibit unconventional superconductivity and correlated insulating states. In this sense, there is a great interest in uncovering the electronic and optical properties, including excitonic properties, of flat band materials, aiming to develop a deeper understanding of these materials. This will contribute to the development of new quantum devices and technological applications. This talk will focus on the electronic and optical properties of flat band materials, with a particular emphasis on Nb3SBr7. We will discuss the influence of excitonic properties. Furthermore, we will examine the effects of structural modifications, including both biaxial and uniaxial strain, on these properties. Through detailed electronic and optical characterizations, our research aims to provide new insights into how structural changes can alter the physical properties and functionalities of these materials. By advancing our understanding of flat band materials, we contribute to the broader field of quantum materials science, paving the way for innovative applications that leverage the exotic behaviors of these quantum systems.

Generation and detection of valley-polarized currents in transport experiments

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Abstract

Coherent control and detection of the valley degree of freedom is a cornerstone for valleytronics and valley-based quantum computation. However, accessing valley-coherent phenomena requires samples without short-range scattering. Recent fabrication advances on gated-defined graphene multilayer devices minimize the effects of inter-valley scattering. Consequently, a series of recent experiments reported control over valley-polarized states. In the first part of my talk, I will introduce a recent experimental effort to generate valley-polarized electric currents in bilayer graphene. We first show the suppression of intervalley scattering in gate-defined quantum point contacts via electron focusing experiments [1]. Then, we use the Fermi surface warping to spatially separate valley-polarized states and present a magnetically controlled source of valley-polarized currents [2]. In the second part of my talk, I will focus on detecting valley-polarized currents. Currently, most experimental efforts to probe valley polarization require an application of external fields and thus are invasive and indirect. To overcome these issues, we propose a gate-defined valley splitter [3]. This splitter works as both a source of valley-polarized current and a probe of valley polarization. We thus propose using this device to detect the valley polarization of quantum dot levels, and as a tool to probe valley-dependent order parameters in graphene multilayers.

References

[1] Josep Ingla-Aynés*, Antonio L. R. Manesco, Talieh S. Ghiasi, Serhii Volosheniuk, Kenji Watanabe, Takashi Taniguchi, and Herre S. J. van der Zant, Nano Lett. 2023, 23, 12, 5453–5459
[2] Josep Ingla-Aynés, Antonio L. R. Manesco, Talieh S. Ghiasi, Kenji Watanabe, Takashi Taniguchi, Herre S. J. van der Zant, arXiv:2310.15293 (preprint)
[3] Juan Daniel Torres Luna, Kostas Vilkelis, Antonio L. R. Manesco, arXiv:2405.00538 (preprint)

GROWTH OF HIGHLY MISMATCHED THIN FILMS AND HETEROSTRUCTURES

Wesley Fiorio Inoch[1], Hudson Alfredo Cardoso Silva[2], Leonarde do Nascmento Rodrigues[2], Clodoaldo Irineu Levartoski de Araújo[2], Sukarno Olavo Ferreira[2]

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This work reviews the growth and properties of II-VI compounds base on Cd, Te and Mn on Silicon(111) substrates using molecular beam epitaxy. The investigated samples were quantum dots, thin films and heterostructures which were characterized by high resolution x-ray diffraction (HR-XRD), high resolution transmission microscopy (HR-TEM), atomic force microscopy (AFM) and photoluminescence (PL). Despite the huge lattice mismatch of almost 19% between CdTe and Si, almost perfect, completely relaxed 3D islands are obtained and the mismatch is probably accommodated by a Tellurium interfacial layer. However, a dense defect network near substrate interface appears during coalescence and the resulting thin films show a surface roughness which depends on growth temperature and time. Using an additional source, more than 50% Mn can be incorporated in substitution of Cd, resulting in a ternary compound (Cd1-xMnxTe) and regardless the high density of interface defects and surface roughness observed in these films, CdMnTe/CdTe/CdMnTe heterostructures grown directly on Si(111) revealed very high PL efficiency. Bi2Te3 thin films grown on Si and GaAs, obtained by Van der Waals epitaxy were also investigated and exhibited very high structural perfection almost independent of the substrate used. Ultra-thin Bi2Te3 thin films grown on GaAs are characterized by HR-XRD, Raman, XPS and ARPES and show the expected surface states of the topological insulator.

We would like to thank the agencies FAPEMIG, CNPq and CAPES for the financial support of these studies by a series of research projects during the last 10 years.

Low carrier mobility next to thermal gate oxides in Silicon Carbide: What's wrong with SiC- MOSFET?

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We report about the combined theoretical and experimental analysis of the interface structure between silicon carbide (SiC) and silicon dioxide (SiO2). We obtain a deeper understanding of impurities, crystal-defects and carbon clusters as they emerge from the thermal oxidation process and affect the electronic performance of the MOS-channel.
Silicon carbide (SiC) a wide-bandgap semiconductor is the major enabling material for advanced high power and high temperature electronic applications. In contrast to the commercially available SiC Schottky rectifier technology, SiC power MOSFETs are still affected by low channel mobilities and threshold voltage instabilities due to the poor quality of the SiC/SiO2 interface. The reason for these defects can be attributed to the complicated oxidation process that necessitates the removal of carbon in the form of CO and CO2. This promotes different defects in SiC (dangling bonds, carbon clusters, near-interface traps, etc.) which modify the electronic properties of the inversion channel and deteriorate the field-effect mobility. Post-oxidation annealing in nitric oxide ambient comprised a breakthrough for improving the SiC MOS performance, but nevertheless the microscopic origin of the passivation mechanism is not yet fully understood. Therefore, we have used a combined “experiment and theory” approach to atomically resolve the structure of the SiC/SiO2 interface, with regard to the electronic structure in the interface-near region and its tunability which is crucial for building Field Effect Transistors in SiC.

Quantum computing with spins in silicon

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In the age of silicon, societal change is driven by compute power. Quantum computers have the potential to bring within reach problems that are currently simply impossible to solve, such as interactions in protein folding and simulations of molecules of modest size. But the technical complexity and necessary level of investment for such an unproven technology cast shadow on the future of quantum computers. In the hope of leveraging the existing transistor industrial capabilities, most qubit makers have retrofitted their technologies to become compatible with CMOS manufacturing, making concessions along the way. Spins are the only exception: they find in silicon their natural habitat and thrive in the materials used in the most advanced foundry nodes. We will show why this technology has significant practical advantages and what the current challenges are, with an emphasis on the scientific opportunities in semiconductor physics.

Quantum oscillations

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

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Topological Insulators (TIs) exhibiting the Quantum Spin Hall effect (QSHE) have emerged as promising candidates for next-generation electronic devices due to their unique electronic properties of an insulating bulk and helical edge channels [1-3]. For a potential usage in device applications, the TI needs to display certain characteristics such as a scalability and reproducibility, a robustness of the helical edge channels against temperature and a tuning possibility (e.g., with electric field). Despite many material systems were predicted to host the QSHE and showed some of these characteristics, none of them could exhibit all of them [1,2]. One prominent example are 2D TIs based on the InAs/GaSb material system. They profit from their compatibility with the semiconductor industry and major growth and processing technology developed. Moreover, the possible phase transition between a TI and normal insulating (NI) phase and the rather temperature-insensitive band ordering make this material system interesting for potential device applications. However, until now the helical edge channels were only demonstrated in the range of a few Kelvin [3]. Here, we present a TI based on an InAs/GaInSb/InAs trilayer quantum well (TQW) and discuss recent advance towards QSHE even at elevated temperatures.

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Raman response of the charge density wave in cuprate superconductors

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Since the 1980s, new superconducting materials, such as copper oxides (cuprates), have been discovered and present a critical temperature around an order of magnitude higher than that of conventional superconductors, being therefore interesting from a technological viewpoint. Despite all the efforts, the mechanism responsible for the unconventional superconductivity of these materials is not well understood. In cuprates, superconductivity appears to be governed by two-dimensional layers of CuO2, where the electrons interact strongly, while the other layers represent charge reservoirs.

In a recent work [Phys. Rev. B108, 165111 (2023)], we have studied the Raman response of the charge density wave (CDW) phase appearing in the underdoped region of cuprate superconductors. We have considered a phenomenological approach to describe the charge order in the CuO2 planes and have calculated the Raman response for both B1g and B2g light-polarization symmetries. Our results for the B2g Raman response show a general dip-hump behavior, which is independent of the system band structure. in sharp contrast with the behavior of the B1g response. This well accounts for the Raman experimental results. Next, we have included in our model another phase of the cuprate phase diagram, the pseudogap (PG) one. We conclude that the PG phase drives the doping dependence of the CDW energy scale, in agreement with experiments. This result is suggestive of the PG phase governing the different energy scales of the exotic phases that appear in the underdoped region of the cuprate phase diagram.

Scanning tunneling spectroscopy of 2D semiconductors and nanomembranes

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In this work we show how the Scanning Tunneling Spectroscopy (STS) technique became a crucial tool to explore the local density of states and electronic structure effects of two-dimensional materials and nanomembranes. Initially used as a derived tool from STM (Scanning Tunneling Microscopy), STS provided major results for the understanding of novel materials and turned out to be independent of the usual atomic resolution goals of the surface STM community. By discussing examples from distinct material classes we show how relevant information is extracted. The observation of Ferroelectricity in few-layer GeS [1], doping fluctuations in SnS2:GeS solar cells [2], Mg surface doping in GaAs nanowires [3] and confined states in InAs quantum dots embedded in GaAs nanomembranes [4] provide direct insight of the technique potential for the materials community. We emphasize how previous limitations in STS use have been overcome with appropriate sample preparation, expanding the use of ambient (non-UHV) STS as well as measurements in oxidized surface conditions.

We would like to thank the FAPEMIG funding agency.

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Shaking up topological crystals with chiral phonons

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The symmetries of crystals play an important role in the properties of their phonons. When the mirror symmetries are broken, the lattice ions can display circular motion with finite angular momentum. These modes, known as chiral phonons, have recently been demonstrated in both rotating and propagating lattice motions. Usually, phonons are insensitive to magnetic fields. On the contrary, chiral phonons carry magnetic moment and directly couple to magnetic fields.

In this talk, I will present a review of the recent progress on the study of chiral phonons using terahertz time-domain spectroscopy. Our contributions to this exciting new field will be highlighted [1-3]. In particular, I will show that the phonon magnetic moment is largely enhanced in topological materials. Furthermore, unpublished results will be discussed to provide future perspectives.

Our research was supported by FAPESP Grants No. 2015/16191-5 and 2018/06142-5, 2021/12470-8, 2023/04245-0, and CNPq Grants No. 307737/2020-9 and 409245/2022-4.

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Single quantum coherent spins in hexagonal boron nitride at ambient conditions

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Colour centres in wide bandgap materials can provide spin-photon interfaces that act as the building blocks in quantum networks and quantum sensing applications. Despite rapid progress reported across several candidate systems, those possessing quantum coherent single spins at room temperature remain extremely rare [1]. Here, we show that hexagonal boron nitride hosts single emitters that combine room-temperature spin coherence and single-photon emission with scalable and compact hardware. Via optical and microwave spectroscopy at room temperature, we investigate the ground-state spin Hamiltonian of these individual emitters. We identify a spin-triplet electronic ground state with zero-field coherences that survive up to microseconds at ambient conditions, and unravel how the symmetry of the spin-Hamiltonian protects the electronic spin from decoherence in the near-zero-field regime [2]. Our results demonstrate the rich spin dynamics underpinning this novel solid-state qubit platform and further reveal the potential of van der Waals materials for quantum information and sensing, where their reduced dimensionality opens exciting routes to new nanoscale quantum devices and sensors.

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Study of self- assembly structures of carbon quantum dots

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Self-assembly (SA) structures arise when discrete elements interact spontaneously with one another to form larger and more complex structures via self-organizing processes. Compared to disorderly systems, self-assembled nanoparticles with specialized functions can have improved or even unique features. One class of nanoparticles that have the ability to generate SAs is carbon quantum dots (Cdots). Cdots are semiconductor nanoparticles with a core/shell structure that exhibit remarkable optical properties, such as light stability, size-dependent energy, and intensity modulation upon particle aggregation. Hence, the organized arrangement of individual Cdots on solid substrates shows potential for the advancement of nanodevices that may act as data storage, sensors, catalysts, or optoelectronic components. In this presentation, I will give an overview of our main experimental findings [1], showing the diverse morphologies of self-assembled structures produced by the evaporation-induced self-assembly technique, using photoluminescent Cdots as the constituent components. We observed distinctive structures and patterns, including diffusion-limited aggregation, river-type and cross-type fractals, sticks, rods, and films, depending on the parameters employed. As I will discuss, we have found that the temperature at which evaporation occurs is a crucial factor that influences the patterns, optical and electric characteristics of SA structures. By employing characterization techniques including scanning electron microscopy, profilometry, and optical and fluorescence microscopy, we were able to discern distinct regimes of evaporation. These results indicate the possibility of controlling the morphology, optical, and electric properties of the SA structures based on Cdots, opening up potential for future applications.

This study was supported by FAPESC and CNPq.

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The polymorphous nature of halide perovskites

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Many halide perovskites exhibit a cubic crystal structure (Pm-3m) at elevated temperatures but transition to lower symmetry structures such as orthorhombic or tetragonal at lower temperatures. Recent theoretical findings have cast doubts upon the cubic structure, as it may exhibit negative phonon modes, unusual band gap trends, and incomplete alignment with PDF measurements. In this context, we propose the concept of polymorphous structures, suggesting that the cubic structure emerges as a result of temporal and spatial averaging of lower symmetry structures. To substantiate this idea, we will employ ab initio and molecular dynamics simulations.

Towards lasing from hexagonal SiGe heterostructures

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Silicon and germanium cannot emit light efficiently due to their indirect bandgap, hampering the development of Si-based photonics. However, alloys of SiGe in the hexagonal phase are predicted to have a direct band gap [1]. In this work, we grow hexagonal SiGe as shells on wurtzite GaAs and/or GaP template wires using the crystal structure transfer method [2]. Efficient light emission from hexagonal SiGe, up to room temperature, accompanied by a short radiative life time of around a nanosecond are shown, which are the hallmarks of a direct band gap material [3]. The band gap energy is tunable in the range of 0.35 till 0.7eV opening a plethora of new applications. One of our next goals is to demonstrate lasing from hexagonal SiGe. We do have first indications of amplified spontaneous emission (ASE) in non-optimized structures, and have revealed the limiting factors for obtaining lasing, among which the crystal quality is an important factor.
Next, we focus on the growth of hexagonal SiGe heterostructures, such as quantum wells (QWs). These QWs are essential to reduce the laser threshold. We study the growth of pure Ge and Si0.1Ge0.9 QWs embedded in Si-rich barrier material in detail as a function of the growth conditions and thickness/strain. We show that the emission energy increases with decreased thickness, indicating confinement of both the electrons and the holes in the QWs. The QWs show bright emission up to room temperature with a short radiative lifetime.

Acknowledgements
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Valley Zeeman physics in van der Waals matter

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The interplay of the spin and the orbital angular momenta of electrons, holes, and their correlated excitonic states, governs the observed Zeeman splitting, which is often described by effective g-factors. In van der Waals systems, transition metal dichalcogenides (TMDCs) host robust exciton features and are ideal candidates to explore the manifestation of coupled spin, valley, and orbital degrees of freedom under external magnetic fields. In this talk, I will cover the basic physics behind the valley Zeeman splitting and effective g-factors, emphasizing the recent first-principles developments in monolayer TMDCs that faithfully reproduce the available experimental data[1], offering robust predictive capabilities. These new theoretical insights demystify the valley Zeeman physics in TMDCs and firmly establish a connection to the vast existing knowledge in the area of III-V materials. Using this full ab initio approach, I will discuss how the spin-valley physics and exciton g-factors provide fundamental insight into the exciton physics in TMDC-based van der Waals matter. Particularly, I will focus on three different examples: (i) strain effects in monolayer TMDCs[2,3,4], (ii) the valley Zeeman splitting of dipolar excitons in MoSe_{2}/WSe_{2} under external electric field[5], and (iii) the proximity-enhanced valley Zeeman effects in WS2/graphene systems[6]. These selected examples demonstrate how the microscopic nuances of the valley Zeeman physics reveal elusive exciton phenomena in van der Waals matter that are particularly relevant to the fields of valleytronics, straintronics, and twistronics. [1] Woźniak, Faria Junior et al., PRB (Editors' Suggestion) 101, 235408 (2020). [2] Faria Junior et al., New J. Phys. 24, 083004 (2022). [3] Covre, Faria Junior et al., Nanoscale 14, 5758 (2022). [4] Blundo, Faria Junior et al., Phys. Rev. Lett. 129, 067402 (2022). [5] Faria Junior, Fabian, Nanomaterials 13, 1187 (2023). [6] Faria Junior et al., 2D Mater. 10, 03400 (2023).

TUTORIALS

Probing Electronic Structure of Quantum Materials with ARPES and Synchrotron Radiation at SAPÊ beamline in SIRIUS

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Quantum materials exhibit phenomena not seen in conventional materials and are at the forefront of next-generation technological innovations. Research into quantum materials drives advances in materials science and engineering, pushing the boundaries of material manipulation, fabrication, and characterization techniques. This opens new pathways for the design and creation of materials with tailored properties. Topological materials are examples of novel quantum states of matter that have topologically protected states, where electrons flow without resistance on the surface of a material. An important tool often used to probe such states is the angle-resolved photoemission spectroscopy technique (ARPES). ARPES probes the band structure of crystals using mainly VUV light which is absorbed by the electrons that are afterwards ejected from the surface of the material and detected by a spectrometer. Synchrotron radiation can be a very useful light source for such measurements. It can generate a continuous range of photon energies which allows to probe the 3D band structure of the solid and make possible to choose a photon energy that maximizes the photoemission signal tunning the higher possible cross-section.
In this presentation, I'm going to show the status of the brand-new beamline, SAPÊ (Angle-resolved PhotoEmission spectroscopy beamline) that is under construction at this very moment in the Brazilian Synchrotron Laboratory. It is a beamline dedicated to ARPES experiments in the Vacuum ultraviolet (VUV) photon energy range. I will also show some ARPES measurements performed, and the results published during the commissioning of the ARPES spectrometer at the old Brazilian Synchrotron machine.

Tutorial: Magnetic field effects on excitons in two dimensional semiconductors

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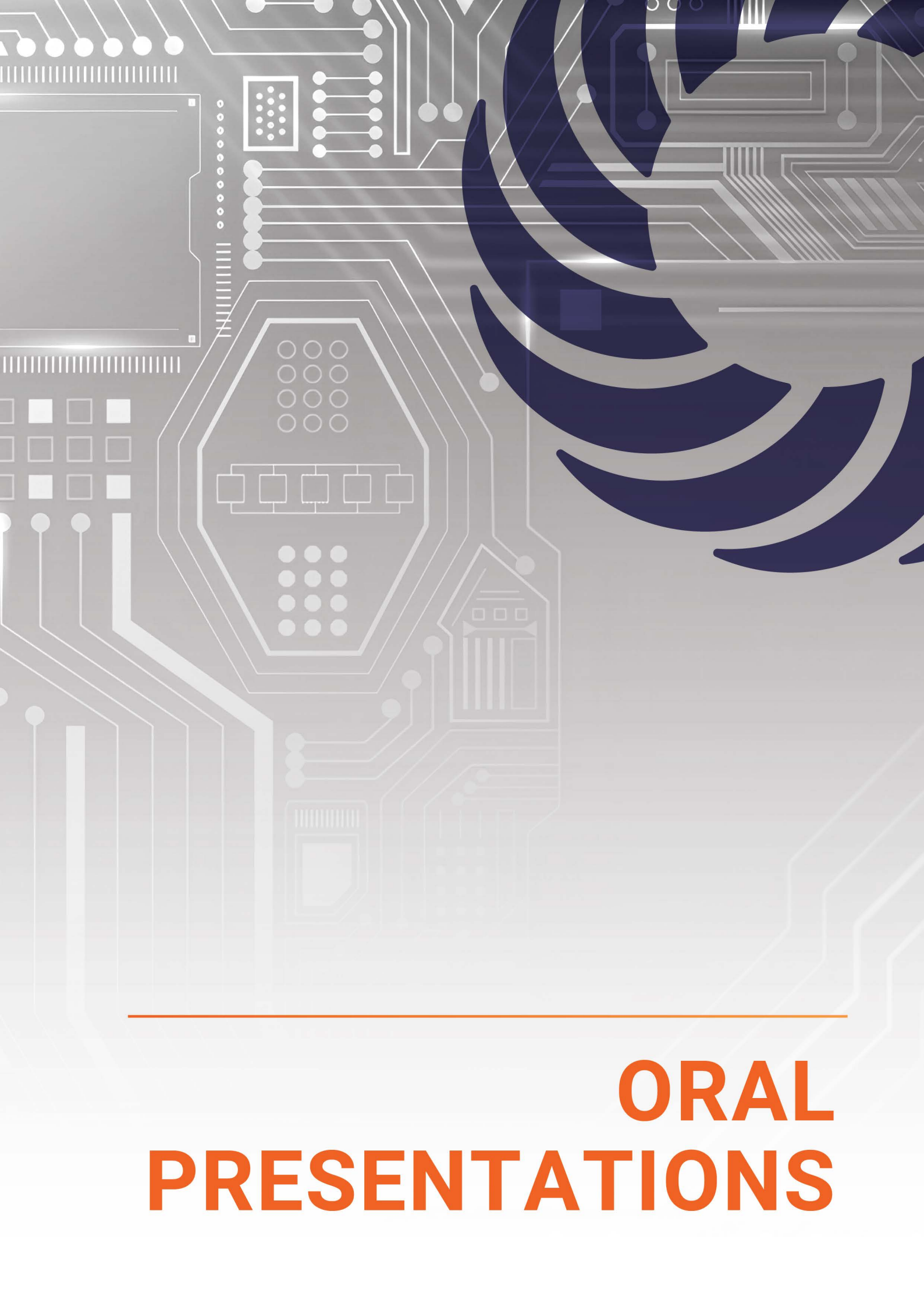
In this tutorial, I will provide an overview of current theoretical models for calculating excitonic states in monolayer semiconductors and van der Waals heterostructures, including those with lattice mismatch that produce moiré patterns. In this part, attendees will learn how to predict the energy of excitonic peaks and their Zeeman g-factors in the presence of a perpendicular magnetic field. This information will then be used in the second part of the tutorial, where I will discuss the use of magneto-photoluminescence (PL) measurements for a better understanding of the nature of excitonic peaks in two dimensional semiconductors and van der Waals heterostructures. Attendees will then learn how to use g-factors obtained in magneto-PL experiments to help unravel PL peaks in the spectra originating from different exciton states (inter- and intra-layer, free or moiré-confined).



ORAL PRESENTATIONS

A Coarse-Grained Geometric Approach to Identify Topological Phases in Three-Dimensions

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We present a novel real-space approach to classify topological states in (disordered) time-reversal symmetric systems [1]. Our framework reinterprets the underlying topological invariant through the lens of coarse geometry, providing a physically motivated setting. This approach offers several advantages: (a) Natural Bulk-Boundary Correspondence: The coarse geometry naturally captures the connection between the bulk properties and surface states, a hallmark of topological systems; (b) Agreement with Physical Knowledge: The framework reproduces established physical understanding of topological insulators, reinforcing its physical validity; (c) Efficient Numerical Calculations: It facilitates the development of efficient numerical methods for calculating topological invariants. The method works for both two (2D) and three-dimensions (3D), pristine and/or disordered topological insulators. It holds particular significance for studying disordered 3D systems, that lack other rigorous methods, and for which the method is computationally very efficient. We demonstrate the power of our approach by applying it to a tight-binding model of a 3D topological insulator. We successfully reproduce the known disorder-free phase diagram and analyze how the topological phase evolves under the influence of disorder. We believe that this new method paves the way for a deeper understanding of disorder effects in topological materials.

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Acoustic modulation of excitonic complexes in hBN/WSe2/hBN heterostructures

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Describing exciton dynamics in transition metal dichalcogenides (TMDs) multi-layer systems remain an area of active investigation gathering attention from the scientific community. TMD monolayers (1L) have already demonstrated their potential as a promising material class for optoelectronic applications, owing to circular-polarized optical selection rules and the existence of excitonic states even at room temperature due to strong Coulomb interaction [1]. Surface acoustic waves (SAWs) have proven to be an efficient means of transporting and manipulating excitonic states via a non-destructive propagating piezoelectric field at rates ranging from Mega to Giga Hertz, in a completely reversible manner [2]. In this study, we manipulate different excitonic complexes in a hBN/WSe2/hBN heterostructure using SAWs. We investigate the dynamics of each individual complex identified by photoluminescence optical power-law dependence, namely the neutral exciton (X0), neutral biexciton (XX0), intra- and intervalley trions (X-intra/inter), dark exciton (XD), and charged biexciton (XX-). We observe a fast response of the excitonic complexes to SAW piezoelectric field, owing to the large carrier mobility of the heterostructure. We also observe stronger interaction of trions with the SAW, moderate interaction of biexcitons, and weaker interaction of the neutral excitons. We attribute the different interaction strengths to a balance between the complex binding energy and its net charge. We examine the dynamic behavior of X0 at different temperatures, revealing reduced mobility as the temperature decreases, suggesting strong localization at 5K, in contrast to the other complexes. Finally, we find no changes in the emitted circular polarization of such complexes even for high acoustic powers, indicating that the SAW affects the spin dynamics of both K and K’ valleys equally.

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Characterization of metal halide perovskites at CARNAÚBA/SIRIUS

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Metal halide perovskite (MHP) received attention due to its optoelectronic properties appropriated to use in several applications, such as X-ray detectors, LEDs, and solar cells. Besides the high efficiency obtained in the last years, several aspects need to be better understood to lead this technology to maturity. In this context, X-ray microscopy plays an important role in allowing the characterization of the MHP in films or complete devices ex-situ, in situ, or operando conditions.[1] CARNAÚBA beamline at the LNLS is a nanoprobe multi-technique beamline that offers great opportunities for MHP characterization.[2] Here, the first scientific results on MHP obtained at CARNAÚBA will be presented. First, the damage caused by the high photon flux of the beamline was investigated. With a multi-technique approach using nano-X-ray fluorescence (nano-XRF), micro-FTIR, AFM, and micro-PL, we revealed the effect of the X-ray beam in the chemical, optical, and morphological properties of the $CsFAMAPb(Br,I)_3$ and proposed strategies to mitigate the damage. In safety conditions, nano-XRF maps reveal a homogenization of the halide distribution on the perovskite film using methylammonium as an additive.[3] The combination of the nano-XRF with X-ray excited optical luminescence (XEOL) also reveals the chemical heterogeneities in perovskites with wrinkles. We also developed a special photovoltaic setup for the operando characterization of perovskite solar cells. The setup allows precise control of the device temperature, atmosphere, illumination, and photovoltaic characterization simultaneously with X-ray characterization.

Acknowledgments: FAPESP (grants 2021/01357-6 and 2017/11986-5). DE-AC02-05CH1123. MicroFab/LNNano (20240713, 20230051, 20230010)

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Co-existence of surface electronic confinement and topological states in Sb4Te3

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Layered materials have attracted significant attention in recent years due to the diverse electronic properties arising from different structural variations. Here, we present Angle-Resolved Photoemission Spectroscopy measurements conducted on the topological material Sb4Te3. This material consists of a composite stacking of two distinct topological materials: the 3D topological insulator Sb2Te3 and the 2D topological insulator Sb2. Our Angle-Resolved Photoemission Spectroscopy measurements combined with density functional theory reveal that the topological behavior exhibited by Sb2Te3 and Sb2 persists, characterized by electronic states from the spin-orbit coupling, hexagonal warping associated with time-reversal symmetry and photon-energy independence in these surface states. By comparing results with the complete bulk and surface bands, we observe parabolic states associated with the existence of stacking faults. The photon-energy independence of this state indicates confinement along the stacking direction. In essence, we revealed the existence of topological states and confined electrons in the material Sb4Te3 using ARPES experiments.
This work was supported by the CNPEM, INCT Carbon Nanomaterials, and the Brazilian agencies Fapemig, CAPES, and CNPq.

Confinement and transport properties of moiré excitons in twisted van der Waals hetero-bilayers

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In the first part of the talk, I will analyze the characteristic dynamics of a moiré exciton wave packet and demonstrate that a rarely seen trembling motion of the exciton center-of-mass, also known as zitterbewegung, is expected as the inter-layer bias reaches a critical value, for which the gap in the moiré exciton band structure is closed. [1] Furthermore, I will explore the moiré exciton conductance quantization via a one-dimensional channel in twist MoS2/WSe2 hetero-bilayers, defining a quantum point contact. Results show a gate-control (device-dependent) and a spin–locked dependence of the moiré excitonic conductance plateaus. We also will show that wavepackets that populate all the regions of gap minima in the moiré superlattice exhibit an elliptic motion, even for zero exciton momentum and in the absence of external forces and/or fields. In the second part of the talk, I will demonstrate theoretically that quantum confinement dotlike and ringlike nanostructures can be electrostatically defined in twisted MoS2/WSe2 junctions by applying two position-dependent bias potentials, which, in turn, introduces an additional control in the moiré exciton trapping. The quantized moiré excitonic energy spectra and the wave functions obtained via the tight-binding model are compared with an analytical solution derived within the continuum model.

Acknowledgments
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Detection of Dirac fermions in crystalline topological insulators using magnetotransport measurements

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The detection of Dirac fermions in topological insulators via transport measurements represents a big challenge for experimentalists. The main reason is that the TIs are not really insulators but mostly highly degenerates narrow-gap semiconductors, which leads to a massive contribution from bulk states to electrical transport. The efforts are focused on separating the contribution from Bulk and topological surface states (TSS) that host the Dirac Fermions. For that, high magnetic fields and low temperatures allow the observation of Shubnikov-de Haas oscillations (SdH) from which valuable information about Fermi surface, effective masses and Berry phase can be extracted. Some years ago, a new class of materials called topological crystalline insulators (TCIs) were discovered, where the TSS are protected by crystal symmetries. Both TIs and TCIs are part of a wider group called quantum materials in which the quantum-mechanical effects fundamentally alter properties of the material leading to new states of condensed matter. The SnTe compound is classified as a TCI, due to its nontrivial electronic topology protected by crystalline symmetry, and it is a promising material for applications in spintronics and quantum computing. In this talk, the results of magnetotransport measurements performed nanostructures based on SnTe will be presented. The investigation will involve the analysis of Shubnikov-de Haas oscillations in SnTe nano-structures1, 2 providing a full description of the important parameters that characterize the electrical transport in these materials.

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Electrical Detection of Chirality in Twisted Bilayer Graphene

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A chiral entity is characterized by the inability to align its mirror image with itself. This fundamental characteristic is observed in twisted bilayer graphene (TBG) structures with opposite twist angles, as confirmed through optical dichroism experiments. Regarding electrical detection of chirality, various techniques are employed, spanning from non-local configurations to non-linear measurements. In this contribution [1], we shown that in the coherent regime a three lead setup is the minimum configuration to detect chirality in twisted bilayers. Specifically, with an in-plane magnetic field, the third lead behaves as a chirality probe, with opposite voltage changes for distinct enantiomers. Without breaking the time reversal symmetry, opposite twist angles manifest as opposite changes in current when the third lead is used as a layer discriminating current probe.

Acknowledgments

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Emergent Electromagnetism in Elemental Tellurium

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The miniaturisation of electronic building blocks is of uttermost importance. Efficient nanoscopic inductors and capacitors could pave the way to better energy economics and therewith more powerful processors. Topological materials which exhibit emergent electromagnetism are promising candidates for such future technologies. Due to its helical crystal structure and strong spin-orbit interaction, tellurium exhibits an experimentally verified internal inductance. By formulating the constitutive equations which describe electromagnetism in tellurium, we show how capacitive and inductive properties naturally emerge in the material. We demonstrate on the basis of AC-impedance measurements that elemental tellurium exhibits an unusually high virtual capacitance and inductance, far exceeding previously studied materials. The highest capacitance we detect in our samples is 130 mF and in one of our samples we measure an extremely impressive virtual inductance of 1.5 H. For low current densities a single piece of tellurium mimics the reactance of an RLC-circuit.

Growth and characterization of new 2D semiconductor materials

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Materials science in the nanoscale domain has become a reality for several applications, from integrated circuits, sensors, catalysts, medicines, and data-storage devices [1]. We achieved the ability to understand materials and, more importantly, command the materials' properties at the atomic level using precise synthesis and growth methods. Therefore, during the last decades, enormous efforts have been made to develop new processes for fabricating, characterizing, and manipulating materials in complex nanoarchitectures with atomic precision, making it possible to express emergent new chemical, electronic, photonic, magnetic, and structural properties. On-surface synthesis becomes a powerful bottom-up technique to fabricate such nanostructures using organic and organometallic precursors as molecular building blocks [1]. In this talk, I will present some strategies we have adopted to produce planar carbon lattice nanostructures, such as porous nanoribbons and doped graphene [3-4]. For a complete understanding of the atomic and electronic properties of the materials, we have combined scanning tunneling microscopy and spectroscopy (STM/STS), X-ray photoelectron spectroscopy (XPS), and numerical simulations based on density functional theory (DFT) calculations.

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Higher-order Fe-Fe exchange interactions in magnetically ordered 2D $Fe_{0.2}Ni_{0.8}$/Ni(001) and $Fe_{0.3}Ni_{0.7}$/Ni(001) alloy systems.

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We develop a theory to study the magnonic properties of the 2D ordered surface alloys $Fe_{0.2}Ni_{0.8}$/Ni(001) and $Fe_{0.3}Ni_{0.7}$ on a Ni(001) material substrate. The surface alloy nanostructures in stable equilibrium are determined by computing the lowest energy configurations of constitutive supercells of the ordered alloys. The magnetic exchange constants of the ground state of the stable systems are calculated to define their Heisenberg Hamiltonians using the DFT Spin-Polarized Relativistic Korringa-Kohn-Rostoker (SPRKKR) method [1] and considering Fe-Fe interactions up to third nearest neighbors. To determine the propagating exchange spin-wave modes, evanescent modes, and the consequent magnonic properties, the spin dynamics of the magnetic surface alloy nanostructures are solved using the phase field matching theory (PFMT) [2]. Our results indicate that the higher-order Fe-Fe exchange interactions are vital for accurately describing their magnonics. In particular, the exchange interactions influence the form of dispersion branches for the high-nergy spin-wave modes of $Fe_{0.2}Ni_{0.8}$/Ni(001) and $Fe_{0.3}Ni_{0.7}$/Ni(001). Appropriate Green's functions are also derived from the PFMT method to compute the local densities of states (LDOS) for the atomic sites at the surface boundary. For the c=0.2 surface alloy, the Fe-Fe exchange interactions shift the Fe LDOS peaks to lower frequency intervals. We also distinguish the emergence of remarkable LDOS peaks for the c=0.3 surface alloy at specific Ni sites. These peaks change positions under second and third-order Fe-Fe interactions, heralding new accessible spin-wave channels. Our results contribute to establishing a systematic understanding of the magnonics of the magnetic surface alloys of transition metal (TM) materials.

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III-Nitrides in the 2D structures and GaN/AlN 2D lateral interfaces: Structural and electronic properties from *ab initio* calculations

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It is well known that the III-Nitrides are the materials for the highly efficient light-emitting diodes, among other optoelectronic devices. Recently, the interest on these materials was renewed, now as a 2D material, when Tsipas and collaborators found that it is possible to grow hexagonal AlN nanolayers on surfaces of Ag (111) [1] and Al Balushi and colleagues found that hexagonal GaN can be obtained via encapsulation of graphene [2]. In the case of III-Nitrides, the structural and electronic properties for both zincblende and wurtzite structures were extensively studied, while their rocksalt and hexagonal closed-packed (hcp) form was not. Moreover, the experimentally observed 2D structures have the same shape of the well-studied BN monolayers. In this work, we report our theoretical results for the structural and electronic properties the hcp form of III-Nitrides, extending our study to the 2D structures of these materials and, finally, to the 2D GaN/AlN lateral interfaces. From our obtained results, we have found that the bulk hcp form of the III-Nitrides is a metastable state which undergoes to the rocksalt or wurtzite structure depending whether an applied pressure is present or not, respectively. However, going to the III-Nitrides 2D structures, the graphene-like structure is most stable one and their electronic structures show an indirect bandgap except for the InN, which has a direct bandgap of ~ 1.9 eV in good agreement with the published experimental data of Pécz *et al.* [3]. Finally, our evaluated electronic properties and band offsets for the 2D lateral GaN/AlN interfaces in both zig-zag and armchair configurations, our results indicate that, in the case of armchair form, the type II superlattices while in the zig-zag form, type I superlattices.

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Indirect Exchange and RKKY Interactions between Magnetic Impurities in Two- and Four-Band Weyl Systems

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Weyl semimetals (WSMs) have attracted significant attention due to their unique topological properties and distinct electronic structure [1]. The breaking of either time-reversal or inversion symmetries in WSMs leads to a separation of Dirac-like cones in the spectrum, resulting in the formation of pairs of chiral Weyl nodes located at different points in k-space. The presence of magnetic impurities in these systems gives rise to Ruderman-Kittel-Kasuya-Yosida (RKKY) and exchange interactions, which can mediated by both bulk Weyl fermions [2] as well as by electrons in surface states forming the so-called *Fermi arcs* [3]. As such, the RKKY interaction in WSMs is a multifaceted phenomenon, influenced by a variety of factors.

In this contribution, we derive analytical expressions for a specific class of systems that describe WSMs involving two and four bands, with up to four Weyl nodes. Going beyond the low-energy linear approximation and including the full band structure, our expressions reveal the emergence of both Heisenberg and Ising terms, as well as an additional Dzyaloshinsky-Moriya term in the absence of inversion symmetry. Moreover, our numerical calculations demonstrate a modulation of the typical RKKY oscillation pattern in different cases and how certain terms are *forbidden* by symmetries. More importantly, we highlight both qualitative and quantitative differences between calculations involving the full band structure and those restricted to the low-energy linear dispersion in the Weyl cones. This underscores the importance of going beyond the linear approximation to obtain accurate results.

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Madelung's approach for obtaining the hydrodynamic model of plasmon-polaritons in anisotropic systems

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A hydrodynamic model based on Madelung's formalism for a collective electronic motion in anisotropic materials was derived, including nonlocal contributions from the Thomas-Fermi quantum pressure and quantum effects from the Bohm potential. Analytical expressions for the magnetoplasmon dispersion and nonlocal optical conductivity were obtained. As a case study for anisotropic two-dimensional electron gas, we apply our model to electrons in the conduction band of monolayer phosphorene. Our hydrodynamic obtained plasmon dispersion results show a very good agreement with \textit{ab-initio} calculations. Our findings demonstrate that including nonlocal and quantum effects in the optical conductivity inhibits phosphorene to host hyperbolic surface plasmon-polaritons. Therefore, it is fundamental to go beyond the local approximation in those anisotropic systems that can support strongly confined plasmon-polaritons.

Navigating Dynamic Nonlinearities and Precision Challenges in the Characterization of Thin Semiconductor Systems

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When there is a variation in electrical output over time, and the response is influenced by both the input and the current state of the system at any given moment, the system is referred to as dynamic. Whether intentional or not, the nonlinear response of conductive materials or the nonlinear operation of electronic devices exhibits widespread properties. These effects can be caused, for example, by redox reactions at the surface of metamaterials, leaking currents in photo-diodes and solar cells, memristive effects in the conduction of semiconductor oxides, and electrochemical processes in thin films. We present the outcomes of our ongoing research efforts, aiming to elucidate the physical origins of these effects and provide a simple and unified theoretical interpretation for various experimental results. Impedance spectroscopy plays a crucial role in characterizing these materials and assessing the performance of electrochemical devices. It allows for real-time analysis of dynamic processes, such as electrode kinetics, electron, hole, or ion transport, and interfacial or defect-driven phenomena. However, the technique's sensitivity to experimental conditions introduces potential variability in results. The intricate interplay of transient effects in spectral impedance analyses adds a layer of complexity, hindering straightforward interpretations. This complexity requires a nuanced approach to refine analytical methodologies and ensure the accuracy of impedance characterization, particularly when dynamic contributions of non-equilibrium components cannot be separated from underlying steady-state characteristics. While inherent systematic errors set a practical limit (accuracy floor) on achievable measurement accuracy, this paper offers both qualitative and quantitative insights into how specific procedures impact this limit. Addressing these errors effectively is essential to surpassing this limitation.
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Novel aspects of Anderson localization: scaling invariance on topological Anderson insulators, and minimal model for the quantum boomerang effect

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Anderson localization, a cornerstone of condensed matter physics, continues to surprise us with counter-intuitive phenomena. This talk explores two recent findings in this field. First, we consider disorder-induced topological phase transitions that yield topological Anderson insulators [1]. Here, disorder plays a key role in renormalizing the band gap and creating topological phases. Our recent work [2] uses the disorder-averaged local Chern marker [3] as a smooth order parameter. This marker unveils a single-parameter scaling function that combines the Dirac mass M, disorder strength W, and system L into a single function, C(M, W, L) = C(z). We show that this scaling function exhibits critical parameters aligning with first-order Born approximation predictions. Second, we present preliminary findings on how electric fields influence the recently discovered quantum boomerang effect [4]. In the absence of an electric field, a wavepacket with initial velocity exhibits a boomerang-like motion in a disordered medium, returning to its origin after initial forward motion. This behavior defies our classical expectation of a finite shift. Our preliminary results for finite electric fields suggest a wavepacket split. Part follows a ballistic trajectory, while the remainder exhibits a boomerang-like return. The split ratio between these components depends on the wavepacket energy, disorder strength, and electric field intensity. Notably, the overall motion deviates from a Drude-like drift. We will discuss the characteristics of this dynamics, and possible extensions for future works.

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Novel Materials from non-van der Waals Solids

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The emergence of graphene created a revolution in materials science and renewed the interest in novel 2D materials. Until recently, due to their easy exfoliation from weak interlayer bonds, most 2D structures were derived from lamellar solids, known as van der Waals solids. However, it was demonstrated [1] that creating 2D materials from non-van der Waals solids is also possible. The first one, named hematene was extracted from hematite [1]. This discovery paved the way for exploring numerous other non-van der Waals solids, such as ilmenite, chromite, magnetite, and pyrite, among others [2]. Recent advancements have extended this exploration to include 2D structures derived from other families, including silicates [3.4]. In this study, we present and discuss the structural and electronic characteristics of these newly developed 2D materials from theoretical and experimental perspectives. Furthermore, we explore their potential applications, particularly in sensor technology and energy harvesting.

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Optical and magneto-optical properties of magnetic van der Waals heterostructures

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Two dimensional (2D) magnetic materials are promising systems for the next generation of spintronics/optospintronic devices. In recent years, there is increasing interest on the physical properties of CrSBr and $CrPS_4$ van der Waals (vdW) magnetic materials[1,2]. The $CrPS_4$ is an air-stable material with layer-dependent ferromagnetic (FM) order and out-of-plane spin orientation[1]. On the other hand, the bulk $CrPS_4$ has an antiferromagnetic ground state (A-type) formed by out-of-plane ferromagnetic monolayers with interlayer antiferromagnetic coupling along the ***c*** axis below the Néel temperature of T_N = 38 K [1]. CrSBr is also an air-stable material which has quasi-1D, semiconducting electronic structure and higher magnetic ordering temperature (Néel temperature, T_N = 132 K) [2,3]. Furthermore, CrSBr has strong coupling between its electronic and magnetic properties[2,3]. Interestingly, 2D magnetic materials can be stacked with monolayers of Group-VI transition metal dichalcogenide (TMDs) materials to form magnetic vdW heterostructures. Their physical properties are very sensitive to the number of layers, strain, twisted angles and magnetic proximity effects, which allows the effective control of their magnetic and optical properties for possible applications in spintronics and opto-spintronics. In this talk, I will present our recent studies on optical and magneto-optical properties of these systems. Particularly, we will focus our attention on the impact of twist angle, charge transfer and proximity effects on the physical properties of TMDs/CrSBr and TMD/$CrPS_4$ van der Waals heterostructures.

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Photoinduced Growth of Tellurium Nanosheets on a $Cd_{1-x}Mn_xTe$ matrix

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$Cd_{1-x}Mn_xTe$ (CMT) is a wide bandgap semiconductor that stands out among the ternary compounds in several industrial applications, such as optoelectronic and solar cell devices. Therefore, it is worth understanding the mechanisms of light interaction with CMT produced by growth techniques. In this work, we investigate the room temperature Raman scattering by longitudinal optical phonon modes CdTe-like (LO_1) and MnTe-like (LO_2) in CMT thin films grown on Si(111) by molecular-beam epitaxy. The well-known linear dependence of LO_1 and LO_2 frequencies on x is observed in Raman spectra when the excitation photon energy is above the bandgap energy. For the excitation energy near the fundamental gap of CMT, the resonance becomes evident in the Raman results. However, for a specific resonance condition due to tuning of the bandgap energy dependence on Mn concentration, the frequencies of the LO_1 and LO_2 phonon modes remain constant as the average manganese concentration increases to values $x \sim 0.30$. From photoluminescence spectroscopy investigations, we concluded that for Mn concentration above 0.3, a broad range of optical transitions provides the required conditions for a resonant Raman scattering selected by the incident photon energy. It introduces a resonant selectivity of regions where the incident excitation energy coincides with a bandgap energy associated with a specific value of *x*, even for samples with nominally different compositions. Finally, based on these previous results, we present a light wavelength-dependent photocrystallization effect of tellurium on the CMT surface. Acknowledgements: We are grateful for the support of Conselho Nacional de Desenvolvimento Científico e Tecnológico, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior, Fundação Arthur Bernardes, and Fundação de Amparo à Pesquisa do Estado de Minas Gerais. Appl. Phys. Lett. 123, 072103 (2023); J. Appl. Phys. 135, 025302 (2024); J. Alloys and Comp, 173830, 983 (2024).

Quantitative point defect density study in atomically-thin materials

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While point defects are atomically small, their significant impact on a material's properties becomes non-negligible in the 2D limit. In this work, we created atomically small defects by controlled irradiation in monolayer MoS_2 crystal. We investigate the optical signature of defects and vacancies via, respectively, Raman spectroscopy and scanning transmission electron microscopy (STEM). We observed that as the ion dose increases, the atomic vacancies merge and form nm-d holes. By using finite crystal length in the defective 2D crystal, the quality of crystal and the characteristic length is determined via STEM image analysis, and then the correlation of the optical signature and the defective structure was discussed. Beyond the creation and the quantification, we have also demonstrated a route to heal the ion irradiation caused atomic vacancy by annealing the defective MoS_2 in hydrogen disulfide atmosphere. The H_2S annealing reduced the defect density to 1/5, and 10% of photoluminescence signal is successfully recovered which was completely quenched by ion irradiation with dose of 2.50×10^{13} ion/cm^2. Finally, it will be briefly discussed how Raman spectroscopy was employed to determine point defect density in graphenic materials. Due to the competition between two double-resonance Raman (DRR) processes, their relative fractions exhibited a universal form against point defect density regardless of layer number, thus the ratio of the DRR bands dictates point defect density.

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Quantum Dots by Droplet Etching Epitaxy as sources of highly entangled photon pairs

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GaAs quantum dots (QDs) grown via the local droplet etching (LDE) method on GaAs (001) substrates emerged as a promising platform for the generation of single photons and entangled photon pairs [1]. Under optimized growth conditions GaAs QDs can be grown with small excitonic fine structure splitting (FSS) [2] enabling the possibility to obtain a near-unity degree of photon entanglement [3]. These dots have shown near-zero multi-photon emission probability under two-photon excitation and the highest two-photon interference visibility among photons emitted by two remote QDs . Using different combinations of barrier material and the filling amount of nanoholes, the QD emission color can be tuned in a range from ~700-810 nm with dot densities around 0.2 µm-2, ideally suited for single QD applications. In this work, we demonstrate the feasibility of extending the emission of QD up to 940 nm by selectively filling the nanoholes with InGaAs with varying concentrations.Compared to established Stranski-Krastanow (SK) InGaAs/GaAs QDs, our InGaAs QDs in AlGaAs can be easily grown with small FSS and low density, allowing (for example) an emission at the wavelength of the D2 transitions of Cs atoms (852nm), which is difficult to achieve with standard InGaAs/GaAs QDs. Moreover, these novel InGaAs dots exhibit a significant reduction in radiative lifetime when compared to SK QDs (from about 1 ns to about 300 ps). We anticipate that this reduction in the radiative lifetime will lead to significant improvement of the performance of InGaAs QDs as sources of polarization entangled photon pairs.

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Raman and Photoluminescence Spectroscopies of in-plane $MoSe_2$-MoS_2 Heterostructures grown by chemical vapor deposition

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Transition metal dichalcogenides (TMDs, such as MoS_2 and WSe_2) and the van der Waals (HS) heterostructures formed by them, either by vertical stacking or in-plane joining, have been widely studied in the last decade due to their physical and chemical characteristics, including strong excitonic effects and the possibility of understanding new phenomena and properties [1]. Lateral heterostructures present a question of scientific interest due to the atomic meeting of the crystal lattices of different TMDs [2], enabling the study of grain boundaries, for example, and also leading to applications in diodes for use in photoelectronics [3]. The heterostructures can be obtained using the chemical vapor deposition (CVD) method, since HS samples obtained by transfer methods present limitations for engineering applications, and the CVD method allows the control of several key parameters for growth, enabling certain changes in synthesis depending on the application required [4]. This work aims to study samples of lateral (in-plane) $MoSe_2$-MoS_2 heterostructures synthed by CVD using salt in a two-step process. These heterostructures were analyzed with Raman spectroscopy at different energies, including laser in the resonant range, and by photoluminescence, in order to understand what happens at the interface of the HS. We will also present some early work on the transport properties of such materials.

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Realistic effective-mass model for III-V Zincblend Semiconductors

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Electronic band structures can be realistically described using effective Hamiltonians, offering low computational cost compared to models using ab initio calculations [1, 2] . For decades, these Hamiltonians have been constructed using the k·p method, resulting in band structures that successfully describe spin-splittings, effective mass parameters and the g-factor of III-V semiconductors. At the Laboratório de Física Computacional (LFC, São Carlos Institute of Physics - USP) we developed a method that extracts parameters by fitting previously calculated band structures, using Löwdin partitioning and effective mass terms that go beyond zero order. Currently, the model that uses the symmetries of the system, is being tuned to allow a better modeling of the spin splittings energies, even applying constraints in the definition of the parameters that allow the correct description of spin orbit terms and also guaranteeing the correctness of signal of the effective massse masses [2] . Using a 14-band model, and non-symmetrical directions, the method allows a more realistic description of Zincblende-GaAs band structure agreeing with the DFT calculation up to 30% of the Brillouin Zone. In addition to an excellent fit, the results made it possible to determine parameters such as the effective mass, the g factor and the Luttinger and Kane parameters, with lower computational costs and in agreement those reported in the literature.

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Structure-driven phase transitions in paracrystalline topological insulators

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We study phase transitions driven by structural disorder in noncrystalline topological insulators. We introduce a procedural generation algorithm, the Perlin noise, typically used in computer graphics, to incorporate disorder to a two-dimensional lattice, allowing for a continuous interpolation between a pristine and a random lattice system, going through all different intermediate structural regimes, such as the paracrystalline and amorphous phases. We define a two-band model [1], including intraorbital and interorbital mixings, on the structures generated by the algorithm and we find a sequence of structure-driven topological phase transitions characterized by changes in the topological Bott index at which the insulating gap dynamically closes while evolving from the Bragg planes of the Brillouin zone towards the center. We interpret our results within the framework of Hosemann's paracrystal theory, in which distortion is included in the lattice structure factor and renormalizes the band-splitting parameter [2].

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Suppressed Kondo screening in two-dimensional altermagnets

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Altermagnets are a class of collinear two- and three-dimensional antiferromagnets that display a large broken spin degeneracy, which have gained considerable attention recently[1]. In this work we have studied the Kondo effect of a spin-1/2 impurity coupled to a two-dimensional altermagnet host material. To acquire the low-temperature many-body Kondo physics of the coupled system, we have performed a numerical renormalization group (NRG) calculations that allows us to access the spectral properties of the system at zero temperature [2]. The impurity spectral function and the Kondo temperature were calculated for different set of parameters, including Rashba spin-orbit coupling (RSOC) and an external magnetic field [3]. Interestingly, in the RSOC and altermagnetic fields, the hybridization function is spin independent, despite the characteristic broken time-reversal symmetry (TRS) of the altermagnet host [4]. This is because the alternating sign of the spin splitting of the bands in the momentum space renders equal contributions for both spin components of the hybridization function. Our results demonstrate that, although the hybridization function is TR symmetric, the Kondo temperature is substantially suppressed by the altermagnet coupling. Moreover, we have investigated the effect of an external magnetic field applied in the altermagnet along different directions. Interestingly, we observe an important restraining of the Kondo peak which strongly depends on the direction of the field. This anisotropic effect is, however, masked if strong Zeeman splitting takes place at the impurity, as it shatter the Kondo-singlet state.

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Synthesis and ionic liquid functionalization of transition metal dichalcogenides

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Transition metal dichalcogenides (TMDs) with lamellar structures similar to that of graphite have received significant attention because some of them are semiconductors with sizable bandgaps and are naturally abundant. Bulk WS_2, for example, exhibits an indirect band gap of 1.2 eV, while single-layer WS_2 exhibits a direct band gap of 1.8 eV. In order to fully exploit this versatility, obtaining layers of these materials over large areas with the desired properties (in particular the number of monolayers composing the stack) is mandatory. Moreover, controlling the interaction of these materials with the environment is a crucial step in any envisaged application. In this context, i) synthesis of WS_2 layers and ii) MoS_2 functionalization were investigated. The most used technique to synthe TMDs is CVD (chemical vapor deposition) where both metal and S precursors are evaporated. An alternative WS_2 synthesis consists of sulfurize WO_3 films deposited on the target substrate. Thus, issues related to the W transport during the process are suppressed. In view of this scenario, we sulfurized sputtered WO_3 films on SiO_2/Si substrates. The influence of sulphur concentration in the gas phase as well as modifications induced in the WO_3 film by its annealing were investigated. Results evidenced that during a certain period, while sulfurization conditions are not efficient, WO_3 annealing induces morphological and structural modifications (mainly crystallization) which modify oxide's reactivity towards S. Concerning functionalization of TMD layers, MoS_2 was functionalized with ionic liquids, aiming at creating a protection layer from oxidizing species like water and oxygen. Results evidenced that Ionic liquid layers were efficient oxidizing barriers. Nevertheless, these layers also induce electronic modifications in the underlying TMD layer.

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Temperature dependent temporal coherence of metallic-nanoparticle-induced single-photon emitters in a WSe_2 monolayer

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In recent years, much research has been undertaken to investigate the suitability of two-dimensional materials to act as single-photon sources with high optical and quantum optical quality. Amongst them, transition-metal dichalcogenides, especially WSe_2, have been one of the subjects of intensive studies. Yet, their single-photon purity and photon indistinguishability remain the most significant challenges to compete with mature semiconducting systems such as self-assembled InGaAs quantum dots. In this work, we explore the emission properties of quantum emitters in a WSe_2 monolayer which are induced by metallic nanoparticles. Under quasi-resonant pulsed excitation, we verify clean single-photon emission with a $g^{(2)}(0) = 0.036 \pm 0.004$. Furthermore, we determine the temperature dependent coherence time via Michelson interferometry, where a value of (13.5 ± 1.0) ps is extracted for the zero-phonon line at 4 K, which reduces to (9 ± 2) ps at 8 K. Associated time-resolved photoluminescence experiments reveal a decrease of the decay time from (2.4 ± 0.1) ns to (0.42 ± 0.05) ns. This change in decay time is explained by a model which considers a Förster-type resonant energy transfer process which yields a strong temperature induced energy loss from the single-photon emitters to the nearby Ag nanoparticle.

Tuning band structure and optical properties by rolling up III-V heterostructures

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Optical resonators fabricated from rolled-up semiconductor membranes are potential candidates to be used in optoelectronics applications. Such structures are obtained by integrating optical emitters like quantum wells and quantum dots into a strained layer system, which is then released from its original substrate and forms a rolled-up micro- or nanotube by strain relaxation. Although the optical emission of the integrated structure can be easily controlled by the appropriate strain distribution of the rolled-up tubes, this engineering possibility has not been extensively utilized in the past. We recently showed that the strain state of the rolled-up tube can alter the selection rules of a rolled-up InGaAs quantum well by inverting the light-hole and heavy-hole energy levels inside the nanostructure.

We also investigated the systematic shift of other emitters, like partially capped and annealed InAs dots embedded into the tube wall, in the framework of a review article. Therefore, we carry out structural and optical characterization as well as band structure calculation to fully characterize their properties. We also calculate the expected strain distribution, which is entered into k•p calculations to predict the band structure of the flat, unrolled structure as well as the rolled-up tube. These calculations allow us to predict transition energies, which can be compared with our photoluminescence results. We can demonstrate that by changing the emission wavelength of the dots by systematically moving their position in the tube wall, we can change the strain experienced by changing the emission wavelength of the dots. We further demonstrate that it is important to determine the exact strain state of the tube to correctly understand the observed behavior of the emitters. The outcomes demonstrate an effective approach for adjusting the emission characteristics of a light emitter through passive techniques, based solely on geometry.

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Universal Machine Learning Interatomic Potentials? Challenges and Directions for Semiconductor Materials' Surfaces

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Machine learning interatomic potentials (MLIPs) are one of the main techniques in the materials science toolbox, able to bridge ab initio accuracy with the computational efficiency of classical force fields. This allows simulations ranging from atoms, molecules, and biosystems, to solid and bulk materials, surfaces, nanomaterials, and their interfaces and complex interactions. A recent class of advanced MLIPs, which use equivariant representations and deep graph neural networks, is known as universal models. These models are proposed as foundational models suitable for any system, covering most elements from the periodic table. Current universal MLIPs (UIPs) have been trained with the largest consistent dataset available nowadays. However, these are composed mostly of bulk materials' DFT calculations. In this presentation, we assess the universality of all openly available UIPs, namely MACE, CHGNet, and M3GNet, in a representative task of generalization: calculation of surface energies. We find that the out-of-the-box foundational models have significant shortcomings in this task, with errors correlated to the total energy of surface simulations, having an out-of-domain distance from the training dataset. Our results show that while UIPs are an efficient starting point for fine-tuning specialized models, we envision the potential of increasing the coverage of the materials space towards universal training datasets for MLIPs.

Reference: [1] arXiv:2403.04217 (2024): https://doi.org/10.48550/arXiv.2403.04217

Unlocking Quantum Materials through Synchrotron Techniques under Extreme Thermodynamic Conditions

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Many of today's most exciting and potentially useful materials display states of matter that seem to be explicable only by applying quantum mechanical models. This is perhaps unsurprising, as these materials can host a complex medley of ingredients that include many-body interactions between spins, electrons, and phonons. The ground states frequently exhibit cooperative properties such as superconductivity, charge or spin order, the Kondo effect, or exotic excitations such as Weyl or Majorana fermions. Besides the fundamental interest in understanding such materials, there is also the prospect of controlling their properties and putting them to use. Therefore, deciphering what causes quantum states of matter to form remains one of the most pressing challenges facing modern physics.

Research exploring the limits of thermodynamic parameters, such as pressure, temperature, and magnetic field, is a rapidly growing and fascinating discipline of science and technology that uncovers many truths and facts about nature that are not possible to observe under ambient conditions. In this talk, I will highlight how we can shed light on the building blocks of quantum materials by combining synchrotron techniques (x-ray absorption, diffraction, and scattering) with external pressure (hydrostatic and uniaxial), low temperature, and high magnetic field to enable a continuous, clean, and reversible tuning of quantum correlations. Our aim with this work is to drive materials through the critical region where the state of matter changes and inherently quantum effects dominate, in order to probe the electronic, magnetic, and structural properties as a function of lattice contraction. We will focus on materials that are on the verge of a phase instability with distinct crystalline structures and electronic behavior that display nontrivial topology.

X-ray photoemission spectroscopy at IPE beamline: from materials to devices

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Understanding the composition and electronic structure of semiconductors is fundamental for advancing various fields, from electronics to renewable energy. The IPE beamline at Sirius [1] offers a platform for exploring the near-surface composition and electronic configuration of materials through synchrotron-based spectroscopic techniques. The combination of X-ray photoemission and absorption spectroscopies provide details of the chemistry, energy levels, density of states and carrier dynamics of semiconductors, which are directly related to their electrical and optical properties. In this work we illustrate the power of advanced X-ray photoemission experiments with examples from recent research at IPE. First, we show how Resonant Photoemission (RPES) evidences the appearance of in-gap states and Ti3+ sites in the SrTiO3 single crystals self-doped with oxygen vacancies. Next, we exploit Resonant Auger spectroscopy (RAS) with the core-hole clock approach to probe the attosecond electron delocalization dynamics in thin films thiophene-based semiconductor polymers [2]. Furthermore, we will also show preliminary results of scanning microprobe XPS/XAS with a spatial resolution of few micrometers and discuss the prospects of performing in situ experiments on devices under operation. In summary, combining X-ray photoemission at IPE with optical spectroscopy and transport measurements, enable researchers to correlate structural, chemical, and electronic properties in semiconductors. This multidisciplinary approach enhances our understanding of semiconductor materials and might assist the development of novel devices with tailored functionalities and improved performance.

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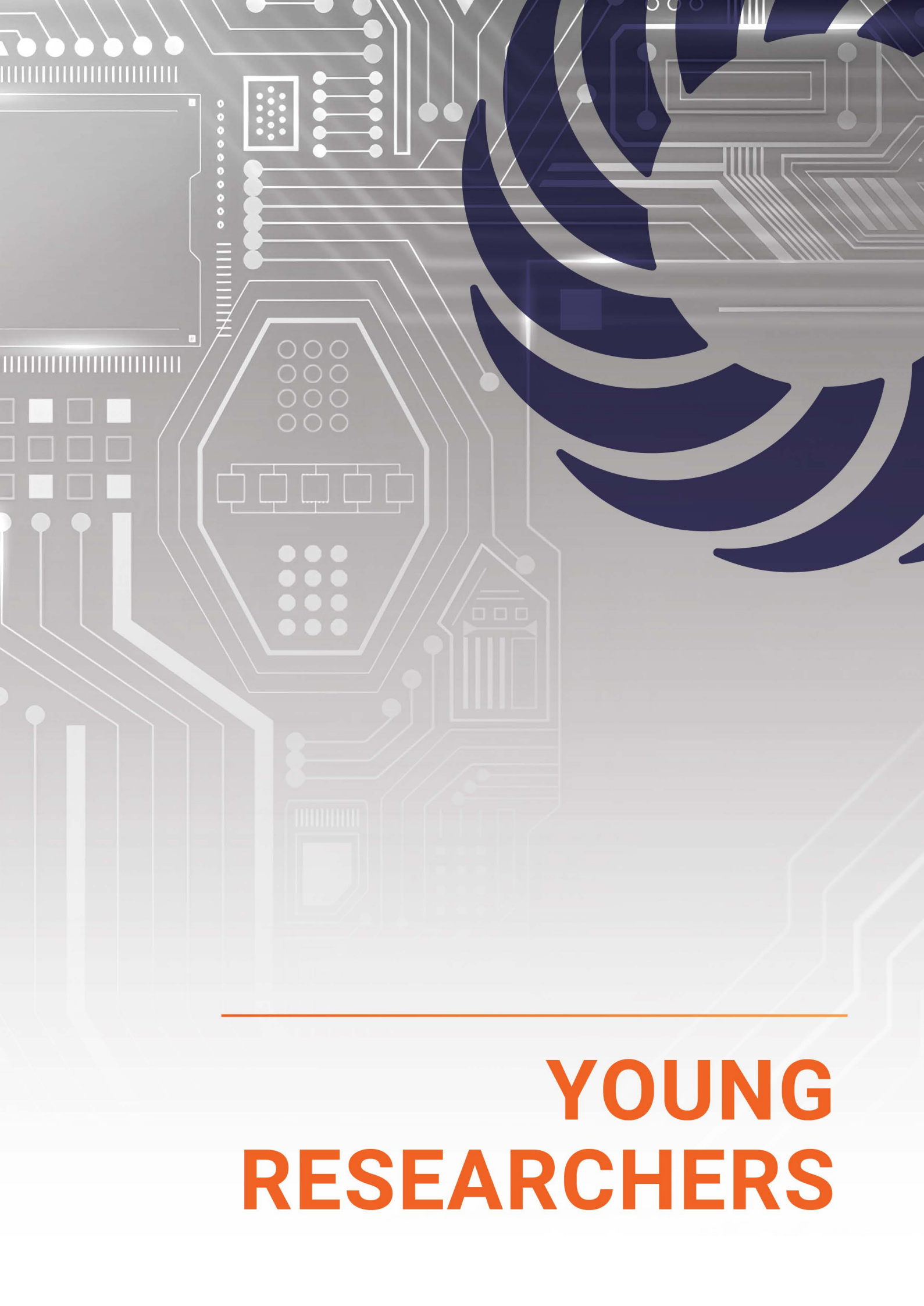

YOUNG RESEARCHERS

Charge dynamics in the 2D/3D semiconductor heterostructure WSe_2/GaAs

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Understanding the relaxation and recombination processes of excited states in two-dimensional (2D)/three-dimensional (3D) semiconductor heterojunctions is essential for developing efficient optical and (opto)electronic devices which integrate new 2D materials with more conventional 3D ones. In this work, we unveil the carrier dynamics and charge transfer in a monolayer of WSe₂ on a GaAs substrate. We use time-resolved differential reflectivity to study the charge relaxation processes involved in the junction and how they change when compared to an electrically decoupled heterostructure, WSe₂/hBN/GaAs. We observe that the monolayer in direct contact with the GaAs substrate presents longer optically-excited carrier lifetimes (3.5 ns) when compared with the hBN-isolated region (1 ns), consistent with a strong reduction of radiative decay and a fast charge transfer of a single polarity. Through low-temperature measurements, we find evidence of a type-II band alignment for this heterostructure with an exciton dissociation that accumulates electrons in the GaAs and holes in the WSe₂. The type-II band alignment and fast photo-excited carrier dissociation shown here indicate that WSe₂/GaAs is a promising junction for new photovoltaic and other optoelectronic devices, making use of the best properties of new (2D) and conventional (3D) semiconductors.
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Directional dependence of the electronic and transport properties of Biphenylene under strain conditions

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Recently, biphenylene (BPN), a novel carbon allotrope, has been successfully synthed using a bottom-up approach involving the lateral fusion of distinct polymeric chains. This synthesis process, known as HF-zipping, entails chemical reactions between pairs of hydrogen and fluorine, which facilitate the formation of C-C bonds between carbon atoms belonging to different chains. This unique chemical mechanism results in the creation of BPN, which possesses an intriguing crystal structure composed of octagonal, tetragonal, and hexagonal carbon rings. One notable characteristic of BPN is its anisotropic nature, as evidenced by the distinct atomic arrangements along the x and y directions. This anisotropy, combined with its unique bonding characteristics, renders BPN a compelling material for further investigation and potential applications in various fields, such as catalysis, anodes for Ion-Lithium and Ion-Sodium Batteries, and other applications. In this work, we investigated the electronic and electronic transport properties of biphenylene (BPN) using first-principles density functional theory (DFT) calculations combined with the non-equilibrium Green's function (NEGF) formalism. We have focused on understanding the electronic properties of BPN, and the anisotropic behavior of electronic transport upon external strain. We found the emergence of electronic stripes (ESs) on the BPN surface and the formation of type-II Dirac cone near the Fermi level. In the sequence, the electronic transport results reveal that such ESs dictate the anisotropic behavior of the transmission function. Finally, we show that the tuning of the (anisotropic) electronic current, mediated by external mechanical strain, is ruled by the energy position of the lowest unoccupied states with wave-vectors perpedicular to the ESs.

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Evidence of Thickness-dependent Surface Induced Ferroelectricity in Few-layer Germanium Sulfide obtained via Scanning Tunneling Spectroscopy

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In this work, we study the surface in-plane ferroelectricity of GeS using Scanning Tunneling Microscopy/Spectroscopy (STM/STS). We obtained remarkable experimental STS evidence of thickness-dependent phenomena surface-induced ferroelectricity in germanium sulfide nano-flakes. We used vapor-phase deposition to synthe ultrathin nano-flakes on a highly oriented pyrolytic graphite substrate (HOPG). Nanostructures of variable thicknesses were studied using scanning tunneling microscopy and spectroscopy and the electronic structure was modeled using density functional theory (DFT) calculations. The tunneling current under forward and backward biases was altered by the thickness of the material. We observe a hysteresis pattern, which we attribute to a two-dimensional ferroelectric behavior, consistent with screening conditions of polarization charges. This effect increases as the number of layers is reduced.

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[1]Evidence of Thickness-dependent Surface Induced Ferroelectricity in Few-layer Germanium Sulfide obtained via Scanning Tunneling Spectroscopy
RR Barreto, TC Ribeiro, G Soares, DR Miquita, GAM Safar, EP Andrade, ... Nanoscale, 2024

FROM LAYERED MINERALS TO 2D MAGNETS - HOW SYNCHROTRON RADIATION CAN SAVE US IN UNDERSTANDING THE ORIGIN OF PROXIMITY EFFECTS

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Two-dimensional (2D) materials have been extensively explored in the fabrication of nanodevices based on van der Waals heterostructures (vdWHs) in which proximity effects can be one of the keys to controlling the system properties. Here, we will show that synchrotron techniques are crucial for an in-depth understanding of the origin of proximity effects, as they are powerful tools in characterizing the chemical composition and electronic structure of 2D materials.

We will begin by demonstrating that the synchrotron infrared nanospectroscopy (SINS) technique based on near-field interactions can provide broadband IR spectra of complex and heterogeneous layered minerals, enabling the analysis of their vibrational modes and retrieving of mineralogical phases [1]. We will show that X-ray fluorescence (XRF) and X-ray absorption near edge structure (XANES) using a synchrotron X-ray nanoprobe are powerful techniques capable of identifying and mapping even trace impurities at the ultrathin limit of layered minerals, also providing the oxidation state and coordination of impurities [2,3].

Proximity effects can arise from impurities, but also from intrinsic properties of a material, as is the case of vdWHs based on 2D magnetic materials. In this sense, we will present how we can access the electronic structure of Cr-based 2D magnetic materials with orbital and element selectivity through resonant inelastic X-ray scattering (RIXS) spectroscopy. We will show that RIXS can reveal changes in the electronic structure and local coordination environment of Cr atoms depending on temperature and polarization that can influence proximity effects.

Acknowledgments

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Hydrodynamic of electron-hole fluid in a mesoscopic GaAs channel

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A manifestation of the hydrodynamic nature is the Venturi effect, where fluid velocity increases as the fluid flows through the constricted section of the pipe. This is a direct consequence of the mass continuity principle and is a key hydrodynamic characteristic observed in electron systems. The dynamics of the diffusion flow of holes photoinjected into a mesoscopic GaAs channel of variable width, where they, together with background electrons, form a hydrodynamic electron-hole fluid, is studied using time-resolved microphotoluminescence. The sample used in this work is a mesoscopic channel of variable width, fabricated based on a single 46 nm thick GaAs quantum well (QW). The hydrodynamic properties were studied using time-resolved photoluminescence (TRPL) microscopy at 4 K and 25 K. The PL transients measured along the channel sections of various widths showed a monoexponential decay, corresponding to the recombination time of heavy holes with background electrons. The recombination time decreased with decreasing channel width, indicative of increased diffusion velocity as predicted by the Venturi effect. The hydrodynamic features of the electron-hole fluid, such as the Venturi effect and the parabolic Hagen-Poiseuille velocity profile are demonstrated. The observed decrease in the recombination time with increasing temperature is unusual and indicates the viscous nature of the investigated electron-hole fluid. A magnetic field induced suppression of viscosity is observed. The presented results manifest to the fundamental role of viscosity in the hydrodynamic flow of an electron-hole fluid in the GaAs mesoscopic channel.

Acknowledgments

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Magneto-optical manipulation of the excitonic complexes in WSe2/CrSBr heterostructures

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Transition metal dichalcogenides (TMDs) are interesting two-dimensional (2D) materials to explore fundamental physics and for device applications. While bulk-TMDs are indirect gap semiconductors, monolayer (ML-) TMDs exhibit direct band gap with strong emission and large exciton binding energy. Recently, other materials, such as van der Waals (vdW) magnetic materials have also attracted important attention, because of their magnetic properties and promising applications in spintronics and quantum technology. 2D magnetic materials can also be combined with ML-TMDs resulting in magnetic van der Waals heterostructures (vdWHs). These vdWHs offer great opportunities for engineering valley properties. In this work, we have performed low temperature photoluminescence (PL) and magneto-PL measurements up to 9T in ML-WSe2/CrSBr heterostructures. We investigated the impact of a bulk-CrSBr, a direct gap semicondutor and A-type antiferromagnetic, on the valley properties of ML-WSe2/CrSBr heterostructures samples. The PL spectrum of the sample reveals different emission peaks such as exciton, trion and several localized dark exciton peaks and a broad defect band. These emission peaks show different behavior with increasing magnetic field and an important influence of the magnetic order of CrSBr. Furthermore, our results indicate that the sample has a broken-gap (type-III) band alignment resulting in an efficient charge transfer process which is sensitive to the magnetic order of CrSBr. In general, our results are explained by the interplay between magnetic proximity interactions and magnetic field dependence of charge transfer in ML-WSe2/CrSBr. Our work suggests that vdWHs with antiferromagnetic-nonmagnetic interfaces are interesting platform to modify the valley properties of TMDs for possible applications in spintronics [1].

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Magneto-optical properties of TMD monolayers induced by defects

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The investigation of defects in two-dimensional (2D) transition metal dichalcogenides (TMDs) has attracted a great attention both for the improvement of growth methods and for tuning their properties to expand their functionalities. For instance, this defect engineering achieved dilute magnetic semiconductors (DMS) by the incorporation of transition metal atoms as substitutional defects in TMD monolayers. It has been recently reported a long-range ferromagnetic ordering even above room temperature in vanadium doped WS2 and WSe2 samples, opening large possibilities for spintronic devices fabrication. Therefore, the optical and electronic characterization of these V doped TMDs become fundamental for future applications. In addition, the optical properties of these doped samples might couple with their magnetic responses, which can be probed boy magneto-optical experiments. Here we present a broadband optical and electronic structure characterizarion of V-doped WS2 monolayers [1] as well as magneto-optical investigations in aged [2] and V-doped WS2 and WSe2 monolayers.

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Many-body effects on the quasiparticle band structure and optical response of single-layer penta-NiN_2

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We present a detailed first-principles study on the optoelectronic properties of the single-layer nickel diazenide (penta-NiN2), a pentagon-based 2D semiconductor with ideal Cairo tessellation, whose bulk counterpart has been recently synthesized. We carry out *ab initio* calculations based on many-body perturbation theory, within the *GW*-BSE formalism, to address the quasiparticle band structure and excitonic effects on the optical absorption spectrum of monolayer penta-NiN2. Our results reveal a quasiparticle band gap of 1.05 eV employing the eigenvalue self-consistent *GW* approach, corroborating its potential in optoelectronics. In addition, its band gap exhibits an anomalous negative dependence on temperature, verified through its pressure coefficient. The acoustic phonon-limited scattering analysis indicates ultra-high hole mobility of ~$87x10^4$ $cm^2V^{-1}s^{-1}$. The most prominent absorption peak of monolayer penta-NiN2 is associated with resonant excitons, corresponding to transitions from VBM to CBM+2, which is explained by analyzing the state symmetry of the bands. Hence, this novel pentagonal 2D semiconductor exhibits compelling and promising properties deserving deeper exploration in optoelectronics and high-speed devices

Multimodal Characterization of Metal Halide Perovskite Films: Correlating Microstructure, Chemical Composition, and Optoelectronic Properties

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This study investigates metal halide perovskite (MHP) materials through a multidimensional approach combining advanced techniques. Nano-fluorescence, photoluminescence (PL) and X-ray excited optical luminescence (XEOL) experiments reveal correlations between microstructure, chemical composition, and optoelectronic properties of Cs_xFA_{1-x}Pb(Br_{0.38}I_{0.62})₃ thin films. XEOL maps show variations in luminescence intensity and energy position correlated with the film's morphology, while PL spectra indicate redshifts in emission energy associated with increased Cs content. The observed shifts in PL, CL, and XEOL are attributed to gradients in fluorescence ratios across the film, influenced by halide composition and morphology. Cathodoluminescence (CL) mapping elucidates optical and structural characteristics, revealing distinct luminescent patterns correlated with the film's microstructure and halide compositions. Comparison between PL, XEOL, and CL techniques underscores disparities in penetration depth and spatial resolution, highlighting their importance for accurate interpretation. X-ray ptychography investigates the influence of incident photon energy on reconstruction outcomes and early-stage degradation processes. Lower energy acquisitions enhance contrast in grain boundaries, while higher energy provides clarity in micrometer morphology. Humid air measurements allow the observation of degradation features, suggesting water intercalation as an early degradation mechanism. This study offers comprehensive insights into the complex behavior of MHP materials, with valuable implications for applications and future research in the field of perovskite materials. The fluorescence ratio gradients across the film explain the observed shifts in PL, CL, and XEOL, providing deeper insights into the optical properties of MHP materials.ACKs: FMCS and MGDG acknowledge CNPq scholarships. RS acknowledges FAPESP (2021/01357-6). Author gratefully acknowledge CNPEM, Shell and ANP.

Noncentrosymmetric two-dimensional Weyl semimetals in porous Si/Ge structures

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In this work, we have investigated nonmagnetic Weyl semimetals (WSMs) in SiGe and Ge porous layered structures. We performed the simulations based on first-principles calculations, using density functional theory (DFT) within the generalized gradient approximation (GGA), and tight-binding method. In both SiGe and Ge atomic configurations, the porous layered structures show a buckling degree with P_6 and P_{622} space group symmetries, respectively. The band structure without spin-orbit coupling (SOC), in both cases, are double degenerated with interesting Dirac-like crossings fourfold degenerated. The SOC split up the degeneracy resulting in pairs of nondegenerate bands crossing each other at two specific points, typically of WSMs. Since the systems are noncentrosymmetric but protected by time-reversal symmetry, they satisfy a requirement for a nonvanishing Berry curvature. The topological character of these crossings was confirmed by 2D Weyl chirality calculation. We verified the formation of six pairs of Weyl nodes at the Brillouin zone for both systems, they are protected by crystal symmetry, as required for 2D WSMs. The bulk-boundary correspondence was studied by the band structure of a nanoribbon and it was noted topological edge bands that connects Weyl points with opposite chiralities, the Fermi arcs.

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Organic Semiconductors as Handles for Optical Tweezers Experiments: Trapping and Manipulating Polyaniline (PANI) Microparticles

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Polyaniline (PANI) is a well-known semiconductor polymer that can change its conductive characteristics by doping and dedoping processes using acidic and basic solutions, respectively. These characteristics allow these polymers to be applied in electronic and optical equipment. To improving the PANI polymer's applicability and efficiency is the production of particles. These structures occurs by adding amphiphilic molecules (stabilizers) such as surfactants and polymers during the aniline polymerization, generating different morphologies as the final product. In this work, our objective was to produce PANI particles using the polymer Poly(vinyl pyrrolidone) (PVP) as a stabilizer and analyze the characteristics of these particles in optical tweezer measurements compared to inorganic semiconductor particles. Using the Dynamic Light Scattering (DLS) technique, it was possible to note that the hydrodynamic radius of the particles varies with pH, showing that when the polymer has a charge, the tendency is for the particles to have a smaller. The scanning electron microscopy technique allowed us to evaluate whether the particles produced are spherical and not amorphous. The results of Raman spectroscopy confirmed the presence of PANI and PVP in the particles. Finally, characterization using optical tweezers showed that the absorption in PANI particles changes with laser power. It is possible to note that the particles do not follow the linear optics for small sizes; however, the behavior of the results was similar to that of the theoretical model for semiconductor inorganic particles.

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Phase transitions and scale invariance in topological Anderson insulators

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Topological Anderson Insulators (TAIs) have garnered significant attention from the condensed matter and material science communities due to their disorder-driven transitions between trivial and topological insulator (TI) phases [1–3]. In our research [4], we delve into these transitions within two-dimensional (2D) systems, focusing on the BHZ model with Anderson disorder, while other standard 2DTI models exhibit similar characteristics. Our simulations indicate that the disorder-driven transitions from trivial to topological insulator phases can be effectively characterized by C_0, the disorder-averaged local Chern marker near the central cell of the system. We show that C_0 follows a single-parameter scaling, expressed as $C_0(M, W, L) \equiv C_0(z)$, where $z = [W^{\mu} - W_c^{\mu}(M)]L$, with M representing the Dirac mass, W denoting the disorder strength and L the system. Here, $W_c(M) \propto \sqrt{M}$ and $\mu \approx 2$ denote the critical disorder strength and critical exponent, respectively. Our numerical findings align well with theoretical predictions based on a first-order Born approximation (1BA) analysis. These observations lead us to speculate that the universal scaling function we have found is rather general for amorphous and disorder-driven topological phase transitions.

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Terahertz spectroscopy applications: unveiling carrier and lattice dynamics of materials

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Terahertz (THz) spectroscopy is now widely used for studying a plethora of condensed matter systems. For instance, terahertz time-domain spectroscopy (THz-TDS) measurements [1] can be used in materials for investigating low-energy excitations, such as phonons and plasmons, through their complex permittivity spectra, thus connecting electrical and optical information. Ever since the successful implementation of a home-built THz-TDS setup in our laboratory [2], it has been a robust tool for unveiling both carrier and lattice physics of a growing collection of systems, with the possibility of exploring their dependencies with variant conditions such as temperature and polarization. In this presentation, we overview the recent results achieved in our lab, showing insightful information on the prospect for investigating semiconductors, minerals, topological insulators, and other thin films [3]. This work is supported by the São Paulo Research Foundation (FAPESP), Grants No. 2018/06142-5, 2021/12470-8, 2023/04245-0, and 2023/11158-6.

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POSTERS

Air Stability and Optical Properties of Hafnium Diselenide ($HfSe_2$)

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Two-dimensional (2D) materials are composed of a single atomic layer and therefore have distinct properties compared to their three-dimensional counterparts. Given this versatility, they can be stacked to form van der Waals heterostructures [1], combining various useful properties for nanocomposites, electronic devices, and solar cells. Among 2D materials, transition metal dichalcogenides (TMDs) stand out for their semiconducting properties, making them ideal for constructing transistors and other electronic devices. TMDs have the general formula MX_2, where M is a transition metal (such as molybdenum, tungsten, hafnium, etc.) and X is a chalcogen (such as selenium, sulfur, tellurium, etc.), and generally exhibit good stability due to the strong covalent bonds between their atoms [2]. Most research in this group of materials focuses on the optical properties of transition metal disulfides (MoS_2, WS_2) and diselenides ($MoSe_2$, WSe_2), neglecting other dichalcogenides, particularly those based on hafnium. Although Hf-based TMDs possess strong absorption in the visible range, high carrier mobility, flexibility, and mechanical robustness, making them suitable for the fabrication of photodetectors and flexible, wearable devices, they degrade under ambient humidity and temperature conditions. Therefore, in this work, a systematic study of the aging process, which results in the formation of spherical structures on the material's surface, was conducted. To this end, we monitored the aging of Hafnium diselenide ($HfSe_2$), the formation of oxides on the surface, and their consequences on optical properties using atomic force microscopy, Raman spectroscopy, and photoluminescence techniques.

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A Kinetic Study on the Laser-Induced Phase Reconstruction and Segregation in CsPbBr3-xIx Nanocrystal Thin Films

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The study of inorganic metal-halide perovskite materials has attracted the interestdue to its low cost and high efficiencies that qualify it for application in high-tech optoelectronic and energy-storage devices, such as light-emitting devices (LED), solar cells and photodetectors. However, the kinetics of ion migration for mixed-halide perovskites of colloidal nanocrystals (NCs) thin films still is not wholly understood. Thus, herein, we combined hyperspectral fluorescence microspectroscopy and computational methods to understand the underlying mechanism of the phase reconstruction and segregation in CsPbBr3-xIx ($0 < x < 3$) thin films. Our outcomes have shown that samples with $x = 1.0$ and $x = 1.5$ exhibits a halide migration favoring Br enrichment locally, in which the photoluminescence peak at 545 nm (from CsPbBr2I) decreases, while a PL band arises at 510 nm, characteristic of the emission of CsPbBr3 nanocrystals. In this case, the laser-induced photothermal effect promotes the expulsion of I- from the perovskite lattice. Thus, thermodynamic parameters such as activation energy and carriers diffusion length were obtained by combining the kinetic parameters from the linear unmixing data, method to compute the halide (Br and I) kinetic separately, and laser-induced temperature calculated using the finite-difference method. On the other hand, for the sample $x = 2.0$, the phase segregation takes place and I- ions diffuse to the nanocrystal core, promoting a red-shift in the PL spectrum. We show that depending on the laser power employed, the threshold for the phase segregation changes.

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Analysis of GaAs for detection of heavy ions in Nuclear Physics

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The objective is to determine the response of Gallium Arsenide (GaAs) cells under the incidence of alpha particles and mostly under heavy-ion radiation. Their characterization will allow for behavioral predictions in high-radiation environments, raising the possibility of using these devices as efficient radiation detectors. A study on the effects of radiation in semiconductor devices was conducted with simulations of range, energy deposition, and damage using SRIM (Stopping and Range of Ions in Matter) in order to calculate the ideal conditions to perform such experiments. Schottky-barrier detectors were produced, one based on n-doped GaAs:Si with a Si concentration of 10^{18} cm^{-3}, and another based on undoped GaAs. The devices were fabricated with a NiGeAu ohmic contact on one side and a Ti/Pt/Au Schottky contact on the other side. Initially, only the undoped device was irradiated with ^{16}O ions having an energy of 45 MeV, ^{28}Si ions having an energy of 53 and 76 MeV, and ^{63}Cu ions having na energy of 83 MeV. The experiments were performed under reverse bias of 30 V and 60 V, and the range and deposition for these conditions were simulated. For a given ion, the induced charge was measured, and the charge-collection time was estimated to be 3–5 ns. New experiments to be carried out soon with other ions and energies will allow a better understanding of the intrinsic characteristics of that semiconductor—as carrier mobility and saturation velocity—and, moreover, its degradation. Afterward, the ECORCE—a TCAD model software—will be used to simulate the physical parameters of the device and evaluate the possibility of using InAs quantum dots in such GaAs-based detectors and the influence of these nanostructures on the response under heavy-ion incidence.

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An innovative light collection device for a Low Temperature Scanning Tunneling Microscope

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The scanning tunneling microscope (STM) is a powerful surface science tool able to image the density of states with atomic spatial resolution and also to trigger local luminescence of materials. Beyond measuring the local density of states (LDOS), within STM, the local tunneling currents can act as local excitation sources, inducing light emission in materials through a combination of elastic and inelastic processes.
Our work introduces an innovative light collection/injection system tailored for low-temperature STM environments. We designed an off-axis parabolic mirror collector which meticulously follows the Étendue conservation principle to achieve an impressive 72% collection efficiency.[1,2] This efficiency ensures optimal light collection while preserving spectral resolution and minimizing signal loss, thereby enabling a wide range of optical experiments within the STM framework.
The performance of our system is validated through atomically resolved imaging and scanning tunneling spectroscopy (STS) on standard sample surfaces. The light injection and collection device was used already in several scientific cases and materials including h-BN, WSe_2, metallic surfaces and quantum dots. Some selected results will be shown.

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Anisotropic optical response of gold-silver alloys

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Gold and silver alloys enable novel opportunities for engineering materials with distinct optical responses. Here we investigate the optical properties of gold and silver (Ag_xAu_{1-x}) structures using First-Principle Density Functional Theory (DFT) for gold concentrations varying from 0% up to 100% with steps of 25%. Results of the optical permittivity are analyzed with the independent particle approximation and compared with previously reported theoretical and experimental works. The pure systems and the ones with unbalanced concentrations exhibit isotropic optical responses. The $Ag_{0.50}Au_{0.50}$ shows an anisotropic response among the y direction and the xz-direction, mainly in the intraband transition energy range. The anisotropy is elucidated in terms of the d-orbitals density of states and the charge distribution with the structure. The anisotropic optical response can be the origin of the discrepancies among reported experimental results for structures with the same stoichiometry.

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Anisotropic transport properties in black phosphorus-based three-terminal ballistic junctions

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Phosphorene sheets can be tailored to produce phosphorene nanoribbons (PNRs) with conventional or skewed zigzag and armchair edges. In this work, we investigate the transport properties of electrons through three-terminal ballistic junctions based on PNRs with different edges in the presence of a perpendicular electric field (PEF) applied to one of the system's branches. The effect of a PEF is to tune the band gap in the band structure, resulting in a modulation of the transmission between the input lead and one of the two output leads. The electronic properties of the structure are studied by tight-binding calculations within the Landauer-Buttiker formalism. The results show that the electric field could modulate the current through the input lead and the two output leads because of matching/mismatching between the energy bands of nanoribbon junctions with different edges. Furthermore, the transport properties in this system are strongly anisotropic depending on the direction in which the nanoribbons are produced. The results provide significant physical insights and a theoretical basis for designing electronic devices based on phosphorene junctions.

Artificial Intelligence in Electron Microscopy Images: Segmentation for Atomic-resolution Analysis

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Electron microscopy is a cornerstone in the nanomaterials field, providing unparalleled resolution for analyzing atomic structures, s, compositions, and interactions [1]. Despite its significant contributions, the vast data generated by electron microscopy often remains underexplored due to the sheer volume and limited time available for manual analysis [2]. Here we illustrate the application of machine learning (ML), specifically deep learning models, to enhance image segmentation and atomic identification, addressing these challenges effectively. We employed advanced ML techniques to process microscopy images, enabling the identification of atomic positions with high precision and uncovering details about defects and other parameters that were previously unattainable. This enables to analyze large datasets rapidly and detect subtle patterns, that may be missed by human observers, therefore bridging the knowledge between experiments and theory in physics. We validate our methodology with multiple datasets, including simulated graphene images created via simulations using python, a simulated MoS2 dataset [3], and experimental Y2O3 and MoS2 datasets obtained at the Brazilian Nanotechnology National Laboratory (LNNano). The diversity of these datasets shows the robustness and versatility of the ML approach in handling various materials and imaging conditions. We demonstrate that integrating ML and microscopy is a powerful tool for enhancing the interpretation of electron microscopy images, accelerating the data analysis process, and providing deeper insights into atomic-scale phenomena, contributing to the advancement of both experimental and theoretical physics.

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Assessing frustration in electronic kagome nanoribbons under strain

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Kagome Antiferromagnets (KAF) [1] are a prime example of frustrated [2] spin systems. The intricacies of their geometric configuration and frustrated spin arrangements have sparked debate about their ground state nature, including the possibility of a quantum spin liquid phase. This study explores the Hubbard model in the presence of a uniform magnetic field on a kagome ribbon subjected to uniform strain. Strain affects hopping parameters and lattice symmetries, modifying the couplings and sometimes even changing a Mott-insulating phase (relaxed system) [3] into a metallic one.

By means of a Tensor Networks platform [4], the density matrix renormalization group (DMRG) was used to investigate zero temperature magnetic properties. In the absence of deformation, the ground state exhibits spin correlations (SCs) that qualitatively resemble a quantum spin liquid (QSL). However, under substantial deformations, distinct correlation structures emerge, including "easy axes" along which free-moments and Néel-like chains coexist. The emergence and intensity of these arrangements can be controlled via strain, demonstrating a versatile approach to modifying correlations in a quantum system.

The system enables an assessment of different frustration measures. One measure, called "parametric frustration", indicates the onset of frustration based on the dispersion of couplings. To confirm its actual presence, a quantifier of "geometric frustration" is used, which depends on SCs and coupling strengths. Their relevance as indicators of distinct ground state phases is investigated via confrontation with DMRG data.

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A Tip Enhancement Photoluminescence Spectroscopy (TEPL) approach on single photon emitters

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Transition-Metal Dichalcogenides (TMDCs) exhibits exceptional photoluminescence when cleaved down to a monolayer[1]. Its spectrum is dominated by the complex excitonic behavior, including dynamics from both bright and dark excítons. When placed on a substrate with nanopillars, the 2D material becomes host of quantum single photon emitters (QSPEs) with sharp lines in cryogenic environment [2]. However, although the emission is localized, its origins are still not well understood. In this work, we develop an alternative way of producing these nanopillars, obtaining a stable organic structure that are also transparent, enabling back illuminated spectrography. We also perform cryogenic photoluminescence, obtaining a single photon emitter spectra with less than 1 nm linewidth that becomes absent when the temperature increases. Despite that, we carry out a Tip Enhanced Photoluminescence Spectroscopy in room temperature, which enabled us to navigate through out our 150 nm nanopillar and map the emissions with a 9 nm resolution, much beyond the diffraction limits of standard optical measurements. Surprisingly, an arising peak was observed on top of the pillar confined in a small region (~40nm) which we believe are associated with the hybridization of dark excítons with the bound excítons (defects level). This new emission are probably correlated to the single photons and could help understand its origins. Because of the amplified signal and nanometer resolution, our study presents a new way of approaching quantum confined excitons that are not observed in normal room temperature photoluminescence experiments.

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Atomic Composition's Impact on TMD Alloy Properties: Theoretical and Experimental Insights into $Mo_{1-x}W_xSe_2$

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The versatility of transition metal dichalcogenides (TMDs) is widely recognized due to the emergence of quantum confinement effects and strong interfacial interactions [1,2]. Compared to other functionalization approaches, the development of TMD alloys enables the continuous tuning of electronic bandgaps over a wide energy range [3]. This theoretical-experimental study aimed to investigate the influence of atomic composition on the modulation of structural, electronic, and optical properties of the 2D alloy $Mo_{1-x}W_xSe_2$. Nanofabrication using local anodic oxidation (by Atomic Force Microscopy - AFM) was employed to create monolayer islands in the 2D alloy $Mo_{1-x}W_xSe_2$, allowing the generation of controlled defects. 2D alloys $Mo_{1-x}W_xSe_2$ with different atomic compositions were extensively analyzed by AFM, optical microscopy, scanning electron microscopy, energy dispersive X-ray spectroscopy, Raman spectroscopy, and photoluminescence spectroscopy. It was observed that it is feasible to create monolayers with controllable , shape, and position, whereby the atomic composition of the alloy directly contributes to the formation of oxide islands. Our results demonstrate increased luminescence in the monolayer island - 2D material heterostructures compared to pristine monolayer. A systematic study of structural and electronic properties was conducted using special quasirandom structures (SQS) and density functional theory (DFT). An increase in the energy gap was observed with the addition of molybdenum concentration in the alloy, along with a strong clustering tendency. Our study provides promising results indicating the potential of the TMD alloy $Mo_{1-x}W_xSe_2$ for applications in nanophotonics and optoelectronics.

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Benchmarking optical pump terahertz probe technicque with GaAs and Si

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In this work we present the establishment of a benchmark for our recently implemented Optical Pump Terahertz Probe (OPTP) technique using gallium arsenide (GaAs) and silicon (Si) semiconductor commercial wafers. The OPTP technique combines optical excitation (~1 eV) and terahertz probing (~ 10 meV) to study ultrafast dynamics of photoconductivity in emerging materials with sub-picosecond resolution [1]. GaAs and Si, well-characterized semiconductors, were chosen as benchmark materials due to their known properties [2]. Through our OPTP setup, we investigated the photoexcited carrier dynamics in GaAs and Si and extracted key parameters such as carrier lifetime and mobility. By comparing our results with established literature values, we validated the accuracy and reliability of our OPTP technique. This benchmarking process ensures the reliability of the OPTP set-up implemented in the Terahertz Photonics Lab at IFGW/Unicamp for studying ultrafast photoconductivity dynamics in various emerging materials (bulk or nano) with a focus on potential applications in renewable energy, such as photovoltaic and photocatalytic materials.

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Biosensors based on single-walled carbon nanotubes

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The study of single-walled carbon nanotubes (SWCNTs) has shown promise for the development of biosensors, given their optoelectronic properties and their ability to interact with organic molecules, enabling the identification and characterization of different analytes bound to their surface. An optical biosensor is a device that detects biochemical substances inserted into a biological medium and converts them into an optical signal; in the case of carbon nanotubes, this results in a change in the emission spectrum via photoluminescence. Each sensor should comprise two parts: the first being
a recognition unit, providing selective interaction with the analyte, and the second being a transduction unit, converting the recognition event into a signal [1]. To synthesize the biosensors, we dispersed the SWCNTs in a saline aqueous solution with ssDNA and processed them with ultrasound for 10 minutes. Subsequently, the solution was centrifuged at 16000g for 90 minutes, separating the supernatant from the undispersed SWCNTs. After synthesis, photoluminescence measurements of the biosensor were conducted to analyze its response to the presence of dopamine. As indicated in the article by Abraham et al. [2], we observed variations in signal intensity according to the concentration of dopamine used. Finally, we analyzed whether the Raman scattering spectrum of the sample would be altered in the presence of varying concentrations of dopamine.

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Broadband terahertz generation in ZnTe and GaP for ultrafast spectroscopy

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Terahertz (THz) technology has emerged as a powerful tool for studying the properties and dynamics of materials across a wide range of disciplines, spanning from fundamental physics to biomedical imaging [1]. Terahertz Time-Domain Spectroscopy (THz-TDS) stands out as a versatile and non-destructive technique for characterizing materials based on their absorption and refractive properties in the THz frequency range, typically from 0.1 to 10 THz. This technique relies on the generation and detection of broadband THz pulses, allowing for high-resolution spectroscopic analysis with applications in semiconductor research, pharmaceuticals, security screening, and beyond. Here, I will present the implementation of optical rectification using near infrared femtosecond pulses (1035 nm) for broadband terahertz generation in zinc telluride (ZnTe) and gallium phosphide (GaP) crystals within our laboratory (Terahertz Photonics Lab - Institute of Physics Gleb Wataghin). I will provide an overview of the experimental setup and key parameters utilized in the generation process, including laser wavelength, pulse energy, crystal orientation, and detection scheme. We demonstrate the generation of broadband THz pulses with sub-picosecond durations and characterize their spectral properties, and show initial spectroscopy characterization results obtained using THz time-domain spectroscopy (TDS) in common semiconductors such as Si and GaAs, where optical constants are extracted and compared to literature values to verify the reliability of our experimental setup.

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Cathodoluminescence and Photoluminescence in a Scanning Tunneling Microscopy applied to the study of semiconductor nanoparticles

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This study focused on understanding the light emission of CdSe/ZnCdS quantum dots (QDs) with high spatial resolution. A low-temperature Scanning Tunneling Microscopy (STM) setup with a 72% efficient off-axis parabolic mirror was used to perform cathodoluminescence (STM-CL) and in situ photoluminescence (PL) experiments on these QDs [1]. The QDs, synthed chemically and suspended in toluene, were diluted and deposited onto a gold substrate for analysis. Ex-situ PL using a 532 nm laser revealed heterogeneous photoluminescence, indicating a high dispersion of QDs. Atomic Force Microscopy (AFM) confirmed nanoparticle s ranging from 5 nm to 10 nm, suitable for STM analysis. STM images were captured at 2 V and 200 pA to maintain tip-sample separation. Combined PL and CL measurements, facilitated by the parabolic mirror, showed similar spectral properties with a peak around 630 nm (1.96 eV) and a slight redshift of 16.6 meV in the CL spectrum, attributed to a confined Stark effect. This spectral shift was consistent with previous observations in CdSe/ZnS QDs and CdSe/CdS composites [2]. However, CL analysis revealed a significant intensity decrease over time, likely due to electron beam damage, even with low energy electrons (300 eV), resulting in a ~50% decrease in intensity after 20 minutes. These findings underscore the necessity of controlling the beam dose in CL experiments on II-VI semiconductors.

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Characterization of Carbon Quantum Dots Produced from Carbon Black

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Carbon quantum dots (Cdots) have dimensions smaller than 10 nm and emit light when UV radiation is applied. Due to their optical and electrical properties, they are used to enhancing photovoltaic cells, producing LEDs, and as biological markers. They are classified into three types: GQDs (few layers of graphene), CNDs (amorphous carbon), and polymeric (polymer aggregates) [1]. The origin of photoluminescence in Cdots is still open. Some authors associate the emission with quantum confinement in graphene nanoislands, while others argue that the emission is due to chemical groups on the surface. We produced Cdots from carbon black (amorphous material) by chemical attack with nitric acid at 100°C for 300 hours. The supernatant with Cdots was collected and subjected to pH neutralization, purification, and separation processes. We characterized the Cdots by absorbance measurements, fluorescence, atomic force microscopy (AFM), and Fourier-transform infrared spectroscopy (FTIR). The results show that the Cdots have an emission spectrum independent of synthesis time and excitation wavelength. Their spectrum consists of two intense emissions at approximately 505 nm and 563 nm, and secondary emissions with peaks located approximately at 372 nm, 391 nm, 408 nm, 431 nm, and 456 nm. AFM investigations showed that the of Cdots decreases with synthesis time, even though there is no change in their emission spectrum. This indicates that the quantum confinement effect does not fully explain their emission. FTIR measurements revealed that Cdots contain amine groups, nitrile, aromatic compounds, carboxylic groups, and nitrogen compounds, which may explain the emission.

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Characterization of Two-Dimensional Metallic Niobium Disulfide (NbS2) by Polarization-Resolved Second Harmonic Generation

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Layered materials, such as transition metal dichalcogenides [1] have been extensively used for second (SHG) and third harmonic generation (THG), which enabled various applications in photonics, including frequency conversion for laser light, all-optical, and light modulation [2,3]. Niobium disulfide (NbS2) is a Group V layered TMD, with the 3R phase being its most stable form, thus naturally exhibiting SHG for any number of layers, and unlike other TMDs NbS2 is metallic. To the best of our knowledge, no study has been reported on the polarization-dependent SHG of NbS2. In this work, we investigated the polarization-resolved SHG in powder-exfoliated NbS2 of different thicknesses and compared our results with SHG from CVD-grown monolayer MoS2. Polarization-resolved SHG measurements were conducted in transmission and reflection modes in a confocal laser microscopy setup, with 1560 nm, 150 fs, 89 MHz pump laser, and signal detection by a grating spectrometer (Andor spectrometer, cooled CCD camera model iDus 416). SHG results of NbS2 for different thicknesses in the range of 1.2-1.3 µm exhibited a signal intensity of up to ~500 times higher than that of monolayer MoS2, indicating that NbS2 is a promising material for photonic applications. Additionally, Raman spectroscopy, optical microscopy, and atomic force microscopy (AFM) characterization were performed to determine the thickness of the investigated flakes, and NbS2 flakes were coated with an alumina layer via atomic layer deposition (ALD) to prevent oxidation during laser excitation.

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Coherent imaging under extreme conditions

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The crystalline structure of nanomaterials under extreme pressure and temperature conditions are affected by processes like phase transition and defect formation, which impact on their basic physical properties. Understanding crystal dynamics in extreme conditions might be the key to further tailoring of potential materials for a range of industrial applications. Sirius, one of the few 4th generation synchrotron sources in the world, allows the use of high brilliant high coherent X-ray beams on experiments able to explore the edges of knowledge in science and technology. The Extreme Methods of Analysis (EMA) beamline offers the opportunity to work with several synchrotron techniques, like X-ray scattering, diffraction, spectroscopy and fluorescence, while submitting materials to high pressure, as well as high and low temperatures [1].
Coherent imaging techniques use computational routines to overcome the phase problem and retrieve local information of nanomaterials with resolution better than the beam [2,3]. Here, we present the imaging setup available at EMA beamline, which is currently available for users worldwide. The use of coherent imaging techniques at EMA offers new opportunities to users interested in exploring local processes with spatial resolution down to the order of ten nanometers. This can reveal properties so far difficult to access, either because they require extreme ambient conditions or simply cannot be spatially resolved by traditional synchrotron techniques.

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Control of a Driven Qubit-Resonator System through Optimization Methods and Neural Networks

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ABSTRACT

In modern days, superconducting quantum circuits emerge as a promising platform for quantum computing. Among these circuits, the transmon qubit can be interfaced with a superconducting resonator that can be used either as a probe of the qubit state or as a storage of continuous-variable quantum states. Within this framework, the circuits are coupled to external drives that provide universal control of the quantum state. The potential applications of such control encompass the realization of quantum gates that enables applications in metrology, simulation, and other quantum computing tasks [1].

The objective of this study is to exert control over a driven qubit-resonator system through a two-independent-stage approach. Firstly, optimization techniques utilizing computer simulation and leveraging the QuTiP and SciPy libraries. Secondly, a control framework developed through the training of Artificial Neural Networks (ANN) and Long Short-Term Memory (LSTM) networks [3]. The protocol for optimization encompasses several stages from system initialization to cost function minimization. In parallel, the neural networks are trained on a curated dataset derived from hundreds of thousands of computational simulations.

Furthermore, the findings demonstrate the feasibility of manipulating the dynamics of a quantum system through classical field optimization, as well as from a proper trained neural network, whereas the results obtained align consistently with the control of the qubit to exhibit a predetermined behavior.

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Convergence Analysis of the Density Matrix Renormalization Group

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The Density Matrix Renormalization Group (DMRG) is a numerical variational technique devised to obtain the low-energy properties of strongly correlated quantum systems in low dimensions, particularly one-dimensional chains and ladders. Traditional techniques, like exact diagonalization, become computationally intractable for large system s due to the exponential growth of the Hilbert space. DMRG circumvents this challenge by iteratively constructing a reduced density matrix that captures the essential physics of the system. This is achieved through a systematic truncation of the Hilbert space, retaining only the states that contribute most significantly to the ground state and low-lying excitations.
Despite the great efficiency of the method, depending on the complexity of the system, DMRG can end up becoming a time and memory consuming method, especially on less powerful machines. In this work, in addition to making a general analysis of the DMRG, we also present some techniques and tricks that can make the DMRG much more efficient.
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Coupling Electrons in Silicon Quantum Dots to a Single Ge Nuclear Spin

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Nuclear spin systems have many desirable properties, as exceptionally-long relaxation times and, fast and precise control. Thus, have been seen as a potential platform for quantum information application. In the present work, we explore the possibility to use 73Ge incorporated into silicon as a nuclear spin qubit. As Ge is isoelectronic with silicon, so we expect electrons can easily shuttle from one Ge atom to another to propagate quantum information via a hyperfine interaction (HFI). So, we use an all-electron linearized augmented plane wave density functional theory calculations to predict the magnitude of HFI and compare with the known result for 29 Si. In addition to it, we also investigate the strain-induced symmetry reduction on nuclear spin which might have a some important influence on the valley pollarization.

Crystalized phases of the excitonic Bose-Einstein condensate in a semiconductor van der Waals heterostructure

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At extremely low temperatures, bosonic atoms can condense into a single quantum state, known as Bose-Einstein Condensation [1]. Initially observed in alkali atoms, there have been recent reports of condensed states achieved by composite particles, formed by electron-hole pairs in semiconductor heterostructures, so-called excitons [2]. Anomalous behaviors, such as the formation of droplets and solids [3], were predicted with dipolar interactions between the particles. Thus, the dipolar nature of inter-layer excitons, where electrons and holes are spatially separated in different layers of material in semiconductor heterostructures, makes the excitonic condensate a promising platform to explore such unusual behaviors and phase transitions. One of these exotic behaviors is the crystallization of the system, where the condensate exhibits both solid and superfluid properties. Our work proposes a device consisting of a van der Waals heterostructure of two-dimensional (2D) transition metal dichalcogenides (TMDs), in proximity to a graphene layer where a 2D electron gas is set. The TMDs hetero-bilayer produces a condensate of inter-layer excitons, which would naturally interact via dipole-dipole repulsion, while the 2D electron gas modifies this interaction by introducing an attractive range in it. Our results show that by tuning the distance between the electron gas and the excitonic condensate, or the density of electrons/excitons, the necessary environment for a self-formed crystal, where the ground state spontaneously organizes itself into an ordered periodic structure, is achieved. We perform a systematic study of this system as to create a phase diagram determining parameter ranges for the formation of crystalized and superfluid states.

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Deposition and Characterization of Co_3O_4 Thin Films for Non-Enzymatic Ascorbic Acid Sensor Applications

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Co_3O_4 thin films were deposited by reactive DC magnetron sputtering onto fluorine-doped tin oxide (FTO) and fused silica (SiO_2) substrates. X-ray diffraction measurements confirmed the spinel Co_3O_4 phase. The surface roughness of the films, as measured by atomic force microscopy, was 4 nm and 20 nm for SiO2 and FTO substrates, respectively. Optical transmission spectra of Co_3O_4 films showed strong absorption in the near-infrared and visible regions. The photoconductivity response of SiO_2/Co_3O_4, using 405 nm excitation and measured at room temperature, was much smaller than that observed at 10 K. The electrochemical activity of FTO/Co_3O_4 for the ascorbic acid (AA) oxidation reaction was investigated by differential pulse voltammetry and chronoamperometry. A model for the oxidation, based on density functional theory calculations for the electronic structure of AA, is proposed. The set of results demonstrates that the assembled FTO/Co_3O_4 electrode can be used as an alternative and remarkable performance non-enzymatic device for ascorbic acid electrooxidation.

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Description of Excitonic Absorption in Metal Tri-Halide Pervoskites using Dispersion Models, a Hydrogen-Polaron Model and First Principles.

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Studies of excitonic absorption of metal tri-halide perovskites have depicted several attention due to its high efficiency rates reaching up to 25%. Correct description of excitons in these systems can lead to improvements to solar cell devices based on them. In this work, we present an optical study and characterization that covers modeling of the spectral curves, an effective model and first principles. First, the modeling of the excitonic absorption is studied in terms of a recently proposed model based on the Elliott equation and the band-fluctuations approach. This analytical model is used to fit the absorption of metal tri-halide perovskites with different concentrations FAPbI_{3-x}Br_x, MAPbI_{3-x}Br_x, CsPbI_{3-x}Br_x and MAPbBr_{3-x}Cl_x. Thus, retrieving information such as bandgap, exciton binding energy and Urbach energy. Secondly, the polar nature of this semiconductors can be modeled in terms of a hydrogen effective model with a potential that mimics the electron-phonon interaction. As a consequence, the exciton-polaron binding energy depends on five parameters. These are the low and high frequency dielectric constant, e₀ and e_∞, the effective masses of electron and hole, m_e and m_h, and the LO phonon energy hω_{LO}. These parameters can be estimated from first principle calculations using the independent particle approximation (IPA) for dielectric response, and the finite differences approach for phonon calculations. Thirdly, we perform an study of excitonic absorption based on first principles by solving the Bethe-Salpeter (BS) equation. Here, we use an approach that solves the BS equation using maximal localized Wannier functions and an analytical screened potential. The advantage of this approach is that it saves computational time up to two order of magnitude so that exciton properties of large systems becomes feasible. The comparison of binding energies and bandgaps of the perovskites show the agreement, capabilities and advantages of each approach.

Design of spin-orbital-textures in ferromagnetic/topological insulator interfaces

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The current interest in topological materials has transitioned from a more fundamental exploration, focused on verifying the topological nature of materials, to a more direct application, such as in the design of new functionalities and/or devices, where knowledge and control of electronic characteristics at the interfaces of realistic systems are of crucial importance in connecting an effect to the observed signal. An area that has shown great advancements in recent years is the study and manipulation of spin-orbit coupling and spin degrees of freedom, especially for spintronic applications, through the manipulation of emerging effects, such as charge/spin conversion mechanisms or spin torque transfer. In this scenario, topological materials have stood out, thanks to the presence of helical interface states, due to spin-momentum locking and symmetry protection against backscattering. In Ref. [1], we combine first-principles calculations with an effective model to investigate how the dispersive image and spin component behavior of surface states in a Topological Insulator can be appropriately adjusted in function of the interfacial coupling with a magnetic layer. We discovered that the modulation of different degrees of freedom in the resulting heterostructure allows for the realization of a rich family of spin textures at the 2D Fermi contours of the Brillouin Zone, leading to efficient control of the spin orientation of topological states depending on the magnetization direction, as well as manipulation of the scattering probability of states as a function of energy.

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Determining the number of layers on transition metal dichalcogenides samples using micro-differential reflectance on LiNbO3, quartz and sapphire substrates

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Transition metal dichalcogenides (TMDs) have gained special interest in recent years within the scientific community due to their novel properties. Piezoelectric substrates, such as LiNbO3, have been used to generate propagating electric and strain waves, the so-called surface acoustic waves (SAWs), to modulate the optical properties of TMD structures. However, the determination of the number of layers on LiNbO3 substrates is not straightforward. Micro-Raman spectroscopy is a widely used technique for that purpose on many substrate materials. For TMDs, this is usually done by measuring the difference between E2g and A1g peaks. LiNbO3 exhibits a rich Raman spectrum, with intensity orders of magnitude larger than the TMDs E2g and A1g peaks, making it difficult to determine the modes spacing with adequate precision. Here, we employ micro-differential reflectance spectroscopy (micro-RD) to determine the number of layers in WSe2 samples on quartz, sapphire and LiNbO3 substrates, as an alternative to micro-Raman spectroscopy. On the sapphire sample we have a region where the TMD is over h-BN. Measurements were conducted at room temperature and 5 K. We observe that overall micro-RD spectrum is strongly dependent of the number of layers in the structure. In particular, we show that the energy of the exciton C peak is extremely sensitive to the number of TMD layers and can be used to precisely differentiate structures of up to five monolayers. This technique, under certain conditions, yields a spectrum which is proportional to the absorption coefficient of the thin film. We observed that these conditions are met for few-layer TMDs on quartz, sapphire and LiNbO3. Even though the theory cannot be strictly applied to the structures with an additional médium, we observed that we can still determine the number of layers in WSe2 layers on h-BN using this procedure.
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DFT2kp: effective kp models from ab-initio data

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The kp method, combined with group theory, is an efficient approach to obtain the low energy effective Hamiltonians of crystalline materials. Although the Hamiltonian coefficients are written as matrix elements of the generalized momentum operator π = p + pSOC (including spin-orbit coupling corrections), their numerical values must be determined from outside sources, such as experiments or ab initio methods. In Ref. [1], we develop a code to explicitly calculate the Kane (linear in crystal momentum) and Luttinger (quadratic in crystal momentum) parameters of kp effective Hamiltonians directly from ab initio wavefunctions provided by Quantum ESPRESSO. Additionally, the code analyzes the symmetry transformations of the wavefunctions to optimize the final Hamiltonian. This is an optional step in the code, where it numerically finds the unitary transformation U that rotates the basis towards an optimal symmetry-adapted representation informed by the user. In this talk, we present the methodology in detail and illustrate the capabilities of the code applying it to a selection of relevant materials. Particularly, we show a "hands-on" example of how to run the code for graphene (with and without spin-orbit coupling). The code is open source and available at https://gitlab.com/dft2kp/dft2kp.

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Diode-like properties of Sb-doped Tellurium single crystals.

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Tellurium is a small band gap semiconductor (Δ=330meV) with a chiral crystal structure. Previous studies have shown that the chirality manifests itself in the transport properties including, magnetochiral effect under the application of external magnetic fields [1] and an antisymmetric non-reciprocal contribution in the magnetoresistance [2]. Here, we present frequency- and offset-dependent transport measurements on Sb-doped tellurium single crystals. In all our experiments the current direction is aligned with the helical screw axis. We see strong indications for a diode like behavior of the single crystalline samples. These include that the samples possess a preferred transport direction, where the resistance is about an order of magnitude lower, and a strong frequency dependence of the impedance of the samples. Thus, we conclude that relatively simples manipulation of tellurium opens the possibility for the creation of novel solid-state devices.

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Direct observation of gramicidin channel filling through electronic HOMO-LUMO signature

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Gramicidin is an ionophoric antibiotic usually extracted from soil bacteria (Brevibacillus brevis). The gramicidin molecule can be understood as a linear pepitide chain with 15 amino acids coiled up in a cylindrical form, resulting in a channel structure. In it's A-form the molecule acts against gram-positive bacteria and is used in low doses in eye drops for topical infections. The ion channel-like pore allows monovalent ions (K+, Na+) to travel freely inside via diffusion, affecting the vital concentration of these ions in bacteria, leading to their cellular death.

In this work we show experimentally that divalent ions are blocked inside the gramicidin channel, docking inside the internal walls and suppressing ion changes. In particular, HOMO-LUMO energy changes were observed in scanning tunneling spectroscopy and calculated by density functions theory (DFT). The quantitative agreement of measurements and DFT calculations indicate that electronic structure simulations in this system, as well as in similar molecules, can be used prior to clinical essays involving simple ions and small molecules.

DOPING CHARACTERIZATION OF ULTRATHIN GRAPHENE HETEROSTRUCTURES BY RAMAN SPECTROSCOPY

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Graphene holds great potential for applications due to its high electrical and thermal conductivities [1-3]. Advances in techniques for obtaining ultra-clean graphene enable the development of ultrathin devices in optoelectronics and photonics [1]. Among these applications, it is possible to exploit the high-energy conversion of p-type doped graphene into van der Waals heterostructures (vdWHs) using two-dimensional materials (2DMs) to create novel solar cells [2]. Additionally, Raman spectroscopy stands out as a widely employed tool for characterizing 2DMs and their vdWHs due to its speed and non-destructive nature. Therefore, using Raman spectroscopy is compelling to identify how 2DMs dope graphene and determine which materials are suitable for fabricating high-quality graphene-based vdWHs [3]. In this project, we developed a Python program to analyze Raman map measurements for various vdWHs, correlating them with doping and/or strain in assembled graphene. Furthermore, the program allows us to pinpoint the most homogeneous regions within the heterostructure, promoting higher quality in the graphene-based devices. In the future, we intend to compare Raman spectroscopy measurements with electrical data to enhance our analysis of developed vdWHs and deepen our understanding of these ultrathin nanostructures. Therefore, our work aims to streamline the process of designing vdWH-based devices using a Python program.

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Edge engineering of quantum spin Hall insulators from first-principle investigations

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Two-dimensional topological insulators (2DTIs) host spin-momentum-locked electronic and transport properties robust against defects and disorder, offering potential solutions to longstanding challenges in spintronic device design [1]. However, recent research has shown different mechanisms capable of altering or mischaracterizing the main signatures of 2DTIs [2,3], raising questions about the viability of device implementations, which demand further investigations. Here, we address the resilience of the topological properties of lead-salt-based quantum spin Hall insulators in the presence of defects, considering its dependence on the edge terminations within the atomistic physical understanding provided by ab initio calculations. We studied defects in lead-salt-based nanoribbons with different edge terminations by performing first-principle calculations based on density-functional theory (DFT), employing semilocal exchange-correlation formalism as proposed by Perdew-Burke-Ernzerhof (PBE-GGA), further considering spin-orbit coupling corrections. Edge-termination-dependent properties are analyzed within a comparative view, shedding light on strategies for edge engineering aimed at optimizing the topological properties of quantum spin Hall insulators and preserving their unique electronic functionalities. Thus, we can provide insights into the experimental realization and integration of lead-salt-based nanoribbons within spintronic devices. The authors acknowledge financial support from the Brazilian agencies FINEP (Ref. No. 0151/21), CNPq (INCT - Materials Informatics, INCT – Nanocarbono), and FAPESP (grant 2023/12336-5).

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Effect of SiO_2 as sintering aid in structural and optical propertiesof Ce:YAG ceramics

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SiO_2 has been widely used as a sintering aid during the fabrication of transparent ceramics, improving its densification and its homogeneity, and reducing pores [1]. In the 1980s, SiO_2 was used for the first time when With and van Dijk produced translucent YAG ceramics [2]. Despite its benefits, careful management of defect formation, such as secondary phase segregation and color center formation, and its influence on the luminescent properties is crucial. This study investigates the impact of varying SiO_2 concentrations, introduced through tetraethoxysilane (TEOS) addition, on the structure of Ce:YAG ceramics during the manufacturing process. The investigation involves comprehensive structural and optical analyses based on X-ray diffraction, scanning electron microscopy, UV-Vis transmittance spectroscopy, and luminescence spectroscopy techniques. The samples analyzed were produced with 0, 14%w.t. and 0, 35%w.t. of SiO_2. The transmittance, after annealing in an atmospheric furnace, achieves 55% and 74% at 960nm, respectively. Both samples exhibit a peak in the luminescence emission spectrum around 550nm and two excitation bands around 340nm and 450nm, which corresponds to Ce3+ behavior into YAG lattice, due to $4f0^5d^1$ excited state electrons to the two ground states transition of the $4f^5d^0$ orbital ($2F_{5/2}$, $2F_{7/2}$)[3]. Our findings further reveal that the addition of SiO_2 can result in the formation of secondary phases along grain boundaries and induce color center effects in Ce:YAG ceramics. Nevertheless, annealing in an atmospheric furnace enabled the attainment of favorable transmittance, and luminescence properties.

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Effect of temperature on optoelectronic properties of NiO_x for applications in perovskite solar cells

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The best efficiencies obtained for perovskite solar cells were achieved with techniques unsuitable for large-area production and using organic layers that show low stability and high costs, limiting the applicability of this emerging technology. This work proposes a study on inorganic materials, with better stability, utilizing the large-area technique of Ion Beam Sputtering (IBS) for the deposition of type-p non-stoichiometric nickel oxide films (NiO_x, x>1), to act as hole transporting layers for perovskite solar cells. The optoelectronic properties of this material are strongly related to the film deposition parameters. Utilizing in-situ photoemission spectroscopy of X-rays and UV (XPS and UPS), we observe that changes in the deposition temperature, or annealing of the film lead to changes in the Fermi level and valence band maximum, without change in the stoichiometry. The excess oxygen in the film formation leads to the formation of Ni^{3+} from the ionization of Ni^{2+} atoms, the presence of Ni^{3+} is related in a complex manner to the conductivity, visible transmittance, band position, and bandgap. Regarding this, a further study employing a series of techniques such as X-ray diffraction (XRD), UV-Vis-NIR spectroscopy, atomic force microscopy (AFM), and also conductivity and carriers measurements is made to characterize the effect of temperature and thermal treatment on the film properties, leading to an efficient transport layer, suitable for hole extraction.

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Effect of the roughness on the photoinduced growth of crystalline tellurium on $MoTe_2$ matrix

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In this work, thin films of molybdenum oxide (MoO_3) were synthed on SiO_2/Si substrates by sputtering technique of molybdenum at low vacuum. These films then were tellurized in a system of closed-space sublimation (CSS). By adjusting the temperature inside the CSS chamber during the growth, 5 nm thick 1T'-$MoTe_2$ (semi-metallic) films were synthed. Surface analyses showed that tellurium spreads over the surface of the as-grown films, forming localized crystalline precipitates whose distribution depends on the tellularization time. It was observed that the prolonged incidence of polarized light on regions of the films with nanometer-d tellurium clusters promotes the growth well-ordered phase of tellurium. The photocrystallization effect observed here is consistent with the Kolmogorov-Johnson-Mehl-Avrami (KJMA) theory for the overall crystallization process. The time dependent intensity of the vibration phonon modes associated with crystalline tellurium were used to describe the evolution of the transformed phase. The characteristic exponent of the growth (Avrami exponent) was obtained. By the characteristic growth exponent, we introduce a more specific model which takes into account the diffusion and the dissociation of tellurium chains, which is used to probe how the effective growth rate is affected by the roughness of the samples.

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Effect of thickness on the RE-doped BiFeO3 multiferroic thin films for low-energy spintronic devices

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For the last few decades, the consumption of electronic devices and the highest demand for data storage has shown such a great opportunity to create new technologies that assure the World needs about computing and development.[1] Multiferroic materials, such as BiFeO3, with simultaneous ferroelectricity and magnetism provide a pathway to achieving strong magnetoelectric coupling with efficient voltage control of magnetism, leading to compact and power efficient electricfield tunable magnetic devices.[2] The 20 nm SrRuO3 thin film was grown on DyScO3 (110) at 700˚C, with a rep rate of 5 Hz and energy of 100 mJ, the La0.10Bi0.90FeO3 was obtained at 700˚C, using a rep rate of 5 Hz and energy of 80 mJ. A ferroelectric layer such as Co0.90Fe0.10 was deposited on the FE layer by sputtering, using a 5x10-3 Torr (Ar) and 10 Watts. All the devices were fabricated by photolithography process and device fabrication. Uniform and smooth surface of 20 nm thick LaBiFeO3 layer was growth by PLD, showing disordered mosaic-like in-plane ferroelectric domain structure. The crystal structure of LBFO was verified by XRD, epitaxial and strained lattice was obtained on SRO/DSO(110). Well-grown and clean interface was achieved between SRO/LBFO layers. Antiferromagnetic ordering state and Neél temperature about 543 K was measured by linear dichroism spectroscopy XMLD. The thickness of LBFO scaling up as d-2/3 factor, according to scaling law. The electrical switching coercive voltage about 0.5 V was achieved in 20 nm LBFO thin film. Thus, we propose to focus on ultra-low energy consumption pathways for such transduction, aiming to develop a new class of multiferroic materials with ultra-low energy consumption for application in FeRAM memory and logic devices.

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Effects of shear strain and external fields on α-T_3 nanoribbons

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The α-T_3 lattice - viewed as a theoretical toy material with a hexagonal structure with an atom in its center whose connections with the adjacent sublattices are modulated by an intrinsic parameter α that allows continuously to morph a honeycomb-like lattice (α=0) into a dice lattice (α=1) - has drawn a lot of attention from the condensed matter physics community due to its extraordinary electronic and transport properties [1]. By this lattice interpolation process, the behavior of charge carriers evolves in lattices α-T_3 from Dirac fermions of spin S=1/2 to Dirac fermions of S=1-from graphene to the dice lattice [2]. Beyond the morphing parameter α, additional ingredients can be considered in order to manipulate the physical properties of the α-T_3 lattice, such as by assuming narrow nanoribbons, deforming the lattice, and applying external perpendicular electric or magnetic fields. Motivated by these morphological characteristics of the α-T3 lattice and by the emerging quantum finite-induced effects, we explore via tight-binding model how the electronic properties of α-T_3 nanoribbons are significantly affected by applying shear strain and external electric and magnetic fields. Different types of edge terminations (zigzag and armchair boundaries), connections between the center atom in the hexagon of α-T_3 lattice with the adjacent neighbors, ribbon widths, and magnitudes of the applied deformation and fields are investigated.

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Efficient spin-to-charge conversion and charge transfer dynamics in graphene/WS2 heterostructures

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The use of graphene in spintronic devices depends, among other things, on its ability to convert a spin excitation into an electric charge signal, a phenomenon that requires a spin-orbit coupling (SOC). We have already reported an investigations of the spin-to-charge current conversion in single-layer graphene deposited on a single crystal film of the ferrimagnetic insulator yttrium iron garnet (YIG-Y3Fe5O12). [1,2] Here we report an investigation of the combination of WS2 flakes with a single-layer graphene for spin-to-charge current conversion. We report an investigation of the combination of WS2 flakes with a graphene layer for spin-to-charge current conversion. The pure spin current was produced by the spin precession in microwave driven ferromagnetic resonance of pemalloy film (Py-Ni81Fe19) and injected into the WS2/graphene heterostructure by the spin pumping process. The spin-to-charge current conversion that occurs in the heterostructure is attributed to Inverse spin Hall effects (ISHE) in WS2 and inverse Rashba-Edelstein (IREE) at the interface of WS2 flakes and the graphene film. The results show that the presence of WS2 flakes improves the current conversion efficiency. Understanding how the interfacial charge transfer and spin-charge conversion process between layered TMDs materials and graphene occur is important for improving the optoelectronic and spintronic device performance. For this purpose, the electron dynamic delocalization and spin-charge conversion in the interface of graphene/WS2 heterostructure was investigated combining the synchrotron-based core hole clock approach and spin pumping process. The results obtained from these methods were supported by density functional theory (DFT) calculations.

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Electrical properties of meso-PS/TiO_2 heterojunctions: the role of the PS thickness.

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Silicon-based semiconductor devices represent the predominant technology in modern electronic equipment. Among these devices, one of the simplest is the junction diode, which consists of the junction of two types of semiconductors, p- and n-type, or a conductor combined with a semiconductor. In the latter case, this junction is commonly referred to as a Schottky junction, and its current-potential curve obeys the thermionic emission model. Diodes made from Titanium dioxide (TiO_2) and Porous Silicon (PS) are well-known because of its potential applications in the photovoltaic cells field and by its energy storage capabilities. In this study, the electrical properties of TiO_2/meso-PS were characterized. For this aim, meso-PS with thickness varying from 3.2 to 15 µm were fabricated by anodizing heavily doped p-Si, where TiO_2 was deposited using the sol-gel method. The fitting procedure of the current-potential measurements using the three-diode model reveals that the charge mechanisms are dependent on the porosity and layer thickness. This dependence is associated with the increase in Schottky barrier potential attributed to the contact/TiO_2 interface, alongside an increase in built-in barrier potential of the TiO_2/meso-PS junction. According to the Mott-Schottky analysis, another factor for diminution in current intensity is linked to the diminution of the charge carrier concentration because of the hole-electron recombination phenomenon at the TiO_2/meso-PS interface.

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Electric Dipole Spin Resonance in Phosphorene Quantum Dots

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Exploring the manipulation of spins through electric fields is crucial for advancing spin-based qubit technology. This work delves into Electric Dipole Spin Resonance (EDSR) [1] induced by oscillating electric fields within a system of double quantum dots formed electrostatically in monolayer phosphorene. Aside from the observed anisotropy in effective masses, phosphorene [2] has recently been anticipated to demonstrate anisotropic spin-orbit coupling [3]. The study focuses on a setup involving two electrons confined within double quantum dots, utilizing a single-band effective Hamiltonian and employing configuration interaction theory to simulate the time evolution of the ground state. The investigation studies spin flips resulting from singlet-triplet transitions driven by external AC electric fields, both within and beyond the Pauli blockade regime, revealing transition times on the sub-nanosecond scale. Additionally, the impact of anisotropy is examined by comparing dots arranged along different axes. The analysis also encompasses discussions on subharmonic higher order transitions and Landau-Zener-Stueckelberg-Majorana transitions [4] near the avoided crossing opened by Rashba spin-orbit coupling.

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Electric Dipole Spin Resonance in Phosphorene Quantum Dots

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Exploring the manipulation of spins through electric fields is crucial for advancing spin-based qubit technology. This work delves into Electric Dipole Spin Resonance (EDSR) [1] induced by oscillating electric fields within a system of double quantum dots formed electrostatically in monolayer phosphorene. Aside from the observed anisotropy in effective masses, phosphorene [2] has recently been anticipated to demonstrate anisotropic spin-orbit coupling [3]. The study focuses on a setup involving two electrons confined within double quantum dots, utilizing a single-band effective Hamiltonian and employing configuration interaction theory to simulate the time evolution of the ground state. The investigation studies spin flips resulting from singlet-triplet transitions driven by external AC electric fields, both within and beyond the Pauli blockade regime, revealing transition times on the sub-nanosecond scale. Additionally, the impact of anisotropy is examined by comparing dots arranged along different axes. The analysis also encompasses discussions on subharmonic higher order transitions and Landau-Zener-Stueckelberg-Majorana transitions [4].

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Electronic properties of multilayered Lieb, transition, and Kagome lattices

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In recent years, there has been a growing interest in researching new materials that can be produced in the form of single or few layers and, in particular, that host unique optoelectronic properties, making them promising for future technological applications. Similarly to multilayer graphene, the physical properties of multilayer two-dimensional (2D) materials can be further tailored by stacking layers of the same or different 2D materials. In the multilayer context and based on the interconvertibility feature shared between monolayer Lieb and Kagome lattices, which allows mapping transition lattice's stages between these two limits, [1] we extend the recently proposed one-control parameter tight-binding model for the case of a multilayer Lieb-Kagome system, by considering the three most-common stacks: AA, AB (Bernal), and ABC. We systematically study the bands' transformation between the two lattices by tuning the interlayer hopping/distance, assuming or not the influence of the next intralayer and interlayer neighbors, and considering different numbers of the stacked layers. The energetic changes are understood in view of the layer dependence of the pseudospin components, the total probability density distributions, and the group theory perspective. The present framework provides an appropriate and simple theoretical way to continuously investigate the evolution in the optoelectronic properties of the multilayer Lieb-Kagome system under any external effect.

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Electronic response of polytypic In_2Se_3: a suitable semiconductor system for wide absorption devices

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Abstract

The investigation of layered III-VI semiconductors continues to attract significant interest due to their potential applications in nano-optoelectronic devices, driven by their atomic-scale thickness, outstanding light absorption properties, high carrier mobility and layer-dependent bandgaps. Among III-VI semiconductors, In_2Se_3 is a promising layered material thanks to its structural and electronic diversity, resulting in possible higher-order topological states, in-plane and out-of-plane ferroelectricity, and a broad range of electronic bandgaps.[1-4] As a result, In_2Se_3 is exceptionally well-suited for applications such as solar cells, high-performance photodetectors, nonvolatile memories, ferroelectric field-effect transistors (FeFETs), gas sensors and more. In this work, we present a semiconductor In-Se system where polycrystalline and polytypic synthesis cannot be easily avoided. By combining scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS) and powder X-ray diffraction (PXRD), we investigate the crystal structure and phase distribution of our In-Se system. Electronic properties were probed using scanning tunneling microscopy and spectroscopy (STM/STS). We present an experimental verification of the coexistence of complementary bandgap energies that cover a broad spectrum (spanning over a wide infrared spectral range), associated with n-type phase-independent doping in the 2:3 In-Se stoichiometry.

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Emerging Technologies: Advances in the Production of Organic Photovoltaic Devices with PTQ-10 Polymer

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Organic photovoltaic devices have attracted significant interest due to their advantages, such as low production costs, flexibility, and potential for large-scale applications, including integration into flexible and semi-rigid materials. However, challenges still exist, such as the need to improve conversion efficiency, long-term stability, and production scale to make these devices even more competitive compared to conventional solar energy technologies. The PTQ-10 polymer has attracted significant interest because, unlike PM6 and D18, which have complex structures, it has a simple structure that makes it industrially advantageous. Additionally, this material has produced devices on a laboratory scale with an efficiency of approximately 16% [1]. In this work, the feasibility of producing devices on an industrial scale is being evaluated, where controlled production under an inert atmosphere is not possible. Therefore, using PTQ-10 synthed through Stille coupling as the donor material, devices were produced in ambient atmosphere. The previous photovoltaic parameters obtained using a low-molar-mass material (Mn = 7835 g/mol) showed a Voc of 0.84 V, Jsc of 11.3 mA/cm2, FF of 60.7%, and efficiency of 5.63%. Some changes in synthesis are being evaluated to obtain a polymer with higher molar mass for the production of even more efficient devices, since the preliminary results were promising.

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Enhanced Electronic Transport Properties of Te Roll-like Nanostructures

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Abstract: In this work, the electronic transport properties of Te roll-like nanostructures were investigated in a broad temperature range by fabricating single-nanostructure back-gated field-effect-transistors via photolithography. These one-dimensional nanostructures, with a unique roll-like morphology, were produced by a facile synthesis and extensively studied by scanning and transmission electron microscopy. The nanostructures are made of pure and crystalline Tellurium with trigonal structure (t-Te), and exhibit p-type conductivity with enhanced field-effect hole mobility between 273 cm^2/Vs at 320 K and 881 cm^2/Vs at 5 K. The thermal ionization of shallow acceptors, with small ionization energy between 2 and 4 meV, leads to free-hole conduction at high temperatures. The free-hole mobility follows a negative power-law temperature behavior, with an exponent between -1.28 and -1.42, indicating strong phonon scattering in this temperature range. At lower temperatures, the electronic conduction is dominated by nearest-neighbor hopping (NNH) conduction in the acceptor band, with a small activation energy $E_{NNH} \approx 0.6$ meV and an acceptor concentration of $N_A \approx 1\times10^{16}$ cm^{-3}. These results demonstrate the enhanced electrical properties of these nanostructures, with a small disorder, and superior quality for nanodevice applications.

Keywords: electrical characterization; hopping conduction; tellurium

Evaluation of the Addition of Porphyrin on the Electrical Properties of the D18:Y6:PCBM Active Layer by c-AFM and KPFM Techniques

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In recent years, advances in synthesis, design, and engineering of devices have driven significant progress in organic semiconductor electronics, resulting in improvements in photovoltaic parameters and, consequently, in overall efficiency. In the context of solar energy research, porphyrins (H2TPP) and their related structures stand out for their remarkable light absorption capacities, thermal stability, and structural flexibility [1]. These characteristics make them especially suitable for optimizing solar energy harvesting. This study adopted a ternary strategy, where the active layer was composed of organic polymers represented by the D18:Y6:PCBM structure. Additionally, complexed porphyrin hybrids (NiTTP and ZnTPP) were included as additives at a concentration of 30%. The aim of this research was to investigate the influence of these additives on nanoscale heterogeneity, using characterization techniques such as AFM, c-AFM, and KPFM. The polymeric films were deposited on ITO substrate using the Blade Coating technique. From the topographical analysis, an increase in phase separation is observed with the addition of additives compared to the (D18:Y6:PCBM) film, along with an increase in surface roughness. It is also noted that surface potential values decreased, suggesting that the addition of porphyrin complexes caused an adjustment in Fermi levels relative to the vacuum level. The magnitude of this variation can impact charge extraction efficiency and, consequently, conversion efficiency. Using the c-AFM technique, it is observed that the addition of porphyrin results in a significant increase in current conduction.

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Evaluation of the graphene-aptamer interaction for the development of a biosensor based on magnetoelastic waves

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The magnetoelastic materials (ME) present strong coupling between their magnetic and elastic properties, which makes them an excellent platform for sensor development. Such materials change their magnetoelastic resonance frequency in response to applied stresses, due to the deposition of a selectively fixed target. These devices offer high sensitivity and wireless detection, particularly useful when direct probe or electrical contact isn't feasible. Graphene, due to its good biocompatibility and high surface area, offers a large surface area for the adsorption of functionalizing molecules such as aptamers, allowing a large number of target molecules to bind to the sensor, which can further increase its sensitivity. The selected aptamer specifically targets the biomolecule of interest to be detected, thus determining the selectivity of the biosensor. Graphene-coated sensors were analyzed, with the aim of investigating how the base material for functionalization affects sensor sensitivity. In this work, graphene was produced using the chemical vapor deposition technique and transferred to the magnetoelastic substrate. An FeNi-based alloy produced by the melt spinning technique was used as a magnetoelastic material. Raman spectroscopy was used to investigate the interaction of graphene with the substrate, with the aptamer (pi-cation-pi interaction) and with the target molecules. For surface characterization, the Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM) techniques were used, followed by magnetoelastic resonance measurements, where it was possible to distinguish the deposition of biomolecules related to the functionalization steps. This approach provided an understanding of interactions at the molecular level and allowed validation of the functionalization process, reinforcing the reliability and accuracy of the proposed biosensor.

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Excitonic complexes confined in lateral two-dimensional heterostructures

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In this work, we conducted a detailed theoretical investigation into the binding energy of excitonic complexes confined at the interface of lateral MoS$_2$/WS$_2$ heterostructures. These heterostructures, crafted from two-dimensional semiconductor materials, feature a distinctive type-II energy band alignment at their interface. Our analysis focused on elucidating the intricate interactions and binding energies associated with excitonic complexes, encompassing excitons and trions. By delving into the nuanced behaviour of these quasiparticles at the heterostructure interface, we aimed to unravel the underlying physics governing their formation, stability, and interplay. The theoretical model considers: \textit{i}. a near-contact interaction between an electron or hole with a dipole, formed by the electron-hole pair (exciton); and \textit{ii}. a long-range interaction for the dipole. Both interactions are mediated by the Rytova-Keldysh potential, which makes it possible to consider effects due to the dielectric shielding length of the monolayers and gradual interfaces of the side junction. To this end, we will use the variational method within the effective mass approximation and the Wannier-Mott theory to calculate the ground state of the charge dipole in a lateral heterostructure of MoS$_2$/WS$_2$. This work contributes valuable insights into the fundamental aspects of excitonic complexes in lateral TMD heterostructures, paving the way for a deeper understanding and potential applications in advanced optoelectronic devices and quantum technologies.

Excitonic Luminescence in Transition-Metal Dichalcogenide Monolayer Domes Using Scanning Tunneling Microscopy

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Scanning tunneling microscopy (STM) enables high-resolution mapping of the local density of states and the determination of occupied and unoccupied states at the atomic scale. In certain materials, the local tunnel current generated by an STM can act as a source of excitation, leading to light emission. As a result, STM can be used to study electronic, morphological, and luminescent properties of nanostructured materials [1]. Here, we focus on the excitonic luminescence of transition-metal dichalcogenide (TMD) monolayer (ML) domes formed via H-ion irradiation of bulk WS2 and WSe2 crystals on Au substrate [2]. Atomic Force Microscopy (AFM) reveals a diverse range of dome s, varying from 1 µm to 50 nm in diameter and 132 nm to 12 nm in height. Our study aims to correlate the nanoscale topography of these ML domes with localized exciton emission. The curved ML shape introduces mechanical stress variations [3], leading to localized strain that could potentially serve as single photon sources. Our approach incorporates a recently developed device featuring a high solid angle off-axis parabolic mirror (72% collection efficiency), integrated with an adapted ultra-high vacuum (UHV) STM [4,5]. This setup allows us to perform optical experiments inside the STM and collect light emission (STM-LE) when the sample experiences tunnel current. This investigation not only contributes to understanding excitonic behavior in TMD materials but also underscores the versatility of STM in probing electronic, morphological, and luminescent properties of nanostructures.

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Exploring 2D Binary Compounds of the III-V Family: Insights from First Principles Calculations and the Tight Binding Method

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In this work, we investigate 2D bynary compounds made by III-V family atomic species, with AB stoichiometry (A = B, Al, Ga; X = N, P, As), in honeycomb phase h-AX. We combined first principle methods, throught density functional theory, with maximally localized wannier functions tight-binding (MLWF-TB) Hamiltonians to investigate excitonic effects by solving Bethe-Salpeter equation (BSE). Our analysis focused on the electronic, optical properties, describing the linear optical processes, taking into account the excitonic effects inherent, due the quantum confinement, in these 2D materials. Firstly, we investigated the crystall stability by phonons in 2D honeycomb phase, our the results revealed that from the 9 investigated systems seven are thermodynamically stable. From the electronic properties, we obtained band gap energies exceeding 0.7 eV, suggesting the potential for forming heterostructures with diverse properties and applications in solar harvesting devices. Our objective is to furnish a thorough comprehension of the fundamental properties and excitonic behaviors within two-dimensional materials of III-V compounds. This work provides valuable insights into the fundamental aspects of synthesizing semiconductor materials formed by group III-V in two-dimensional structures and heterostructures, exploring new possibilities.

Exploring biocidal properties of Ag-based semiconductors using high-throughput Density Functional Theory

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The ongoing SARS-CoV2 pandemic has posed a significant challenge to global health, leading researchers to search for effective materials that can combat its spread [1]. Ag-based semiconductor oxides have been identified as a promising solution due to their ability to generate Reactive Oxygen Species (ROS) that can kill microorganisms and prevent their transmission [2]. This research aims to further explore the potential of Ag-based semiconductors in combating the SARS-CoV2 virus and other microorganisms by applying a high-throughput computational approach using Density Functional Theory to analyze the surface stabilities and reactivities of these Ag-based materials [3]. The ultimate goal of this research is to improve public health outcomes by providing insights into the most effective Ag-based materials for ROS formation and the inhibition of microorganism transmission.

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Exploring Interface Phenomena in Persistent Luminescent Glass Matrix Composites via Synchrotron Light and Cathodoluminescence

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Persistent phosphors, known for their outstanding luminescent properties, have gained significant attention in various scientific and industrial domains. However, there is a critical need to improve their stability and expand their range of applications. In this study, we created a translucent persistent glass matrix composite (PeL-GMC) through pressureless viscous sintering, using silicate glass as the base material and embedding persistent luminescent microparticles (PeL-MPs) of strontium magnesium silicate with the composition $Sr_2MgSi_2O_7:Eu^{2+}$; Dy^{3+}. We investigated the PeL-GMC using synchrotron radiation-based techniques and cathodoluminescence intensity maps. Specifically, we analyzed emission spectra changes in a polished cross-section of the composites to identify structural changes after PeL-MP incorporation, focusing on the glass-PeL-MPs interface. Additionally, we compared cathodoluminescence and X-ray excited optical luminescence (XEOL) results in spectral mode to evaluate the sensitivity of each technique, highlighting their respective strengths and limitations. X-ray fluorescence (XRF), scanning transmission X-ray microscopy (STXM), and X-ray absorption near edge structure (XANES) were also employed to reinforce our findings.

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Exploring the use of earth-abundant layered materials in 2D-based studies: from natural mines to van der Waals applications

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Phyllosilicate minerals are an emerging class of naturally occurring layered insulators with large bandgap energy that have gained considerable attention from the scientific community. This layered materials (LMs) class has been explored recently at the ultrathin two-dimensional (2D) level due to their specific mechanical and optoelectronic properties, which are crucial for engineering novel devices. Phyllosilicates have lamellar structures and can be embedded into van der Waals heterostructures due to the possibility of exfoliation down to monolayers (MLs) and easy handling. Here, we will present a high throughput characterization of some naturally occurring LMs by employing several experimental techniques and first-principles calculations. We will demonstrate that these LMs can be applied in different nanotechnological areas [1-6]. Consequently, phyllosilicate minerals can be considered promising low-cost nanomaterials for electronics, photonics, and optoelectronics future 2D-based device applications. We will also present features of these nanomaterials relevant to their use in potential 2D-based applications, discussing the major challenges in working with them.

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Exploring Topological Transport Properties in Pt_2HgSe_3 Nanoribbons

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The quantum spin Hall effect paved the way for the design and development of spintronic devices [1]. On the other hand, researchers are interested in finding new materials that could host such electronic properties. Here, we theoretically investigated the electronic conductance of a realistic quantum spin Hall system, Pt_2HgSe_3 [2] nanoribbon, presenting a large topological gap [3,4,5]. Through an ab initio approach, we investigated the material's edge states, finding a penetration depth of about 0.9 nm, in contrast with much smaller ones predicted in other 2D topological systems [3]. This allows the exploitation of Pt_2HgSe_3 nanoribbons as a viable platform for topological electronic transport realization. We studied the electron conductivity using non-equilibrium Green's functions calculations, including SeHg antistructure defects randomly distributed within the Pt_2HgSe_3 scattering region. We investigated different scattering lengths up to 109 nm, thus finding localization lengths that can surpass µm dimensions for narrow-width nanoribbons (9 nm). Our findings can contribute to further understanding the behavior of topological insulators under realistic conditions, as well as their integration within electronic and spintronic devices.

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Fabrication technique of graphene-based modulator over side-polished fiber.

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As communication and transmission systems continue to advance, the demand for compact and efficient devices becomes crucial [1]. Optical modulators, essential components in these systems, can be made with various materials InGaAsP, InP, Si, and more. Notably, recent research has explored the integration of graphene monolayers for electro-optical modulator fabrication [2]. In this study, we concentrate on crafting a graphene-based modulator featuring a capacitive structure. This structure uses conductive plates composed of two graphene monolayers produced via Chemical Vapor Deposition (CVD) on a side-polished fiber (SPF). The dimensions are tailored to the optical fiber's core area, approximately 8 µm in diameter, to modulate the TE mode of the light beam, typically at a wavelength of 1550 nm. The graphene, synthed via CVD, is transferred to the side-polished surface using the wet transfer method [3]. Subsequently, chromium and gold layers are deposited for electrical contact. Following this, Atomic Layer Deposition (ALD) is employed to create a thin layer of Al2O3, serving as the dielectric of the capacitor. Finally, the second graphene monolayer and the upper electrical contact are stacked. To enhance modulation efficiency, a layer of PMMA is added over the capacitor. This modulator design mirrors established graphene-based capacitive structures from literature, aiming to empirically validate findings from simulations on SPF [4].

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Femtosecond vacuum ultraviolet source for time-resolved ARPES

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This work presents the development of a vacuum ultraviolet (VUV) femtosecond pulse source tailored for time- and angle-resolved photoemission spectroscopy (ARPES) [1]. We present the initial outcomes of our efforts, with a focus on generating 7.2 eV and 10.8 eV pulses, corresponding to the 6th and 9th harmonics of our fundamental laser energy (1.2 eV), respectively. These pulses are synthed through a cascade nonlinear frequency conversion setup utilizing nonlinear crystals and noble gases, facilitating high repetition rates (> 50 kHz) to counteract potential space charge effects. Such effects, if unaddressed, could degrade the energy and momentum resolution crucial for accurate ARPES measurements. The laser driver for our VUV source is an industrial-grade femtosecond laser system with long-term energy and beam pointing stability. Such stability is paramount for conducting prolonged acquisition measurements, which are a common necessity in various photoemission spectroscopic techniques. Furthermore, we aim to find an optimal balance between energy and time resolution, while ensuring a high photon flux at increased repetition rates. The main goal of this VUV ultrashort pulse source is to support future time resolved ARPES studies on quantum materials, using a setup that combines an optical pump with a photoemission probe. By integrating this source with an ARPES spectrometer in a pump-probe configuration, we will be able to access the equilibrium unoccupied band structure and gain profound insights into the dynamics of photoexcited carriers with simultaneous energy and momentum resolution in quantum materials.

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Fitting method for band structures using k·p Hamiltonians and symmetry properties to obtain effective mass parameters and g-factor

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Effective Hamiltonians are used to describe realistic band structures at a lower computational cost than ab initio calculation[1,2,3]. The k·p method has been used by the IFSC's Laboratório de Física Computacional (LFC) and collaborators, combined with Löwdin partitioning and effective mass terms that go beyond zero order, making fittings to previously calculated band structures [1]. The group has been updating the method to include the use of the system's symmetries, to determine odd terms of the Hamiltonian for better modeling of spin-splitting, and using restrictions that allow the spatial inversion symmetry of the Hamiltonian to be described. The computational package was developed in Python and uses as input previously calculated energy values in specific directions in the BZ, obtained with DFT for example. The calculations are then carried out using the minimization process in the curve fitting using the lmfit package and, for each parameter involved in the interband interactions, an analysis is carried out concerning the parabolic behavior of the bands. In this way, the other bands are inserted into the model and the g-factor values are recalculated. The method was applied to a 14-band model for GaAs in the Zincblende form. The results provided excellent curve fits and parameter values such as effective mass and g factor, as well as the Luttinger and Kane parameters, in accordance with the literature and with low computational cost.

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Formation of entangled states in phonon-polaritons interacting system

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Many of the quasiparticles found in semiconductors play a fundamental role in describing the properties that arise in many-body systems. In 1972, Keldysh and Ivanov [1] predicted the emission of phonoritons, quasiparticles emerging from the strong coupling between photons, phonons, and excitons, that were recently detected [2]. Here we investigate quantum dynamics and quantum entanglement in a system composed by phonons and polaritons quasiparticles, forming a tripartite bosonic system, given by one phononic subsystem and two polaritonic subsystems. The hamiltonian of the system contains the non-interacting term H_0, that describes each of the three modes separately and an interacting term H_{int}, that accounts for the coupling between the three subsystems. The coupling between phonons and polaritons is given by two distinct process, g_1 that accounts for each polariton population coupled to the lattice dipole induced by acoustic phonons, and g_2 that describes inter polariton subsystems hopping, mediated by creation or annihilation of acoustic phonons. Based on density matrix formalism we search for evidences of entanglement, analyzing quantifiers such as negativity, Von Neumann entropy, and quantum mutual information (QMI). Preliminary results reveal the presence of entangled states in the tripartite system, mediated by g_2 interaction. Additionally, the role of phonoritons in the formation of highly entangled states will be discussed.

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Fotoconductivity effect on epitaxially Bi2Te3 films doped with Eu atoms

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In this work, we present measurements of the photoconductivity effect performed on bismuth telluride films doped with Eu atoms (Bi2Te3:Eu) using different wavelengths of light and temperatures ranging from room temperature to the temperature of liquid nitrogen. Bi2Te3 is a narrow gap semiconductor that has been extensively studied in recent decades due to its potential application in the development of thermoelectric devices.[1] Recently, Bi2Te3 was theoretically predicted and experimentally demonstrated as a three-dimensional topological insulator (TI), a new class of materials with unique quantum mechanical properties. Such properties are related to the band structure of these materials that exhibit a finite band gap in the bulk and band-free surface states with linear Dirac cone-shaped dispersion.[3] Regarding the photoconductivity effects in this material, a negative photoconductivity transition for positive it was found around 125K for 150nm thick Bi2Te3. The transition effect was analyzed using the recombination and generation equations, and the associated activation energy, calculated from the recombination time, obtained from experimental photoconduction decay curves.[3] This work will investigate, for the first time, the role of Eu atoms in the electrical transport properties of films and photoconductivity amplitudes over a wide range of temperatures. From the transport properties, an overview will be presented of the effect of photoconductivity on Bi2Te3:Eu films and how its properties can lead to the development of new high-performance near-infrared (IR) photodetectors.

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General Hamiltonian learning through neural network

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Recently, significant attention has been directed towards artificial intelligence (AI), with machine learning (ML) emerging as a crucial tool for extracting insights from vast datasets. While ML has found widespread application in various fields, its integration with physics has only recently gained momentum.One of the pioneering applications of ML in physics involved analyzing particle physics experiments. Additionally, ML techniques have been successfully applied in condensed matter systems, AdS/CFT correspondence, and phase transition determination.In this study, we leverage ML, particularly the Physics-Informed Neural Network (PINN), to determine the physical parameters of a general system comprising N-qubits. The PINN approach relies on the universal approximation theorem, which asserts that neural networks can approximate any function given sufficient complexity. By utilizing additional data provided by the user, intrinsic physical parameters can be extracted from experimental data through inverse-PINN. We first apply inverse-PINN to extract all physical parameters constituting a two-qubit Hamiltonian. Our findings demonstrate the method's efficiency, even in the presence of small errors in experimental data. While the inverse-PINN technique could theoretically be extended to N-qubit systems, the computational cost increases exponentially with the number of qubits. As an alternative approach, we propose a scheme where we learn the total Hamiltonian by analyzing pairs of qubits individually, effectively freezing interactions with other qubits. This freezing is achieved through a method akin to dynamical decoupling, wherein proper external fields are applied to N-2 qubits.

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Growth and characterization of CdCl2-doped CdTe by hot wall epitaxy for future applications in solar cells

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CdTe is one of the candidates for more efficient solar cells due to band gap of 1.5 eV, high absorption coefficient and relative ease in forming thin films. Solar cells utilizing CdTe/CdS films have demonstrated efficiencies exceeding 20%, employing CdTe deposited through various methods such as thermal evaporation, sputtering, chemical vapor deposition (CVD). This study focuses on investigating the growth and characterization of CdTe, with particular emphasis on the CdCl2 treatment process. In this study, our focus is the growth of CdTe on ITO glass substrates using the hot wall epitaxy (HWE) method. This technique offers notable benefits, including precise temperature control during deposition, enabling the optimization of thin film properties. Additionally, it provides more uniform and high-quality deposition compared to conventional thermal evaporation techniques. A critical aspect of this study is the subsequent thermal treatment with CdCl2 after CdTe deposition. This process has been shown to be crucial for improving the properties of CdTe films. In addition to enhancing grain growth and reducing defect density, CdCl2 treatment promotes interdiffusion at the CdTe/CdS junction interface, directly impacting solar cell efficiency. The work is dedicated to a detailed analysis of the effects of this treatment, particularly regarding CdTe grain and the associated reduction in resistivity. X-ray diffraction (XRD), atomic force microscopy (AFM) and Raman spectroscopy were used in the characterization of the CdTe film. Additionally, photoinduced effects due to laser excitation during Raman measurements which induce the growth of the crystalline phase of tellurium are discussed.

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Growth of epitaxial ZnS ultrathin films on Ag(111) using two different growth methodologies

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Zinc Sulfide (ZnS) is an important semiconductor compound studied in materials science with several applications like sensors, photocatalysis, solar cells, etc [1]. Bulk ZnS crystallizes in either zincblende (ZB) or wurtzite (WZ) structures, with the cubic ZB form being the more stable phase at ambient conditions. In an attempt to modify the properties of regular ZnS bulk materials, the synthesis and growth of various nanostructured ZnS have attracted considerable interest. However, in the literature, there are only a few reports of ultrathin film growth [2] and theoretical investigations [3]. In this study, a single layer of ZnS consisting of a few atomic layers of ZnS(111) plane has been grown on Ag(111) using the gas source molecular beam epitaxy(GSMBE) technique with two different methodologies called “Room Temperature Growth” and “Hot Growth”. The ultrathin film was characterized using X-ray photoelectron spectroscopy (XPS), X-ray photoelectron diffraction (XPD), low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM). In “Room Temperature Growth”, a small shift in Zn 2p3/2 core-level indicates the formation of ZnS in XPS; LEED measurements indicate the predominance of the superstructure of ZnS-(3x3)/Ag-(4x4); STM proposes the coexistence with ZnS(2x2)/Ag(4x4) structure and XPD proposes the formation of two layers of ZnS with Zn termination. In “Hot Growth” we also found the formation of ZnS in XPS; LEED indicates now the predominance of the superstructure of ZnS-(2x2)/Ag-(4x4), and STM corroborates these results. XPS was also used to investigate how the system evolves thermodynamically with increasing temperature, demonstrating that the ultrathin film ZnS/Ag(111) is stable until it reaches 285 °C.

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Growth of High-Quality CdTe on SOI (111) Substrates for Integrated Devices

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Silicon substrate has been widely used for many years as one of the main platforms for basic physics research as well as the fabrication of nanostructured devices. High-quality heteroepitaxial growth of group II-VI semiconductor as CdTe on Si substrates has an important role due to potential as infrared and gamma ray detectors. Furthermore, CdTe self-assembled QDs and CdTe diode-type device optimization for X-ray detectors [3] on Si substrates have been explored in last years. Recently, CdTe/CdMnTe heterostructures grown on Si(111) substrate [1] have demonstrated potential as optical materials, even with large lattice mismatch of almost 20% compared to silicon. Recent advancements in flexible electronics have opened new possibilities for integrating CdTe into flexible devices, such as bendable and conformable electronics, lightweight and portable devices, and integration with curved structures. In this study, we focus on the growth of CdTe thin films on Silicon on Insulator (SOI) substrates oriented along the (111) plane by molecular beam epitaxy (MBE). Despite the significant lattice mismatch and the typically lower quality of SOI compared to standard Silicon wafers, our results from AFM, Raman and X-ray diffraction reveal the formation of high-quality CdTe <111> oriented thin films. We demonstrate the successful transfer of the released CdTe/Si membrane heterostructure to a flexible new host substrate without compromising its structural integrity. This research opens new possibilities demonstrating a potential for flexible devices integrating high-quality CdTe in several areas such as silicon-based photonics and photovoltaic devices.

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Growth of High-Quality cubic MnTe on GaAs (001) by molecular beam epitaxy

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MnTe is a magnetic semiconductor which presents stable and metastable crystal phase. The stable MnTe phase crystallizes typically in the hexagonal structure, while the metastable MnTe phase arises as zinc blende structure. Antiferromagnetic materials as MnTe has been widely studied due to their role as next-generation spintronic devices and quantum computing. Furthermore, basic studies have been developed using epitaxial MnTe structure such as observation of spontaneous anomalous Hall effect [1] and the recently discovered of the “altermagnetism” phenomenon [2]. This work conducts a study on the growth and properties of cubic MnTe which were grown on GaAs (001) substrates by molecular beam epitaxy (MBE). The metastable MnTe structure is not usual to reach. However, the nonequilibrium growth by MBE has been used to grow cubic MnTe on GaAs substrate. The investigated samples consisted of thin films of MnTe produced by individual sources of Mn and Te, which were analyzed by X-ray diffraction (XRD), atomic force microscopy (AFM) and Raman spectroscopy. Despite the large lattice mismatch between MnTe and GaAs (almost 13%), it is possible to control the growth of high-quality films on this substrate.

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Halting Thermalization in Spin Chains with Single-Ion Anisotropy

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The concept of thermalization in physics describes how a macroscopic system evolves over time towards balance. For instance, a hot cup of coffee in a cold room eventually reaches thermal equilibrium as it cools to room temperature. In quantum mechanics, a closed system progresses according to its Hamiltonian from an initial state. Statistical physics suggests that closed quantum systems with many particles naturally achieve thermal equilibrium as different parts interact, evenly spreading energy. However, in the 1950s, P. W. Anderson showed that disorder can confine non-interacting systems, halting the attainment of thermal equilibrium. This led to the concept of Anderson Localization (AL) [1]. Subsequent research unveiled Localization in Many-Body Systems (MBL) [2] in disordered systems. M. Schutz later demonstrated that thermalization breakdown is possible even without disorder, introducing Stark Many-Body Localization (SMBL) [3]. This phenomenon, observable in various systems like Heisenberg spin chains, remains robust when nearest-neighbor couplings are included. In this study [4], we investigate SMBL in spin chains with spin S=3/2 under single-ion anisotropy. We find that anisotropy alters SMBL in non-trivial ways and can independently suppress spin dynamics, leading to localization for substantial anisotropy values. When magnetic field gradient and anisotropy are comparable, they compete, resulting in poor system localization.

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Highly uncommon fluorescence phenomena in organic materials

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Photoluminescent pure organic materials represent an intriguing low-cost alternative, characterized by ease of handling and the potential for modulation its optical properties through conformational or substituent changes. This study presents a diverse set of molecules with different functional groups exhibiting rare photoluminescent properties. A series of carbazole-based molecules display phosphorescence at room temperature. Another series based on thiazole exhibits white fluorescence and deviates from the Kasha rule. A comprehensive photophysical study was conducted to characterize and elucidate the origins of these effects. Including time-resolved spectra, lifetimes, and photoluminescence in various matrices, for example.

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How does the pressure of sputtering chamber affects the structural, optical, morphological and photocurrent properties of ZnO thin films

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Nanostructured oxide materials are currently used as biosensors in technological applications. These materials are of great interest due to their potential for use in medical diagnostics, as they enable rapid, non-invasive, and low-cost evaluations. In this work, zinc oxide (ZnO) films were produced by the sputtering deposition method, varying the working pressure [1] [2], in order to obtain materials with specific features which can be used as gas sensors. Surface analysis using SEM revealed the formation of microrods and grains. The average width and diameter seem to be independent of the working pressure and remained at ~300 nm and ~200 nm, respectively. X-ray diffraction analysis revealed the formation of ZnO's wurtzite phase with preferential orientation along the [002] direction. It was determined that the film thickness decreases as the working pressure is increased. XRD data analysis also indicates that the mean crystallite and lattices constants decreases as the working pressure is increased. UV-Vis spectroscopy results revealed that the band gap energy of the films does not show a clear tendency with the working pressure. However, Urbach Energy increases from 0.1 to 0.3 eV, suggesting the formation of more defects as the film thickness becomes thinner. The temperature dependence of the resistivity of the films in the range from 300 to 573K shows a typical semiconducting behavior and indicates the presence of two activation energies. Photocurrent measurements for the films showed a good sensitivity to UV light [3]. Data analysis indicates the presence of trap energies at 0.58 and 0.63 eV, suggesting fast and slow response, respectively. Tests of sensor response using methane gas were carried out, which showed that the ZnO films can be used as a gas sensor material.

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Hybrid organic-inorganic heterostructures based on graphene and phthalocyanine molecules to improve the sensitivity and selectivity of contaminant gas sensors

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Toxic gas sensors are products of great relevance for human health safety. Therefore, ideas that solve or facilitate the obtaining of these sensors are necessary. However, the materials commonly used in the production of gas sensors are semiconductor metal oxides [1]. These materials have the disadvantage of thermal instability, irreversibility and low sensitivity [2]. In this work, organic/inorganic hybrid heterostructures based on graphene obtained by chemical vapor deposition (CVD) will be used for application in gas sensors. Our goal is by combing these two materials be able to modulate, modify, and improve the physicochemical properties of the hybrid materials studied with respect to pristine cases. By functionalizing graphene with organic molecules and nanoparticles, it is possible to preserve many of the original properties of these materials, as this increases the compatibility and binding capacity with ions or biomolecules of the heterostructures formed and thus, an improvement in the efficiency of the sensor. The deposition of organic molecules on graphene will be carried out through evaporation in high vacuum chambers gy using physical vapor deposition (PVD). Characterizations of the hybrid heterostructures will be carried out using Raman spectroscopy, XPS, UPS, among others. Afterwards, we inted to fabricated field-effect transistors composed by these hybrid materials and test it towards gas sensor and compare with respect to pristine graphene devices. This work will contribute to the area of gas sensors, producing products that are more efficient and beneficial compared to current ones.

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Improvements in Exciton Lifetime in Perovskite Nanowires: A Study of Temperature and Strain Effects.

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There remains a significant controversy in materials science about whether ferroelectricity or ferroelasticity more critically defines the optoelectronic attributes of metal halide perovskites. This study examines the temperature-dependent photoluminescence of CsPb(Br(1-x)Clx)3 nanowires and their heterojunctions. We discovered that exciton lifetimes are prolonged due to phase transitions within the crystal structure, independent of the halide mix and its influence on transition temperatures. This phenomenon could potentially enhance the functionality of perovskite-based solar devices under conditions of elevated light concentration at temperatures above standard room temperature. The nanowires are conceptualized as disordered strain superlattices where flexoelectric spatial modulation significantly influences their luminescent characteristics. This conceptual model might also apply to other metal halide perovskite configurations, suggesting a broader applicability to understanding and improving perovskite optoelectronics.

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Influence of sublattice symmetry alteration on the electronic behavior of Lieb, transition, and Kagome structures and nanostructures

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Since the isolation of graphene in 2004, the scientific community has been looking for new two-dimensional (2D) materials aimed at different technological applications. It is known that the chemical components involved, the type of hybridization, and the geometry formed are key factors for the resulting electronic band structures. This led to a theoretical investigation into possible designed crystals with desired geometries and interesting physical properties. Examples of 2D materials engineering are the Lieb and Kagome lattices, in which their band structures are formed by the coexistence of a conical Dirac energy band and a flat (non-dispersive) band. [1] Motivated by the growing interest in flat band systems, by the experimental ways to induce sublattice symmetry breaking, for example, due to substrate in graphene [2], and inspired by studies exploring finite effects and ways to manipulate their energy spectra, here we systematically study the effects of sublattice symmetry breaking on the electronic properties of nanoribbons and infinite sheets of Lieb, transition, and Kagome lattices. Our theoretical framework is based on a generic tight-binding Hamiltonian, which allows us to investigate evolutionary stages between Lieb and Kagome lattices. Results for three nanoribbon terminations are discussed: straight, bearded, and asymmetric edges. By considering different on-site energy configurations, we analyze, for infinite Lieb-kagome lattices, the degeneracy lifting of the energy bands, changes in the dispersive spectrum of the flat band, and Dirac cone shifting in momentum space, and in addition, for their nanoribbons, the spatial distribution of the wave functions and changes on the curvature of the edge states are explored for different types of edges.

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In situ thermal annealing of MoS2 thin films deposited by RF sputtering for spintronics applications.

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Spintronics is an emerging field that relies on electron spin properties for information storage and transmission. Specifically, one of the most promising material for spintronics is molybdenum disulfide (MoS2), due to its unique properties as intrinsic spin-orbit coupling (SOC), which enables its use in studies involving spin effects [1]. This work reports the fabrication and characterization of MoS2 thin films and hybrid magnetic nanostructures based on MoS2 applied in the detection and conversion of spin-to-charge current. MoS2 thin films were deposited by RF sputtering on Si/SiO2 substrates at room temperature and subjected to an in situ thermal annealing varying temperature after deposition. Results from AFM, SEM, Raman analysis, and XRD indicate that MoS2 thin films treated at high temperatures (>500 ºC) show better morphological, superficial structure, crystallinity and quality when compared to as-deposited thin films. Furthermore, by XRD it was observed that these films have a preferential growth orientation in the (002) plane. Characterization with HRTEM images was also conducted, showed good crystalline quality, and layered structure in samples of different thicknesses heat-treated at 600 ºC. These results show that the sputtering technique is suitable for the synthesis of good quality MoS2 thin films when subjected to thermal post-treatment. Finally, we report the conversion of spin to charge in a magnetic hybrid nanostructure composed of a thin film of MoS2 coupled with a NiFe film at room temperature through the generation of spin currents by microwave-driven ferromagnetic resonance spin pumping.

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Investigating Weak (Anti)Localization and Negative Magnetoresistance in Few-flake Reduced Graphene Oxide

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Since the isolation of graphene in 2004 and the experimental observation of its unique electronic properties, the research field of two-dimensional materials has received enormous scientific interest. Among the large variety of existing 2D materials, graphene oxide (GO) has emerged as a crucial material for scalable manufacturing of diverse applications. However, GO is an insulating material and to improve its conductivity, one can rely on diverse reduction methods (e.g. thermal, chemical, electrochemical, etc.) to obtain reduced graphene oxide (rGO). It is already known that in two-dimensional graphene, the peculiar nature of low-energy electronic states yields a wealth of anomalous transport features such as Klein tunneling, weak localization and antilocalization, unconventional quantum Hall effect, or new ways to guide charge flows [1]. Therefore, in this study we aim to investigate the influence of the reduction process on the electrical transport properties of multilayered rGO thin films which were prepared by different methods such as electrochemical and thermal reduction. From magnetotransport measurements, we observed normal magnetoresistance, negative magnetoresistance, weak localization and weak antilocalization phenomena in such films. These anomalous transport properties are typical of disordered systems, being essentially caused by quantum-interference of the charge carriers [2]. In our discussion, we will analyze such effects in rGO films, considering the underlying physics and possible implications on the performance of rGO-based electronic devices.

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INVESTIGATION OF THE ELECTRONIC AND MAGNETIC PROPERTIES OF FEWLAYER CrPS4

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Ferromagnetic van der Waals crystals are two-dimensional materials (2D materials) that have been attracting great interest for applications in spin and valleytronic devices [1,2]. These 2D materials appear as promising candidates for spin valves, spin field-effect transistors, and magnetic tunnel junction devices. More interestingly, their magnetic properties are susceptible to external tuning via the application of electrostatic doping and magnetic fields, but narrow energy bands present in most of these 2D materials pose a significant challenge in transport investigation. In this work, we chose to study monolayer samples of CrPS4, a lamellar semiconductor with a band gap close to 1.745 eV. Initially, we explored methods for isolating, characterizing, and transferring a single layer of the material. From there, we aimed to develop field-effect transistors capable of adjusting the Fermi energy by controlling the band gap, and next, we intend to investigate transport and magnetoresistance influenced by the external magnetic field. Future perspectives include expanding these techniques to other two-dimensional materials, such as CrSBr, and applications in heterostructured devices.

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Investigation of transition metal dichalcogenide monolayers using CMOS-compatible field-effect-transistors

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Graphene's discovery resulted in an uprising of two-dimensional (2D) material studies and applications, mainly in electronics and optoelectronics [1]. Among them are the transition metal dichalcogenides (TMDs), 2D materials made of layers of covalent bonds between the transition metal and the dichalcogenide. In the monolayer (ML) form, tungsten disulfide (WS2) is a direct bandgap material, which does not apply to its multi-layer counterpart [2]. Moreover, the low bandgap value (~2eV) makes ML-WS2 applicable in electronic devices, such as field effect transistors (FETs) [3]. Its operation consists of controlling the current between two terminals (drain and source) by applying of a voltage on another terminal (gate) [4]. In this sense, the main objective of this work is to fabricate FETs using WS2 as the active material on a hexagonal boron nitride (hBN) passivating layer. These devices allow for extracting of the ML-WS2 electrical properties such as carrier mobility. This requires adequate contact engineering for contact resistance reduction between the TMD and the metal electrodes [3]. We also aim to chemically characterize the ML-WS2 material using non-destructive techniques such as photoluminescence and Raman spectroscopy. In addition, as a perspective work, we aim to fabricate FETs from other TMD materials to investigate the carrier mobility during cooling experiments from 300K to 2K.

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Investigation on the vibrational and electric properties of PbI2 2D crystals

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Lead Iodide (PbI2) is a metal halide semiconductor with a direct gap in its bulk form and presents strong applications as high-energy photodetectors and photovoltaic cells [1,2]. It has trigonal symmetry belonging to the P3¯m1 space group, with one lead atom and two iodine atoms covalently bonded in its unit cell. This material possesses weak van der Waals interactions between layers where different ordination forms give rise to different phases of the material. The most common phases observed in normal temperature and pressure conditions are the 2H and 4H polytypes. There are four optical modes predicted by group theory, two of them being Raman active, belonging to the irreducible representation E_g and A_1g, and another two being infra-red active belonging to the irreducible representation E_u and A_2u. The four vibrational modes are localized in crescent order of frequency in approximately 72 cm^(-1), 94 cm^(-1), 106 cm^(-1) and 113 cm^(-1), respectively. In this work, we observed a phase transition from the 2H to 4H crystalline phase at a temperature of 415K, as mentioned in the literature [3]. Moreover, we investigate the Raman and Photoluminescence spectra of 2D crystal samples with different thicknesses determined by atomic force microscopy (AFM). We observe a strong dependence on the intensity ratio of the Raman modes with respect to the sample thickness as well as a blueshift of the bandgap of the material, as the samples get thinner, in accordance with theoretical predictions previous reported in the literature [4].

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Investigations of the photoconductivity effect in bismuth-doped Pb0.5Sn0.5Te films

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In this work, we investigated the photoconductivity effect in undoped and doped Pb0.5Sn0.5Te epitaxial films, with bismuth (Bi) atoms, at temperatures of 77 K and 300 K. The results show that the samples show negative photoconductivity effect (NPC) and persistent photoconductivity (PPC). A detailed study was performed on Pb0.5Sn0.5Te sample doped with 0.15% Bi, which presented higher photoconductivity amplitude than the other samples, by performing Hall effect and photoconductivity measurements in the temperature range of 77 – 300 K under dark and illuminated conditions. Using Arrhenius model, trap activation energy was extracted and compared with energies found in literature. From the Hall measurement we found that the NPC effect observed is due to a decrease in the mobility when the sample is illuminated while the carrier concentrations are nearly unaltered. It was also found that Pb0.5Sn0.5Te:Bi presented photoconductivity response for a wide range of wavelengths, indicating that it is potentially interesting for application in optic sensor devices.

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Light-assisted resistive memory effect in ZnO:Na film

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Some semiconductor oxides are notable for exhibiting a resistive memory effect, characterized by the changes of device electrical resistance during an I–V sweep. The transition from low to high resistances, may be driven by a variety of conduction mechanisms [1,2]. This study explores the effects of optical excitation on the memristive properties of a sodium-doped ZnO film (ZnO:Na) grown by spray pyrolysis. The cyclic I-V curves measurements conducted in a free atmosphere and at room temperature reveal that the observed memory effect strongly correlates with the interaction of the film surface with the atmosphere. By employing lateral planar electrical contacts, the ZnO:Na film, when optically stimulated with UV laser of different intensities, we demonstrate a conductance increase and a change in the profiles of the hysteresis loop in contrast with the I-V curves observed in the absence of light stimulation. Additionally, to establish the optimal range for I-V sweeps under illumination, photoconduction measurements were conducted under UV excitation, allowing the identification of the period at which generation and recombination rates of photoexcited carriers stabilize. In this context, understanding the electronic conduction mechanisms influenced by light not only provides insights for developing faster and more efficient energy storage devices but also leads to innovations in the field of optoelectronics.

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Localized-states Quantum Confinement Induced by Roughnessin CdMnTe/CdTe Heterostructures Grown on Si(111) Substrates

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This work shows that despite a lattice mismatch of almost 20%, CdMnTe/CdTe/CdMnTe heterostructures grown directly on Si(111) have surprisingly good optical emission properties. The investigated structures were grown by molecular beam epitaxy and characterized by scanning transmission electron microscopy, macro- and micro-photoluminescence. Low temperature macro-photoluminescence experiments reveal three emission bands which depend on the CdTe layer thickness and have different confinement characteristics. Temperature measurements reveal that the lower energy emission band (at 1.48eV) is associated to defects and bound exciton states, while the main emission at 1.61eV has a weak 2D character (two-dimensional confinement) and the higher energy one at 1.71eV has a well-defined 3D nature (three-dimensional confinement). Micro-photoluminescence measurements show the existence of sharp and strongly circularly polarized (up to 40%) emission lines which can be related to the presence of Mn in the heterostructure. This result opens the possibility of producing photon sources with the typical spin control of the diluted magnetic semiconductors using the low cost silicon technology.

Longitudinal Spin Seebeck Effect Thermopiles Based on Flexible Co-Rich Amorphous Ribbons/Pt Thin-Film Heterostructures

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Thermoelectric phenomena, such as the Anomalous Nernst and Longitudinal Spin Seebeck Effects, are promising for sensor applications in the area of renewable energy. In the case of flexible electronic materials, the request is even larger because they can be integrated into devices having complex shape surfaces. Here, we reveal that Pt promotes an enhancement of the thermoelectric response in Co-rich ribbon/Pt heterostructures due to the spin-to-charge conversion. Moreover, we demonstrated that the employment of the thermopiles configuration in this system increases the induced thermoelectric current, a fact related to the considerable decrease in the electric resistance of the system. By comparing present findings with the literature, we were able to design a flexible thermopile based on LSSE without the lithography process. Additionally, the thermoelectric voltage found in the studied flexible heterostructures is comparable to the ones verified for rigid systems.

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Magnetic field effect on the symmetry-breaking induced chiral states in $\alpha - T_3$ lattice

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Similarly to graphene, sublattice-symmetry breaking in the $\alpha - T_3$ lattice leads to a bandgap opening. In addition, when one introduces a defect line in the substrate where the $\alpha - T_3$ lattice is deposited, viewed as a topological change in the substrate that induces translational in-plane symmetry breaking, middle-gap states emerge. These topologically protected states are confined along the defect line and exhibit a chiral behavior, i.e. presenting a preferential group velocity, with different signs for the different Dirac valleys. In this work, we investigate how these unidirectional localized states are affected in the presence of a perpendicular magnetic field and how they can be tuned by varying the controlling system parameter responsible for merging the $\alpha - T_3$ structure from a honeycomb-like lattice ($\alpha=0$) to a dice lattice ($\alpha=1$). Our theoretical framework is based on the continuum approximation described by a 3×3 matrix with sublattice symmetry-breaking term given by $\Delta(x)$ diag(1 -1 1), assuming two different settings for the $\Delta(x)$ function: (i) kink-like and (ii) kink/anti-kink mass potential profiles. Landau levels of $\alpha - T_3$ lattice under sublattice symmetry-breaking are shown in the dispersion relations to clarify the energetic states' origin and the valley degeneracy lifting. Results for dispersion relations and wavefunction distributions for different α parameters, magnetic field amplitudes, and domain wall lengths are discussed.

Magneto Dependent Exciton-Phonon Coupling in Twisted WSe2

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Monolayer transition metal dichalcogenides (TMDs) exhibit rich physics related to their excitonic complexes. In these materials, the reduction of the dielectric screening collaborates with the intensification of Coulomb interaction and, consequently, the formation of exciton with high binding energy and other complexes involving more carriers. In particular, TMDs present spin-orbit coupling, promoting valence and conduction band splitting, and valley structure can be verified with circularly polarized light. In a slightly different system, the band structure and the excitonic properties can be tuned if two layers of TMDs are placed, one on top of the other with a twist angle, producing a twisted WSe2 material (t-WSe2). In our work, we investigate the excitonic states of high-quality t-WSe2 encapsulated in hBN crystals. We inspect the photoluminescence's polarization and magneto dependency at low temperatures. Comparing with the monolayer case, we observe a new emission that rises for high magnetic fields (B > 7 T) that is very likely related to the E” phonon in the K point and an electronic state of the moiré pattern. Our results may reveal this electron-phonon interaction owing to the formation of a hybridized exciton phonon replica with a real state in the moiré electronic structure in twisted semiconducting 2D heterostructures. Also, we observe emissions from the non-active hBN ZO phonon mode and its sum with A1g WSe2 phonon mode caused by coupling in the interface between the materials.

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Magneto-optical properties and thermal stability of twisted moiré homobilayers

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Moiré homobilayers present a promising avenue for manipulating electron-phonon properties by adjusting the twist angle. At specific twist angles, known as magic angles, bilayers of transition metal dichalcogenides exhibit exciton confinement, holding potential for scalable quantum state production. Our research focuses on investigating a novel magic angle in twisted bilayers of MoS_2, showcasing long-lived moiré excitons. Given the necessity for variable temperatures in processing twisted bilayer MoS_2 into devices, particularly concerning twist angle adjustments, we delve into the thermal stability of this system using Raman and photoluminescence spectroscopies. Additionally, with the aim of utilizing twisted bilayer MoS_2 in switchable devices, we explore the tunability of moiré excitons under magnetic fields and varying polarizations. Our study provides an experimental roadmap for fabricating moiré homobilayers and harnessing their potential in quantum information devices.

Manipulation and excitation of semiconductor particles by means of optical tweezers experiments

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An optical tweezer is formed by a highly focused laser beam through a high numerical aperture objective, capable of trapping particles near the focal region by means of the gradient force. The gradient force in the focal region can be quantified by the parameter trap stiffness (κ), which depends on the optical properties of the semiconductor material. In this work, we present a new interpretation where the laser used to construct the optical trap also excites the semiconductor particles, increasing their carrier density and consequently modifying their optical properties. The nature of the optically generated carriers, whether electron-hole pairs (predominant in inorganic semiconductors like Ge and Si) or excitons (predominant in organic semiconductors like MEH-PPV), directly influences the modification of optical properties, resulting in different responses in the parameter κ. While the generation of electron-hole pairs decreases the refractive index (and, consequently, κ), the generation of excitons increases the refractive index (and, consequently, κ). In both cases, κ is a function of the carrier density N. Our study with MEH-PPV demonstrated that κ is sensitive to variations in the third decimal place of the refractive index for particles approximately 200 nm in radius. Furthermore, for inorganic semiconductors, when the carrier density is sufficient to bring the material's plasma frequency (ω_p) close to the laser frequency (ω), an oscillatory dynamic can be induced in the material due to the nature of the gradient force, which is attractive for $\omega >> \omega_p$ and repulsive for $\omega \approx \omega_p$. Such oscillatory dynamics are consistent with our observations for Ge, Si, Bi_2Te_3 , and Bi_2Se_3.

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Microfabrication of Integrated Cavities in Thin Film Lithium Niobate for Generating Entangled States

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Quantum information science has been an ever growing field in the last decades and has received even more after the first demonstrations of quantum computation advantage. While there is an ongoing debate about the best platform for quantum computation, is it clear that light is the best choive for communication. Quantum communication is based on building a quantum network that reliably shares states between its nodes. Entanglement plays a key role in communications protocols such as quantum teleportation. In this work, we propose the generation of entangled states of light in lithium niobate thin film (TFLN) through the nonlinear process of parametric down conversion (PDC). The generated states are entangled, because the photons are created at the same time. These process depends on phase-matching conditions and overlap between the pump, signal and idler fields. We present finite element method (FEM) simulation showing when it is possible to have phase-matching conditions for the pump, signal and idler fields. Additionally our simulations show that the phase-matching conditions are robust to fabrication errors and how we can to modulate the difference in frequency of generated fields. Besides FEM simulations, we show the best measured quality factors of our cavities.

microRNA Biosensing Through the Functionalization of Semiconducting Reduced Graphene Oxide Employing an Electrolyte-gated Transistor Platform

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Reduced oxide graphene (rGO) is a material that presents electrical properties ranging (semi)conducting to conductor depending on the degree of reduction. When employed as the active layer in thin film transistors (TFTs), rGO devices exhibit ambipolar operation, which can be useful for developing new electronic applications. When rGO TFTs are used in electrolyte-gated transistors EGTs, they represent a powerful device for biosensing applications [1]. The functionalization of the rGO oxygen groups can add several functionalities to such devices. This work aims to functionalize rGO EGTs with ad-hoc bioreceptors to detect biomarkers of stress-related diseases. rGO was produced either via thermal reduction or electrochemical reduction of few-layer graphene oxide (GO) thin films. Two functionalization routes were used to attach a single-stranded DNA receptor (DNAcp), the non-covalent 1-pyrenebutyric acid N-hydroxysuccinimide ester (PBASE) and the covalent 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride (EDC)/N-hydroxysuccinimide(NHS). Different incubation times and concentrations of ssDNA with a sequence similar to the complement of the DNAcp biomarker were used as a negative control. The analytical curves were obtained from 0.01 to 500 fmol L−1 in phosphate-buffered saline (10 mmol L−1, pH 7.4) derived from the EGT transfer curves which were obtained by recording the device source-drain current as a function of the gate-source voltage varing from +0.5 to −0.5 V, with a constant source-drain voltage of 0.2 V. PBASE rGO thermal reduction obtained the best results with a linear range from 0.01 to 500 fmol L−1, R2 = 0.996, and attomol-level sensitivity (limit of detection = 9.0 amol L−1). Our approach aims to contribute to the development of new semiconducting devices for point of care biosensing.

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Nanophotonics properties of Low-dimensional Sn3O4 nanobelts with Synchrotron Infrared Nanospectroscopy.

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Phonon polaritons (PhPs) result from coupling electromagnetic fields and crystal lattice vibrations, creating bosonic quasi-particles analogous to photons confined at the crystalline lattices interfaces with opposite signs of permittivity. They exist from THz to mid-IR spectral frequencies within Reststrahlen bands (RBs), between transversal (ω_{TO}) and longitudinal(ω_{LO}) optical phonon frequencies. PhPs enable light confinement beyond the diffraction limit in nanostructured polar dielectric materials. Their advantages stem from inherently higher quality factors and lower optical losses than plasmon polaritonics. In the far and mid-infrared regime, particular attention has been drawn to strongly confined phonon polaritons (HPhPs) observed in materials like h-BN[1], α-MoO3[2], and SnO2[3] due to their natural hyperbolicity and enhanced waveguiding properties. In the scope of photonics, Sn3O4 exhibits negative permittivity within specific spectral ranges, from far to mid-IR, where various polaritons coexist. We introduces low-dimensional Sn3O4 nanobelts as a lithography-free nanophotonic platform suitable for the cavity confinement of infrared radiation. Leveraging scattering scanning near-field optical microscopy (s-SNOM) in conjunction with Synchrotron Infrared accelerator-based sources, we used broadband Infrared Nanospectroscopy (SINS) to access PhPs cavity modes experimentally. Sn3O4 as a photonic material naturally optimized for the realization of subdiffractional resonators and potentially for waveguiding in the far-IR range.

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Neural network quantum many-body state of a 1D quantum spin chains: a tomographic analysis

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The use of artificial neural networks (NN) for representing quantum many-body states has garnered recent interest as a promising approach to address intricate many-body problems. An important challenge in the application of machine learning techniques to quantum many-body systems is the absence of training sets. This becomes specially important when we want to use a machine learning approach to large interacting systems where exact solutions are not available. This is, for instance, the case of quantum frustrated phases in 1D quantum spin-chains, which are of particular significance in the field of condensed matter physics. In this study, we adopt the neural network quantum state (NNQS) approach to obtain the ground state of 1D spin chains modeled by a J1-J2 model and conduct a comparative analysis with exact diagonalization and density matrix renormalization group (DRMG) technique. We are particularly interested on how can we apply an unsupervised machine learning approach to attain quantum phase transitions in 1D spin chains in the frustrated regime. We observe that there is clearly a sector in the parameter space in which the neural network presents a better performance. By performing a a tomographic analysis of the evolution of the synaptic weights of the NN we aim at identifying why in some regions of parameter space, the NN presents a poorer performance as compared to other regions. This NN tomography may allow us to propose improvement of the current NNs which can open up the possibility of using them to tackle quantum phase transitions in higher order systems, where other methods are known to be inefficient. Our work may not only contribute to the growing body of research exploring the application of neural networks in quantum physics but also may be used to shed light on the intricate dynamics of the frustrated phase in one-dimensional quantum systems.

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Observing Parrondo's effect in continuous-time quantum walks with non-periodic alternation

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The continuous-time quantum walk (CTQW) is a lattice-based model for the propagation of a particle (walker) [1] with diverse applications [2] and experimentally implemented in several ways [3].
The Parrondo effect is a paradoxical phenomenon, where the combination of games with negative outcomes can lead to a scenario with favorable results.
We reported the first mechanism capable of producing a Parrondo effect using CTQWs [4].
It was demonstrated that the periodic alternation between defects, which individually retard the wavepacket propagation, can counterintuitively improve the wavepacket spreading. Here, we present an extension of our previous work [4] by considering a protocol with non-periodic alternation interchange between time-dependent transition defects. The results show that the Parrondo effect in the CTQW remains resilient even with random switching between defects. Thus, it is not necessary to construct a protocol with a specific order in the defect alternation sequence to obtain a Parrondo effect that can enhance the wavepacket spreading.

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One-step hydrothermal facile synthesis of cellulose-titanate-Ag membranes from sugar-cane bagasse

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Cellulose has received a lot of attention as the most abundant natural material on the planet. It is used as a raw material for the production of paper, biomaterials, composites and also for the production of synthetic fibers. In this study, we carried a one-step hydrothermal synthesis to extract the cellulose from sugar cane bagasse and produce cellulose-titanate-Ag membranes. The process involved dried sugar cane bagasse, 5.6 mL of titanium isopropoxide, 50 mL of 10M NaOH and Ag^+ solution, that were mixed and placed in a stainless steel reactor for 24 hours at 110 °C. The samples were washed with distilled water until pH 7 and dried at room temperature. Infrared spectroscopy, ATR mode, showed that in the sample doped with 4% Ag there was a reduction in the band near 3500 cm^{-1}, indicating that the hydroxyl groups of cellulose had been replaced by acetyl groups, associated with the appearance of bands at 1745 cm^{-1} and 1356 cm^{-1} corresponding to the symmetrical stretching of the carbonyl (C=O) present in the acetyl group. The C-O-C vibrations of the cellulose macromolecule were observed in the 1050 cm^{-1} range, with a peak at 900 cm^{-1} in the region attributed to the characteristic stretching modes of the M-O (Ti-O) bond, which for the sample containing 4% Ag the peak was less pronounced, thus involving oxygen atoms, the band at 2350 cm^{-1} refers to the vibration of CO_2 common for both. The results of the photocatalysis of methylene blue under UV-C irradiation showed that the Ag presence (1% and 4%) has increased photocatalytic dye removal as compared the control sample.

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Optical Activity Heterogeneity in 2D/3D Perovskite Heterointerfaces and the Impact of Molecular Flexibility on Device Efficiency

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Metal Halide Perovskites (MHP) have emerged in the photovoltaics field due to their high Power Conversion Efficiency (PCE), high charge carrier mobility, and low exciton binding energy [1]. Perovskite Solar Cells (PSCs) have demonstrated promising PCE of up to 25%, comparable to the widely commercialized monocrystalline silicon counterparts. However, achieving highly efficient PSCs requires careful optimization of the perovskite absorbing layer and interfaces with charge-selective contacts.

Introducing ammonium-based organic molecules in post-surface treatments forms low-dimensional 2D perovskite structures that influence the quantum confinement regime and mitigate surface trap states [2-3]. This study explores the correlation between molecular flexibility and 2D/3D perovskite heterointerfaces formation, exploring the 2D phase spatial distribution and its effects on PCE.

The analyses reveal, through nanoscale mapping of optical activity [4], that the 2D phases present a heterogeneous distribution over the 3D surface and provide compelling evidence for the preferential formation of the 2D perovskite at the boundaries. In addition, local CL analysis suggests preferential accumulation of n=1 or n=2 phases. Also, the 2D/3D interface enhances the device's PCE, and the more flexible molecule exhibits a device with higher efficiency, close to 21%.

Moreover, collaborative efforts yielded insights into the impact of novel organic molecules' stiffness on PCE and 2D/3D heterointerface formation mechanisms. The findings offer guidance for designing more efficient and stable PSCs, making progress in next-generation photovoltaic technologies.

Acknowledgments

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Optical Properties and its dependence with temperature of CsPbBr3 films prepared by spin coating.

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Fully inorganic metal halide perovskites are a stable material compared to the hybrids ones, competing with them for their convenient photoelectronic properties. Because of this their application in the next generation of optoelectronic devices is foreseen. Among them, CsPbBr3 perovskites, studied in this work, show absorption edge and intense photoluminescence in the green spectrum region.

Samples were prepared on a glass substrate with fluorine-doped tin oxide (FTO) by spin-coating of PbBr2 and CsBr, varying from 3 to 8 cycles. Between each cycle, heat treatments of 250 °C and 120 °C for 5 minutes were performed. At the end, annealing was done at 250 °C for 20 minutes.

Optical transmittance and photoluminescence (PL) were measured at different temperatures. Their absorption spectra are dominated by the presence of an excitonic peak. Fitting the Elliott function [1] to these spectra gives the bandgap energy Eg and the binding energy of the exciton EB. At room temperature Eg = 2.43 eV and EB = 40 meV and both increase with temperature. For Eg this tendency is opposite to the one in conventional tetragonal semiconductors. The PL shows a quantum efficiency of about 1% as expected in bulk materials. Through this analysis we found a Stokes shift of several tens of meV, which is desirable for no reabsorption.

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Optical properties of localized excitons in WSe2/β-Ga2O3

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Two-dimensional (2D) transition metal dichalcogenides (TMDs) materials are attractive systems for fundamental physics and possible applications in optoelectronics and quantum technology. Monoclinic gallium oxide (β-Ga2O3) is an ultra-wide band-gap semiconductor that despite of not being a van der Waals material and having highly strong ionic bonding, β-Ga2O3 crystal can be mechanically exfoliated along the (100) favorable surfaces to make ultra-thin layers. In this work, we have investigated optical and magneto-optical properties of a monolayer (ML) WSe2/β-Ga2O3 /SiO2 under a perpendicular magnetic field up to 9T [1]. Remarkably, we observed that Ga2O3 substrates improve the optical properties of WSe2 by reducing the doping and PL linewidth of the exciton peak. Furthermore, several sharp emission peaks were revealed at lower energy which were related to localized excitons. Their g-factors values were found to be close to -4 which is an unusual result for localized excitons in WSe2. Moreover, we observed that few PL sharp peaks have shown higher g-factor values of ≈ -7 and ≈ -12 which were associated with the hybridization of strain-localized dark excitons and defects in WSe2. In general, our studies provide fundamental insights into the impact of exfoliated β-Ga2O3 and point defects on the optical properties of monolayer WSe2/β-Ga2O3/SiO2 heterostructures which is relevant for the development of devices for optoelectronics and quantum information technology

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OPTICAL STUDY OF GRAPHENE/WATER INTERACTION

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Among all the 2D materials, graphene is the most studied, it is the first isolated 2D material, and further to its atomically thin structure, it also presents admirable electrical, thermal, and mechanical properties. Those properties motivate using graphene as a membrane in liquid interfaces for applications such as transparent windows, filtering, flow sensing, and DNA sequencing. A better comprehension of the interactions between graphene/liquid interfaces needs to be improved to enhance the design of applied devices. Raman spectroscopy has a significant role in studying graphene and the interactions between graphene and the surrounding medium, such as substrates, gases, and liquids. Since Raman spectroscopy is
sensitive to defects, doping, strain, and strain variations, it can access crucial information about the interaction of graphene/liquid interface. In this work, we present a microfluidic channel with windows covered with suspended graphene to study the interactions of the air/graphene/air (dry) and air/graphene/water (wet) interfaces. Also, we aim to study the dynamics of the optical response of the graphene when we insert water into the channel and let it spontaneously evaporate. Our results show that the optical response is sensitive to graphene and water''s mechanical and electronic interactions. As a highlight result, we observe the generation of metastable defects in graphene; those defects increase with time when graphene is in contact with water in the channel. Finally, we transfer an h-BN flake over a graphene window to understand the difference between this window and the
free-suspended membrane; we observe that the h-BN flake makes the graphene sample much more stable mechanically and suppresses some of the interaction signatures. This study’s results attract a deeper understanding of 2D materials interactions with liquids.

Optimizing Organic Photovoltaic Devices: Fluorinated Donor-Acceptor Polymer Variants Based on PTB7Th

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Conjugated polymers have garnered significant attention in materials science due to their electronic properties, making them suitable for a wide range of applications, including organic electronics, photovoltaics, and optoelectronics (1). The chemical structure of polymers containing donor-acceptor (DA) monomer units within the same molecular chain is crucial for adjusting properties such as energy gap, energy levels, and charge separation (2). This study describes the synthesis of semiconductor polymers based on PTB7Th and its variants, for producing solar cell devices. D-A polymers were synthed, maintaining the acceptor unit and varying the donor units through the introduction of fluorine atoms into the benzodithiophene structure. Specifically, the units containing fluorinated thiophene (SC-ThF) and doubly fluorinated benzene (SC-BDT4F) were studied in comparison to PTB7Th. The analysis of the optoelectronic parameters showed a slight increase in the optical bandgap with the introduction of F atoms: PTB7Th= 1.43 eV; SC-TF= 1.48 eV, and SC-BDT4F= 1.51 eV. A reduction in the values of HOMO and LUMO for both fluorinated structures was also observed. OPV devices were prepared with a conventional architecture of PET-IMI/ZnO/DA:Y6:PCBM/PEDOT/Ag. The values of Voc, Jsc, FF, and PCE were evaluated, highlighting PCE (%)= 1.43 (PTB7Th), 1.84 (SC-TF), and 1.10 (SC-BDT4F). The increase in PCE was also accompanied by an increase in polymer molar mass (Mn, g/mol) from 13,591 (PTB7Th) to 17,609 (SC-ThF) with the introduction of F into the thiophene ring (Th).

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Optoelectronic properties of multilayered 2D talc in the presence of substitutional defects

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Talc, a natural mineral with the chemical formula $Mg_3Si_4O_{10}(OH)_2$, belongs to the phyllosilicate family and exhibits a Si:O ratio of 2:5. It can be found either hydrated with water or with hydroxyl groups attached. In its bulk form, talc acts as an insulator, with a direct band gap of 5.35 eV and a high dielectric constant [1]. Known for its softness, smoothness, and moisture absorption capabilities, talc has recently attracted important attention due to the successful isolation of a monolayer via mechanical exfoliation [2]. This process considers talc's weak interlayer bonds, classifying it as a van der Waals (vdW) material. Mechanically exfoliated talc flakes have been utilized as substrates or encapsulating layers in graphene-based electronic devices, taking advantage of advanced techniques for stacking 2D materials [3]. In this work, we investigate the optoelectronic properties of monolayer, bilayer, trilayer, and tetralayer talc with two different stacking configurations. We examine band structures, projected density of states, absorption coefficients, and refractive indexes, using first-principle calculations within the density functional theory framework. Furthermore, we explore the effects of substitutional defects composed of Fe^{2+} and Fe^{3+}. Our results show variations in the optoelectronic properties with the number of layers and stacking configurations, which play an important role in the application of talc-based materials. The presence of Fe defects further influences these properties, indicating potential for fine-tuning the material’s behavior in electronic and optoelectronic devices. This study contributes to the improvement of knowledge of vdW materials and their potential integration into future electronic and optoelectronic systems.

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Organic Devices Based on PM6 Produced in Ambient Atmosphere with Photovoltaic Efficiency

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PM6 is an organic semiconductor polymer constructed from monomeric units of benzodithiophene and benzodione dithiophene, which has garnered significant interest for the production of photovoltaic devices. This polymer was developed by Zhang et al., 2015 [1]. Initially, in blends with PCBM, it exhibited efficiencies ranging from 5.7% to 8%. Currently, with advancements in non-fullerene acceptors, there are PM6-based devices (PM6:Y6) with efficiencies exceeding 18% [2]. However, this efficiency was achieved in an inert environment, which cannot be replicated under industrial production conditions. Therefore, in this project, PM6-based devices were produced in an ambient atmosphere to study the feasibility of applying this polymer on an industrial manufacturing scale. Additionally, the polymers were synthed under various reaction conditions to obtain materials with different molar masses. This allowed for an evaluation of which material exhibits the most suitable characteristics for the intended application. Regarding UV-Vis absorption parameters, bandgap, and energy levels, there were no significant differences among the synthed polymers due to the similarity in chemical structure. However, it was observed that the polymer synthed with a higher amount of solvent and longer reaction time exhibited the highest molar mass (Mw = 38,856 g/mol). This material also demonstrated the highest photovoltaic efficiency value of 5.2% in devices produced in an ambient atmosphere, in addition to a Voc of 0.818 V, Jsc of 13.26 mA/cm2, and FF of 52.91. Further alterations are being studied regarding the quantity of catalyst for subsequent evaluation of the obtained materials.

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Ozone sensor based on SnO2 nanowires

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This project aims to develop and characterize an electronic device based on SnO2 semiconductor nanowires for ozone detection. In order to do that, we propose to investigate the electronic properties of individual nanowire devices and nanowire films, as well as to analyze their responses under different controlled environments, in which the temperature, exposure time to the gas of interest, and ultraviolet light illumination conditions could be varied. To this end, several samples of gold-deposited nanowires were grown on silicon substrates, and their electrical properties, considered ohmic, were analyzed using electrical contacts. In addition, the sensitivity of these samples to ultraviolet light and ozone gas was confirmed, with very short responses observed after exposure, which characterizes them as good gas-sensitive devices. Finally, based on the analysis of the characteristics of the nanowires produced and characterized, an ozone sensor was developed.

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Partial boomerang effect in the presence of a constant electric field

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Within the context of Anderson localization [1], a recent study has observed a novel phenomenon: a particle launched with a non-zero initial momentum in a system with random potential exhibits an initial forward motion followed by a return to the system's origin, this phenomenon has been named "quantum boomerang" [2]. In our work, we introduced a constant electric field into this scenario and discovered a surprising result: part of the particle's wave function remains localized near the origin, while another part behaves as free free particle, moving with constant acceleration. This dynamic, where one part of the wave packet remains localized while another part moves freely, contradicts classical expectations of a particle eventually reaching a terminal velocity due to potential drag. Our main goal is to elucidate the reason behind this separation in the wave function and explore applications of this phenomenon in more complex systems, including those with spin-orbit coupling in higher dimensions.

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Photoassisted electrodeposition of copper micro-islands for SERS application.

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Photoelectrodeposition on p-type silicon has been explored as a cost-effective method for controlling deposits of various materials on the silicon surface since the previous century. This study focuses on utilizing photoelectrodeposition on p-type silicon (111) to control copper microdeposits. In a specially constructed electrochemical cell, the silicon was immersed in a CuSO4 solution and selectively illuminated by a HeNe laser, precisely directed by a microscope within a Raman Setup [2]. The characteristics and morphology of the deposits were manipulated by adjusting parameters such as laser intensity, exposure duration, and electrochemical cell potential. Despite initial implementation challenges, the results highlight significant potential for forming and adjusting electrochemical deposits. These deposits' properties are notably sensitive to process parameters, facilitating diverse applications including lithography and sensor fabrication. In addition to examining the morphology and properties of the deposits through parameter variations, their utility in Surface-Enhanced Raman Spectroscopy (SERS) was explored. SERS, which often overcomes limitations of conventional Raman spectroscopy, is observed on metallic surfaces like gold, silver, and copper, with its efficacy dependent on surface properties and chemical affinity with the analyzed material [3].

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Photoconductivity of Ag-functionalized ZnO/Pani hybrid heterojunctions

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Hybrid oxide/organic heterojunctions are an emerging system for developing optoelectronic devices. In particular, ZnO has a high photogeneration of electron-hole pairs in the UV region. In turn, polyaniline (PANI), in its emeraldine-salt phase, acts as a p-type conductive polymer. The heterojunction ZnO/PANI thus emerges as an attractive system for constructing optical sensors. In this study, we present strategies to explore the photoconductivity of this heterojunction. The samples were fabricated using spray-pyrolysis to grow oxides on top of ITO/glass substrates and a chemical route to prepare emeraldine-salt PANI. For comparison, single ZnO films exhibit ultraviolet (UV) photoresponse (PR) around 0.1 with strong persistence. The formation of ZnO/PANI heterojunctions inhibits the persistence and improves PR by at least 15 times. To investigate plasmonic effects, we incorporated silver in the heterojunction using two approaches: doping ZnO (ZnO:Ag) and decorating the oxide/polymer interface with Ag submicron islands (Ag-ZnO). In both cases, optical absorbance around 520 nm indicates plasmon bands associated with Ag nanoparticles. In the case of a single ZnO:Ag layer, the persistence is mitigated with a twice increase in PR. However, ZnO:Ag/PANI heterojunction exhibits persistence besides a substantial increase in PR. Conversely, Ag-decorated ZnO single layers exhibit inherent persistence, which deteriorates the PR profile in Ag-ZnO/PANI heterojunctions. Finally, insights about the electronic transport mechanism of hybrid heterojunctions are explored with an approach of co-assisted photoconductivity using resonant wavelengths to PANI and Ag structures.

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POLARIPY: A new python-based package for the calculation of surface electromagnetic waves

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Surface polaritons, electromagnetic modes hybridized with matter excitations, have garnered renewed interest with the emergence of low-dimensional materials [1]. They can be stacked together to create a diversity of polaritonic modes. As new van der Waals materials are characterized and combined, there arises a need for accessible computational tools. To address this issue, we propose Polaripy, a python-based package that is simple to use, designed for the calculation of surface electromagnetic waves. We present a scattering matrix-based method for calculating the electromagnetic response of arbitrary stacked one-dimensional (1D) anisotropic materials, leveraging a 4 X 4 formalism tailored for surface plasmon-polaritons. Polaripy is a python package, built upon numpy, that is able to calculate the Fresnel coefficients, Purcell factors and loss function of 1D stacks with arbitrary dielectric permittivities and magnetic permeabilities. It is written in a modular structure, with the goal to be easy to add new functionalities, such as nonlinear and nonlocal responses and in-plane periodicity.

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Porous silicon characterization: porosity and thickness determination via SLIM

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Porous silicon (PS) has gain significant interest since its discovery due to its unique optical properties, which enable its use as anti-reflective, for instance, depending on the morphological characteristics of its porous structure. In different applications, knowledge of the thickness, d, and porosity, p, is of paramount importance because they define its optical behavior, reason for which various techniques have been developed to measure them. In this context, the use of optical methods has been suggested. In this study, we have used the method known as SLIM, which is based on reflectance measurements of PS in the presence of air and liquids (ethanol, methanol, toluene. Etc) within the pores. SLIM allows the simultaneous determination of both d and p, with the aid of the Bruggeman or Looyenga effective medium approach. For this purpose, mesoporous silicon samples were fabricated through the anodization of p+-Si, with a resistivity of 0.001 Ω·cm, in an HF:ethanol (3:7) solution, applying a current density of 5 mA/cm^2 to 50 mA/cm^2 for 5 minutes to 15 minutes. The results of d obtained via SLIM are comparable to those obtained via scanning electron microscopy (SEM), with thickness ranging from 2500 nm to 5300 nm, and porosity from 64% to 89%, respectively.

Reconstruction of the experimental data using these values, alongside the effective medium-based refractive index models shows a deviation of less than 5%. However, it was observed that the values of d obtained via SLIM exhibit a significant deviation from the expected value at wavelengths shorter than 700 nm. This is attributed to the high absorbance of liquids in this region.

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Potential application of PBS as electrolyte in Organic Electrochemical Transistors

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Abstract: Phosphate-buffered saline (PBS) is an electrolytic solution that aims to mimic phisiological conditions, in addition to having neutral pH, which preserves biological samples [1]. Due to this characteristic, PBS is used for various biological analysis, like Enzyme-Linked Immunosorbent Assay (ELISA), for example [2]. In this work, the potential application of the PBS as electrolyte in electrolyte-gated transistors (EGTs) was studied, because these devices are great candidates for the development of point-of-care technologies (PoCTs) [3]. A planar architecture was used, consisting of indium-tin oxide (ITO) interdigitated source and drain electrodes, poly-3-hexylthiophene (P3HT) as organic semiconductor channel, a Pt wire as gate electrode and PBS as electrolyte. Based on the parameters extracted from typical EGT's electrical measurements, like on/off ratio, transconductance and threshold voltage, for example, it was possible to observe that the EGT operates as an organic electrochemical transistor (OECT). Thus, this study demonstrates the feasibility to fabricate OECTs with PBS as electrolyte, opening the possibility to introduce different biological substances into this electrolytic solution and envision sensing platforms applied to biosensing.

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Probing the cw-Laser Induced Fluorescence Enhancement in CsPbBr3 Nanocrystal Thin Films: An Interplay Between Photo and Thermal Activation

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Perovskite nanocrystals hold significant promise for a wide range of applications, including solar cells, LEDs, photocatalysts, humidity and temperature sensors, memory devices, and low-cost photodetectors. Such technological potential stems from their exceptional quantum efficiency and charge carrier conduction capability. Nevertheless, the underlying mechanisms of photoexcitation, such as phase segregation, annealing and ionic diffusion, remain insufficiently understood. In this context, we harnessed hyperspectral fluorescence microspectroscopy to advance our comprehension of fluorescence enhancement triggered by UV continuous-wave (cw) laser irradiation of CsPbBr3 colloidal nanocrystal thin films. Initially, we explored the kinetics of fluorescence enhancement and observed that its efficiency (φ_{ph}) correlates with the laser power (P), following the relationship $\varphi_{ph} = 7.7 <P>^{0.5}$. Subsequently, we estimated the local temperature induced by the laser, utilizing the finite-difference method framework, and calculated the activation energy (Ea) required for fluorescence enhancement to occur. Our findings revealed a very low activation energy, Ea ~9 kJ/mol. Moreover, we mapped the fluorescence photoenhancement by spatial scanning and real-time static mode to determine its microscale length. Below a laser power of 60 µW, the photothermal diffusion length exhibited nearly constant values of approximately (22 ± 5) µm, while a significant increase was observed at higher laser power levels. These results were ascribed to the formation of nanocrystal superclusters within the film, which involves the interparticle spacing reduction, creating the so-called quantum dot solids configuration along with laser-induced annealing for higher laser powers.

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Production of Luminescent Nanoparticles Based on Graphite Obtained as a Byproduct of Acheson Process

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Carbon-based nanomaterials have drawn the attention of the scientific community due to their physical properties and numerous applications. An example of these materials is the graphene, which can be produced from several techniques such as, for example, chemical vapor deposition, sublimation of Si atoms from SiC wafers, and liquid phase exfoliation of graphite. Previous works have reported that the precursor of graphene can be synthed at high temperatures using raw materials such as petroleum coke. Herein, the effect of heat treatment of carbon-based structures, obtained as a byproduct of the synthesis of silicon carbide by the Acheson process, was investigated. For this, two treatments were compared using a tubular furnace in two different configurations: one in an argon atmosphere and the other at a low vacuum. In both configurations, the carbon structures were subjected to different heat treatment temperatures. Through Raman spectroscopy, it was possible to obtain the well-ordered domain as a function of temperature used in the heat treatment. These results were compared with the Scherrer length obtained from X-ray diffraction (XRD) measurements, which showed an evolution of the crystalline phase of graphite due to the increase in temperature. The morphological and structural characterizations of the modified material were performed by scanning electron microscopy (SEM). It is worth mentioning that in this work high-quality graphite was obtained at relatively low heat-temperature treatments when compared with previous works. We applied the graphite compound produced at low vacuum to synthe carbon-based quantum dots with intense luminescence between 430 and 510 nm. From atomic force microscopy measurements, we investigated the effect of the carbon precursors roughness on the emission of the synthed nanoparticles.

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PRODUCTION OF ULTRATHIN HETEROSTRUCTURES AND DEVICES FOR NANOELECTRONICS

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Isolated two-dimensional materials (2DMs) have been widely studied due to their intrinsic electrical, mechanical, and optical properties [1]. Recently, the combination of two or more 2DMs in the so-called van der Waals heterostructures (vdWHs) has allowed improvements in the optoelectronic quality of multifunctional devices and in the observation of new quantum phenomena that do not exist in isolated forms [2]. Consequently, this has boosted the use of these 2DMs, as well as technological applications of these ultrathin and hybrid vdWHs, mainly in areas related to nanoelectronics [3]. In this project, we manufactured and characterized samples of graphene encapsulated in biotite natural crystals from a Brazilian mine and compared the results with the 2D crystal most used in the literature, hexagonal boron nitride (hBN). We demonstrated that natural 2DMs can be easily incorporated into ultrathin vdWHs with graphene. Our Raman spectroscopy analysis showed that biotite crystals induce a spontaneous charge transfer to the graphene, inducing doping without applying external gate bias. The results were then compared to the electrical characterization of field effect transistor (FETs) nanodevices, thus corroborating the total charge density transferred to graphene, as well as the type of charge carrier. Therefore, our study seeks to contribute to the area of electronic devices with low production costs using natural 2DMs from Brazilian soil.

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Quantum dots as an active resevoir for longer effective lifetimes in GaAs bulk

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AlInAs/AlGaAs quantum dots (QDs) have emerged as excellent emitters across the visible spectral range, showcasing highly tunable electronic properties through variations in composition and size [1]. This versatility allows for diverse band alignments within the same system. In this study, we present compelling evidence for the coexistence of type-I indirect and direct emissions from QDs, supported by comprehensive analyses of their photoluminescence responses to excitation power, temperature, and time, along with band structure calculations. The high-density QD system exhibits signs of lateral coupling [2], facilitated by carrier transfer between dots, modulated by energy barriers and recombination times. Additionally, we can unequivocally prove that the QDs act as carrier reservoirs that progressively feed optically active states in the bulk GaAs at low temperatures—an attractive prospect for hot-carrier photovoltaics [3]. Above certain temperatures, the bulk system reverts to the anticipated predominantly radiative recombination dynamics. Our theoretical framework, accounting for the coexistence of QD specimens with varying recombination times, successfully elucidates the optical response at different temperatures, emphasizing the pivotal role of QD excitation in enhancing the effective lifetime of carriers in the bulk.

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Radiation Effects on Solid-State Electronics: Impacts in Space and Terrestrial Environments

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Electronic devices can experience undesired effects and failures when operating in radiation environments, such as outer space and Earth's atmosphere. In space, heavy ions are the primary agents causing destructive radiation effects in electronic devices [1]. In terrestrial environments, neutrons are the primary cause of radiation effects in electronic devices operating at ground level and avionic altitudes [1]. Transistors are crucial to modern electronics, although the susceptibility to radiation-induced failures and related mechanisms in advanced technologies are often unknown [2].

This study directly compares the radiation effects induced by energetic particles on traditional and modern transistor technologies. Regarding space applications, devices were irradiated with alpha particles and energetic heavy ion beams. Regarding avionics and ground-level applications, transistors were exposed to monoenergetic and state-of-the-art quasi-atmospheric neutron beams. By considering fundamental semiconductor properties and using computational codes for ion transport and interaction in matter, we developed a comprehensive test protocol for qualifying electronic devices made from various semiconductor materials, such as Si, SiC, GaAs, GaN, Ge, and Diamond, for space applications. Furthermore, computational simulations of the interaction of fast neutrons with transistors were conducted to investigate the contribution of nuclear reaction products capable of triggering failure modes. Finally, future perspectives on radiation effects in emerging technologies, such as solid-state systems for quantum information, will be briefly discussed.

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Rashba effect on the optoelectronic properties of twisted multilayer anisotropic two-dimensional semicondutors

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Resumo

Within an effective mass approximation, we theoretically investigate the effects of Rashba-type interactions on the band structures, wave functions, density of states, and optical conductivities of hetero-bilayer systems made out of anisotropic 2D semiconductors, i.e., with different effective masses along the x and y directions and with the layers being twisted relative to each other. We analyze how these optoelectronic properties change by taking different interlayer twisting angles and surrounding environments, such as the width and dielectric constant of the spacer located between the two layers, as well as by assuming different orientations of the applied in-plane magnetic field related to the crystallographic directions. The optical conductivity associated with interband transitions between the Rashba-induced splitting bands as a function of the frequency for arbitrary polarization angles is calculated using Kubo formalism [1,2].

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Scanning probe studies of local surface potential and density of states in CdTe/InGaAs nanomembranes

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Kelvin probe force microscopy (KPFM) is a novel avenue of research onto electrical and electronic properties of materials. Using a typical atomic force microscope (AFM) setup with a specially coated cantilever, it becomes feasible to probe the local surface potential and conversely measure the surface's work function. Such setup delivers spatial resolution equivalent to those of the conventional AFM through an electronic feedback and lock in system available in commercial AFM kits.
In this project we aim to investigate the effects of strain in semiconductor nanomembranes of InGaAs and CdTe using KPFM along with scanning tunneling microscopy (STM) and spectroscopy (STS). Our results reveal the dependence of the local surface work function and electric potential at the nanomembrane surface with the quality of the CdTe/InGaAs interface and provide insights for future device development. Changes in the electronic density of states were probed with STS and results are discussed.

Semiconductor-Ferromagnetic nature of rare-earth based ferrocobaltite $SmFe_{0.5}Co_{0.5}O_3$

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Materials in which electronic spin manipulation is possible for the tuning of charge and spin currents are intensively pursued due to the multifunctionality of their potential applications in spintronics technology. In this work, the synthesis and characterization of the crystallographic, optical, electrical and magnetic properties of $SmFe_{0.5}Co_{0.5}O_3$ material is reported. Structural analysis reveals its crystallization in an orthorhombic cell (Pnma space group) with disordered distribution of Fe and Co cations. The optical response evidences the occurrence of a bandgap E_g= 1.0 eV, typical of semiconductor materials, which is corroborated by electrical resistivity measurements and J-E curves, where a varistor-type curve is recorded. Magnetic analysis suggests a predominant antiferromagnetic behavior at low temperatures with weak ferromagnetic response, which strengthens at high temperatures as a result of interactions described by the super-exchange model. Ab-initio calculations of the density of states and electronic band structure predict the semiconductor type response, with an asymmetry of the bandgap between the two spin polarizations, opening channels for tuning polarized spin currents, which is characteristic of ferromagnetic semiconductor type materials.

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Shubnikov de-Haas Oscillations in 2D Topological Insulators

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Topological Insulators (TIs) were introduced in 2006 by Bernevig, Hughes, and Zhang (BHZ) on the study of the quantum spin Hall effect in HgTe quantum wells. TIs are described by the BHZ model, and are known for their topological edge states with protected conductivity against weak disorder, thus being promising for spintronics applications. In TIs, the theoretical interpretation of quantum oscillations, e.g., Shubnikov de-Haas oscillations (SdH), relies on the Lifshits-Kosevich (LK) equation. However, analytical LK-type equations for the BHZ Hamiltonian are not possible in the presence of both spin-orbit coupling (SOC) and Zeeman terms, and significant approximations are necessary for obtaining analytical solutions. This research aims to numerically study the effects of SOC and Zeeman terms on SdH oscillations of TIs described by the BHZ Hamiltonian [1,2]. Considering the Drude model and Fermi's golden rule in the first Born approximation, we rewrite the longitudinal resistivity of the quantum Hall effect in terms of the density of states (DOS) at the Fermi level [3]. Python's Kwant package is employed to numerically evaluate the DOS, and hence the SdH oscillations in 2D TIs. SdH oscillations serve as a fundamental tool to characterize transport-related quantities in different materials, enabling measurement of charge density, DOS, and bands' effective masses from oscillation frequencies and amplitude.

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Simulating single-electron transistor in the presence of electron-electron interaction

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Carbon-based structures such as nanotubes, and more recently graphene, have attracted great attention from the scientific community both from the point of view of basic science and possible applications in photonics and electronics. In the particular case of graphene, a two-dimensional carbon structure organized in a hexagonal lattice, we have an extremely strong material with unparalleled electrical and thermal transport properties. Graphene nanoribbons can be obtained by confining graphene in one dimension. These one-dimensional structures retain many of the properties of graphene in a wire at the nanoscale. In particular, given recent experimental advances, it was possible to fabricate atomically precise graphene nanoribbons (GNR) in a multi-gate device architecture using carbon nanotubes (SWNT) as electrodes. This SWNT-GNR-SWNT retains many of the properties of single-electron transistors. In this work, inspired by this recent experimental advance, we propose a single-electron transistor based on carbon nanotube (metallic) as electrodes, coupled to a graphene nanoribbon (semiconductor). Here, we seek to understand how the electron-electron interaction alters the electronic and transport properties of this device. To this end, we perform calculations using the out-of-equilibrium Green function method, describing the interacting states through an Anderson impurity model together with the so-called non-crossing approximation (NCA) and a generalization to the Meir-Wingreen formula for non-proportional coupling regime. Using this methodology we are able to recover experimentally observed phenomena, such as the Coulomb blockade, as well as the corresponding Coulomb diamonds. Furthermore, we are able to separate the different contributions to transport and show that incoherent effects due to the interaction play a crucial role in the transport properties depending on the region of the stability diagram being considered.

Size-Dependent Bandgap and Particle Size Distribution of Colloidal CsPbBr3 Perovskite Quantum Dots: A New Theoretical-Experimental Approach

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A new analytical expression for the -dependent bandgap of ultrasmall CsPbBr3 perovskite quantum dots is developed within the framework of the finite-depth square-well effective mass approximation.[1] A theoretical-experimental approach is then proposed to convert optical spectroscopic data (photoluminescence spectrum) into accurate estimates for the particle distribution of colloidal systems by correlating two main problems: the corrected -dependence of the first excitonic transition of a single cube-shaped quantum dot and the broadening of the fluorescence lineshape of a colloidal ensemble containing a population of quantum dots with different s. By applying the reported methodology to CsPbBr3 quantum dot samples belonging to the strong and intermediate confinement regimes, the distributions are predicted and compared directly to those obtained from transmission electron microscopy. The presented calculation scheme is based on general theoretical considerations so that it can be readily adapted to semiconductor quantum dots of many other systems from all inorganic metal halides to hybrid perovskite materials, regardless of the adopted chemical synthesis route.

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Spray pyrolysis synthesis and characterization of $Zn_{0.05}Cd_{0.95}O$/CdO heterostructure

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Cadmium oxide (CdO) and zinc oxide (ZnO) are polycrystalline semiconductors that belong to the family of transparent conducting oxides (TCOs) and are used in several optoelectronic applications, such as in the production of solar cells and phototransistors [1]. Electrical transport in these semiconductors is influenced by disorder, grain , potential barriers between them, doping and vacancy concentration. In this work, three samples grown on a glass substrate using the spray pyrolysis technique were studied: two films (CdO and $Zn_{0.05}Cd_{0.95}O$) and a heterostructure ($Zn_{0.05}Cd_{0.95}O$/CdO). X-ray diffraction showed that the heterostructure is more crystalline and has a larger crystallite compared to films. Scanning electron microscopy revealed a well-defined interface in the heterostructure. The electrical characterization was carried out at temperatures between 100 and 1.9 K and all samples showed semiconductor behavior. In the heterostructure, below 4.2 K, a logarithmic drop in electrical resistance was observed, which was attributed to the presence of the spin-orbit coupling effect. Applying field up to 9 T at different temperatures, all samples exhibited negative magnetoresistance (MR) which was attributed to weak localization, while the antilocalization effect was observed only in the heterostructure below 4.2 K, possibly due to interface formation. By fitting the MR curves of the heterostructure with the Fukuyama-3D model, the parameters were obtained: inelastic scattering time (τ_φ) and spin-orbit scattering time (τ_{so}) with values of $(24.44 \pm 4.03)\times10^{-12}$ s and $(2.89 \pm 0.28)\times10^{-12}$ s, at T = 2.5 K, suggesting the potential of this material for applications in the area of spintronics.

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Stability and optoelectronic properties of two-dimensional gallium phosphide

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Since the discovery of graphene in 2004, research on two-dimensional materials has made significant advancements. While graphene's zero energy band and semimetallic nature have limited its applications in electronic devices, researchers have been compelled to seek out new two-dimensional materials. Among these materials, semiconductor nanostructures have garnered attention. For instance, two-dimensional gallium phosphide (GaP-2D), a member of the III-V family of the periodic table, emerges as a promising alternative for optoelectronic device applications due to its adjustable physical properties. In this work, using first-principle calculations, density functional theory, and tight-binding method, we investigate the optoelectronic properties of two-dimensional gallium phosphide (2D GaP). Our investigation covers electronic properties, such as band structure and electronic band gap, and optical properties, including absorption spectra, refractive index, and reflectivity, considering excitonic effects. Additionally, structural aspects, such as stability, elastic properties, are also analysed. This comprehensive study brings up valuable insights into 2D GaP physics, evincing the key features that make it a potential material for optoelectronic applications like photodetectors and solar cells.

Structural and electronic properties of MoS_2/$MoSe_2$ lateral and vertical interfaces from DFT calculations

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Transition metal di-chalcogenides (TMDC) are one of the most studied 2D materials with interesting electronic and optoelectronic properties which, due to the modulation of their bandgaps, that are in the visible region of the electromagnetic spectra, can be applied in new optoelectronic devices. Concerning the electronic devices, there is a lot of both theoretical and experimental studies about interlayer interfaces involving TMDC and other materials, such as graphene or h-BN. However, intralayer (or lateral) interfaces were less considered in the conception of new devices, while the interlayer interfaces are well studied. In this work, we report our *ab initio* Density Functional Theory results (with van der Waals corrections included) for the structural and electronic properties of MoS_2/$MoSe_2$ lateral interfaces in both zig-zag and armchair configurations, and vertical interfaces as well. Band offsets and alignment of these interfaces were also obtained. Our results have shown that the band offsets of the lateral interfaces have small values, 76.0 and 23.3 meV for both zig-zag and armchair configurations, respectively. This feature favors the formation of type II superlattices and quantum wells, with good application for optoelectronic devices independent of its configuration. In the case of vertical interfaces, independent how $MoSe_2$ stacks over the MoS_2, there is a thin energy barrier (~ 2 Å) of around 15 eV, which can be used to control the generation of interlayer excitons formation.

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Structural characterization and Local surface electronic response of sputtered Bi_2Se_3 thin films grown on MgO (100) substrate

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This work presents a systematically study of RF-sputtered growth Bi_2Se_3 thin film at room temperature on (100)-oriented MgO substrate. The structural and chemical properties of Bi_2Se_3 films are characterized by high resolution transmission electron microscopy (HRTEM), in-depth energy dispersion x-ray spectroscopy, x-ray photoemission spectroscopy (XPS), x-ray diffraction (XRD), x-ray reflectivity (XRR) and Raman spectroscopy techniques which confirm the growth of high quality and stoichiometry compound. Atomic force microscopy (AFM) and scanning tunnelling microscopy (STM) revealed films characterized by a granular surface morphology. Scanning Tunnelling spectroscopy (STS) technique that measure the surface local density of states (LDOS) confirms the growth of Bi_2Se_3 film with topological insulator properties. The intrinsic spin orbit coupling and dissipationless surface states topologically protected of Bi_2Se_3 might lead to spintronic devices with fast and efficient spin-charge conversion [1,2].

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Structural investigation and thermal stability of Al2(MoO4)3 obtained by the coprecipitation method

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The $A_2(MO_4)_3$ inorganic compounds have many uses in microelectronics, optics, and photocatalysis [1,2]. These compounds properties and potential applications depend on their structures, which can be controlled through synthesis. $Al_2(MoO_4)_3$ was synthed using coprecipitation and followed thermal treatment in this study. This material structure and thermal stability were analyzed in detail using techniques such as Thermogravimetric (TG), Differential Scanning Calorimetry (DSC) and X-Ray Diffraction (XRD). Thermal analysis was used to determine the optimal heat treatment temperature for studying the crystalline evolution of the amorphous precipitate. Monoclinic crystals of $Al_2(MoO_4)_3$ were obtained by at 570 °C/1h with the P121/a1 space group. The crystal was further analyzed using the Rietveld method to precisely determine the crystal system, lattice parameters, and unit cell volume. In addition, the unit cell of $Al_2(MoO_4)_3$ was modeled using atomic coordinates, distances, and angles. The study found that the heat treatment caused varying degrees of distortion in the AlO_6 and/or MoO_4 tetrahedral polyhedra. The crystal increased from 63 to 73 nm as the temperature increased from 700 to 770 °C/1h, measured by the Scherrer method. The thermal stability of $Al_2(MoO_4)_3$ was studied and observed an incongruent sublimation at 1000 °C, leading to the formation of different intermediate phases of Al_2O_3. No phase related to molybdenum was observed, indicating a sublimation of molybdenum oxide. This reaction is not predicted by the Al_2O_3-MoO_3 phase diagram and hasn't been reported before.

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Study of Conductivity in Reduced Graphene Oxide Thin Films

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The conductivity of graphene oxide (GO) can be adjusted by its degree of reduction and/or doping, making it a versatile material for various applications, such as capacitors, batteries, transistors, and sensors [1]. Understanding the electrical properties of GO is crucial for directing its use according to the material's characteristics. This study aimed to investigate how the electrical properties of graphene oxide are influenced by its oxidation level and the presence of other two-dimensional materials on its surface. The films were prepared from GO on a glass substrate using an automated spray coating technique at different thicknesses (specified by the number of passes), followed by thermal treatment at 200°C for one hour in an inert atmosphere. The sheet resistance was measured using the Van der Pauw method [2]. Subsequently, the majority charge carrier type was determined through the Hall effect [3], using a static magnetic field of approximately 1 Tesla. The results showed an average sheet resistance of 7.1 kΩ/□ for films with 10 passes and 5.8 kΩ/□ for films with 30 passes. Additionally, it was found that the majority charge carrier is negative and that after depositing a suspension containing talc on the rGO film, there was an increase in the number of carriers.

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Study of defects created by FIB in $MoSe_2$ monolayers by Raman and Photoluminescence spectroscopy

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TMDs have been intensively synthed/studied thus linking their morphological aspect to their physical properties, and consequently leading to the understanding of the possible benefits of defects in such materials. Nevertheless, for future applications, quantifying and identifying defects in TMDs is still a milestone to reach in order to better employ these materials in optoelectronic devices. Raman Spectroscopy has been successfully employed in graphene to quantify punctual or line defects. In this work [2], we bombarded monolayer $MoSe_2$ with He ions and found out the existence of three defect activated Raman bands around 250–300 cm^{-1}. DFT calculations were employed to obtain the electronic and phonon dispersion bands, making it possible to infer that these bands arise from inter-valley Raman double resonance processes. Interestingly, the same punctual defect model, that allows one to predict the defect concentration at which graphene starts to become amorphous, also works for TMDs. Now for two series of irradiated samples we are studying the relationship of low frequency modes for Raman spectroscopy and the relationship of defects with PL. In both cases, with temperature dependence Hence, this work opens the door to the macroscopic quantification of defects in TMDs, which is essential for technological.
applications.

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STUDY OF ELECTRICAL PROPERTIES OF THE ACTIVE LAYER OF A BHJ CELL CONTAINING P3HT:PCBM NANOFIBERS OBTAINED BY CO-AXIAL ELECTROPHATION USING KPFM and C-AFM.

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Electrospinning is a technique that allows the production of nanofibers by applying an electric field to a polymer solution. However, the electrospinning of conductive polymers needs to be done via coaxial electrospinning. This process involves two nozzles that are concentrically aligned with the solutions for the core layer (P3HT:PCBM) and the shell layer (PMMA). To improve the photovoltaic parameters of BHJ-type solar cells, as well as the thickness of the active layer of this device and to reduce exciton recombination [1], one proposed alternative is the insertion of nanofibers of the donor polymer and acceptor material within the active layer. In this work, the obtained nanofibers underwent washing with a solvent to remove the shell layer. Subsequently, for the interconnection of the nanofibers, spin-coating deposition with aP3HT:PCBM solution on an ITO substrate was performed. Additionally, a reference sample (blank) containing only the thin film of P3HT:PCBM was prepared. The AFM study was conducted at CNPEM facilities. The first result revealed that the difference in roughness between the samples is significant, with the sample containing nanofibers showing double the roughness compared to the reference sample. Furthermore, Kelvin probe force microscopy (KPFM) and conductive atomic force microscopy (c-AFM) techniques were able to map the conductivity and the extraction current of positive charges (holes). Using the hybrid AFM-IR technique, it was possible to map the distribution of the donor material and the acceptor material and confirm the absence of the shell layer after washing.

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Study of multilayers Bernal and Rhombohedral graphene and its applications in biological systems

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The physicochemical characteristics of graphite with Bernal and rhombohedral phases at different concentrations have been explored in different fields such as electronic. Bernal graphite (2H), with its ABAB stacking order, shows semi-metallic behavior with zero bandgap, good in-plane mechanical properties, high in-plane thermal conductivity, and characteristic optical and magnetic properties, all derived from its unique electronic structure. On the other hand, rhombohedral graphite (3R), with ABCABC stacking order, also exhibits semi-metallic behavior, but with a slightly different electronic band structure, although it shares with Bernal graphite similar high in-plane thermal conductivity and diamagnetic behavior, the different stacking order can lead to varied mechanical and optical properties [1,2]. Both types of graphite are chemically stable, yet their reactivity might be influenced at the edges or defects due to the different stacking orders. The unique properties arising from these distinct stacking orders make Bernal and Rhombohedral graphite suitable for a variety of applications in electronics, photonics, and other technological fields. In this work, we have elucidated the potential of MBRG (Bernal-Rhombohedral multilayer graphite) to increase in biological systems like plants. The systematic study of MBRG unveils its significant contribution to material science, particularly in agricultural applications, bridging the gap between advanced materials and sustainable agriculture practices. The distinctive stacking orders of Bernal and Rhombohedral graphite, embodied in MBRG, underpin its unique material properties, which in turn, foster enhanced seed germination and root growth [3].

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Superconductivity from spin fluctuations and long-range interactions in magic-angle twisted bilayer graphene

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At a certain magic angle, twisted bilayer graphene showcases a a maximum superconducting critical temperature, charge, and magnetic orders, which are arguably caused to electron-electron interactions. In this work, we present a theory of spin and charge fluctuations, incorporating higher order corrections to account for interactions beyond the usual Hartree-Fock or random-phase approximation, and consider off-site interactions in magic-angle twisted bilayer graphene. Our investigation reveals that incorporating off-site interactions introduces an additional dependence on scattering momenta for the interaction strengths. This dependence can manifest attractive components in some momentum regions and repulsive components in others. Notably, the momentum dependence is sensitive to lattice geometry and gives rise to a novel mechanism that promotes superconductivity over magnetism. If the potential nesting vector, as determined by the non-interacting band structure (i.e., the symmetry of the normal state), lies within the region characterized by repulsive components, electron-electron interactions favor this nesting vector, leading to the ordering of a magnetic state. Conversely, if the potential nesting vector falls within the region characterized by attractive components, electron-electron interactions suppress this nesting vector, delaying the magnetic ordering while enhancing superconducting pairing strength. We predic this magnetic-superconducting-magnetic transition as the off-site interactions are tuned within a filling dome.

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SUPPRESSION OF THE CHARGE DENSITY WAVE IN $TiSe_2$ BY ATOMIC LAYER DEPOSITION

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Titanium Diselenide (TiSe2) possesses a hexagonal close-packed (hcp) structure and is part of the Transition-metal Dichalcogenide group. It exhibits a charge density wave (CDW) below 200K, a phenomenon resulting from Coulomb and electron-phonon interactions. This CDW causes a distortion of the lattice, generating a very small electronic gap, which classifies Titanium Diselenide as either a quasi-metal or a small-gap semiconductor. The rapid oxidation of TiSe2, presents significant challenge in preserving their unique electronic and structural properties under ambient conditions. A successful strategy to stabilize the oxidation of TiSe2 is by utilizing a surface capping layer. An atomic layer deposition (ALD) of Al2O3 thin film has already been applied to effectively protect the TiSe2 thin flakes from environmental degradation [1]. Our approach is to investigate and characterize the sample with different methods other than the ones already used. Initially, we are characterizing the sample that has already been exposed to the air, initiating its oxidation. For this purpose, we are using Atomic Force Microscopy (AFM) and Scanning Tunneling Microscopy and Spectroscopy (STM/STS) techniques, and we are repeating this process for the newly exfoliated sample. In the second part of our study, we will encapsulate the TiSe2 sample performing the same experiment to observe all the modifications that occur within the material. With the experiment complete, we can finally study the changes in the Charge Density Waves (CDW) with STS by comparing the spectra with and without ALD at different temperatures.

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Surface and electronic response of β-polymorph Indium Selenide.

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Indium Selenide (In2Se3) is a versatile material that can be obtained in a wide range of polytypes and polymorphs each one with distinct structural and electronic properties. The study of the surface response of its polytypes and polymorphs is crucial for understanding possible technological applications, which often leads to exciting novel structural and electronic behaviors. This material is known to exhibit interesting properties, such as in-plane and out-of-plane ferroelectricity, high-order topological properties, bandgaps that depend on the number of layers and high carrier mobility [1, 2].

In this work, we present a theoretical and experimental investigation of the β(1T)- and β(3R)-In2Se3 structural, surface and electronic responses. The structural and chemical characterization of the sample was performed using X-Ray Powder Diffraction (XRD) and X-ray Photoemission Spectroscopy (XPS), respectively. To probe the surface electronic response, Density Functional Theory (DFT) calculations with experimental results of Angle-Resolved Photoemission Spectroscopy (ARPES) were employed.

Due to the similar structure of the quintuple layers (QL) of these polymorphs along the c-direction and beam resolution, ARPES was not able to paint the full picture of the phase distribution in the surface. Moreover, the UV light used in this experiment is unable to penetrate more than just a couple of QLs into the sample, failing to eject bulk electrons. Electron-BackScatter Diffraction (EBSD) was then employed to understand the phase distribution on the surface of the sample.

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Surface structure and water intercalation analysis in phyllosilicates by Crystal Truncation Rod scattering

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The lamellar structure of naturally occurring phyllosilicates has attracted attention from the scientific community in the past years. These materials can be easily thinned down to few atomic layers due to the existence of Van de Waals bonds between adjacent stacked structures. Although they exhibit interesting insulating properties there are intrinsic issues to overcome in order to apply them in future devices. Among such limitations we can point out the chemical doping, lattice defects and water adsorption.
In this work we have investigated three types of phyllosilicates with distinct structure: talc, which is the simplest structure among this mineral class, consisting of a Mg oxide octahedra located between two layers of Si oxide tetrahedra (hereafter called TOT layer); phlogopite, which has TOT layers intercalated with K ions and; Clinochlore, a material that intercalates TOT and brucite (Mg octahedra) layers. In each case water presence at the surface and sub-surface layers were inferred by Kelvin Probe Force Microscopy (KPFM) and Infrared spectroscopy measurements. The coexistence of different water incorporation models and ice-like structured H2O molecules between layers is analyzed here using surface-sensitive synchrotron X-ray diffraction. A kinematical model is implemented and the presence of water evaluated through fits of the (00L) Crysal Truncation Rod (CTR) data collected at the EMA beamline (Sirius, Campinas). We discuss the variations of water content and correlate its out-of-plane conformation (from CTR) with in-plane conditions retrieved by KPFM, providing a comprehensive scenario required for potential device-oriented use of this material class.

Synthesis and investigation of the optical properties of $Cs_{1-x}Rb_xPbBr_3$ perovskite microcrystals

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Inorganic halide perovskites have attracted interest due to their ease of synthesis and their extraordinary optical and electronic properties with potential technological applications. They have the chemical formula ABX_3, where A and B are cations and X is a halogen ion.[1] In this work, we synthed microcrystals $Cs_{1-x}Rb_xPbBr_3$ by the method of slow evaporation of solution at a fixed temperature. The same environmental conditions are used to obtain crystals with different concentrations of rubidium in the range from 0% to 30%. The chemical composition of the crystals was determined by energy dispersive spectroscopy measurements to verify the concentration of rubidium introduced into the samples. We also grew microcrystals with higher molar ratios of $RbBr_2$ in the solution to ensure greater inclusion of rubidium in the structure. X-ray diffraction measurements confirmed the orthorhombic crystal structure belonging to the Pnma space group at room temperature for all rubidium concentrations. The lattice parameters were determined by the Rietveld Method using the Fullprof software, in which observed variations in the lattice parameters as seen by Linaburg et al.[2] We firstly have been investigated the vibrational properties of these materials by Raman Spectroscopy measurements in the spectral region from 20 to 400cm^{-1} at room temperature. We carried out the symmetry assignment of vibrational modes of the pure $CsPbBr_3$ crystal and to studied the dependence of the modes position with the rubidium concentration.[2] We have started the synthesis of two-dimensional $CsPbBr_3$ crystals to produce heterostructures composed of transition metal dichalcogenides and perovskites in the future.

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Synthesis of D18-Based Photovoltaic Copolymers for Device Fabrication in Ambient Atmospheres

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Polymeric photovoltaic devices reach energy conversion efficiency values close to 19%. The conjugated copolymer D18 reached the mentioned efficiency values, but still presents limitations regarding the preparation of homogeneous thin films, especially in an ambient atmosphere. Therefore, the synthesis of photovoltaic polymers that present better processability and optoelectronic properties is extremely important. Three photovoltaic copolymers based on D18 were synthed by varying the amount of solvent or adding 5% hexylthiophene to the reaction medium. Subsequently, the copolymers were purified by Soxhlet extraction, using different solvents in sequence. The sample with a greater volume of solvent in the reaction medium favored an increase in dispersity (Mw/Mn = 2.08). On the other hand, the addition of 5% hexylthiophene resulted in an increase in the molar mass of the resulting polymer (Mn = 52925 g/mol, Mw = 93100 g/mol), concomitantly with a reduction in dispersity (1.76). In general, the polymers presented an optical bandgap around 1.95 eV, but the ultraviolet-visible absorption profile underwent significant variations, related to both the molecular weight and the presence of the termonomer. When analyzed by cyclic voltammetry, it was observed that the insertion of the termonomer raised the HOMO level, while the increase in the volume of solvent in the reaction medium lowered it. The addition of hexylthiophene increased the molar mass, reduced dispersity and improved processability, obtaining more homogeneous thin films, as observed in optical microscopy. This resulted in good photovoltaic devices with energy conversion efficiency of up to 7.96%, even manufactured in an ambient atmosphere, with a large substrate (5x5 cm) and a larger pixel area (0.55 cm2).

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Synthesis of manganese vanadate by precipitation method and study of its photocatalytic activity

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Photocatalysis is part of the Advanced Oxidative Processes. It is possible to use semiconductors that can be excited by visible or ultraviolet radiation, generating radicals that act to degrade organic pollutants [1]. In this study, Mn2V2O7 crystals were formed by homogeneus solution precipitation method with urea as the precipitating agent [2]. The precipitates obtained were submitted to thermal analysis to determine the heat treatment. Subsequently, the samples were structurally characterized by X-Ray Diffraction (XRD) and refinement by the Rietveld method. From the thermal analysis (DSC), it was possible to determine that from 410 °C/1h, there was the formation of monophasic β- Mn2V2O7 crystals. At 560 °C/1h, a phase transition was observed, referring to the α- Mn2V2O7 phase. Transmission Electron Microscopy (TEM) made it possible to visualize that the single-phase particles have the shape of plates. These are formed by smaller crystallites, suggesting a growth mechanism by oriented attachment. The characterization by UV-vis spectroscopy, it was possible to calculate the band gap energy of the samples, presenting values between 4.08 and 4.11 eV. The photocatalytic potential of these crystals was evaluated through the degradation rate of Rhodamine B and Methylene Blue dyes in an aqueous solution in the presence of UVc radiation [3], in which degradation was not observed for the rhodamine B dye. The methylene blue dye showed a percentage of 47% degradation.

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Temperature dependence on the Bandgap energies in MoS_2 : A Photoluminescence Investigation

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In this study, we investigated the photoluminescence (PL) of the transition metal dichalcogenide molybdenum disulfide (MoS_2) monolayers diluted in ethanol. The solution is drop casted on a silicon dioxide (SiO_2) substrate to create a thin film of monolayers, and later characterized by Atomic Force Microscopy (AFM), Raman spectroscopy and UV-vis spectroscopy. The PL of the film was then measured at temperatures ranging from 20 K to 400 K. The temperature dependence of the energy band gaps extracted from the PL spectra follows the Pässler and Oelgar´s model for exciton peak positions in semiconductors (**J. Appl. Phys**. 82 (5), 1, 1997). The temperature dependence of the model parameters, like the effective phonon energy, is also discussed.

TERAHERTZ LATTICE AND CHARGE DYNAMICS OF THE BISMUTH-DOPED TOPOLOGICAL INSULATOR $Pb_{1-x}Sn_xTe$

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Topological insulators are quantum materials that have attracted large attention of the scientific community. Recent studies shown the importance of the strong coupling between the deformation of the crystal lattice and the electronic states for controlling versatile topological phases [1]. Furthermore, the ferroelectric phase that arises from the distortion of the lattice with decreasing temperature was associated with the different degrees of phonon magnetic circular dichroism observed in Pb1-xSnxTe thin films [2]. To uncover the role of ferroelectric and topological phases in this dynamic process, we studied bismuth-doped Pb1-xSnxTe thin films grown by molecular beam epitaxy [3]. The films permittivity was evaluated using a home-built terahertz time-domain spectrometer in transmission geometry [4]. By monitoring the dependence of the terahertz permittivity with the temperature, a ferroelectric phase transition was observed. The dynamics of the transverse optical phonon mode and the parameters of the charge carriers were extracted by fitting the data with a Drude-Lorentz model. We demonstrated the possibility to control the critical temperature of the ferroelectric transition by tuning the type and concentration of charge carriers with bismuth doping. In conclusion, our work provides a material platform for the study of chiral phonons in a system with controllable ferroelectric and topological phases.

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The Impact of Gaussian Gate Voltage Pulse on Quantum Entanglement in Electronic Qubits

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The effects of electronic initialization of quantum states on the entanglement in electronic systems remain an open question. Our research focuses on a system model comprising of quantum dot molecules attached to electronic reservoirs[1]. Two electronic qubits interact with each other via Coulomb repulsion. The interplay between Coulomb and hopping process results on the formation of entangled states. Here we analyse how a Gaussian gate voltage pulse, that injects electrons into the qubits in a time controlled way, can interfere on the entanglement degree. To this aim we calculate different quantities such as fidelity, Von Neumann entropy and negativity. Ours results show that the proper adjustment of the initialization pulse width is crucial to the formation of highly entangled states, thus shining light on possible future experimental implementation of electronic qubits. The authors acknowledge FAPEMIG, CNPq (Grant No. 422350/2021-4) and UK STFC "Quantum Technologies for Fundamental Physics" program (Grant no. ST/T006404/1) for financial support.

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The impact of thermal annealing treatment on the optical properties of β-Ga_2O_3 crystals

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Gallium oxide (Ga_2O_3) is a promising ultra wide band semiconductor for possible applications in power electronics and UV optoelectronics[1,2]. In this work, we have investigated optical properties of Si-doped β-Ga_2O_3 crystals using photoluminescence (PL) and Raman techniques. We observed that the Raman spectra at 300K of the fresh and thermal annealed Ga_2O_3 samples are similar showing that there is no important change in the crystalline structure after thermal treatment. The PL spectra showed a stronger blue band at around 3.0 eV with a weaker green tail at lower energies centered at around 2.48 eV. This blue band in undoped β-Ga_2O_3 samples was observed previously and associated with the recombination of electrons and holes trapped at an acceptor site. However, the type of donors that contribute to the PL are not well understood but they are usually associated with shallow donors such as unintentional doping or Ga_i (Ga interstitial). On the other hand, the green PL band is usually associated with the presence of oxygen-related defects originating from the recombination of electrons with holes trapped by interstitial oxygen (O_i). The observed results indicate an increase of V_{Ga} vacancies after thermal annealing. On the other hand, the green PL band, which is correlated to holes trapped at O_i, has shown a decrease of the relative PL intensity after thermal annealing. In general, our optical results are explained by a possible enhancement in the density of gallium vacancies after thermal annealing treatment. However, the observed changes in the relative intensity of PL bands in β-Ga_2O_3 are not well understood in detail and further investigations would be needed to investigate their nature[1].

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The Mott transition in the particle-hole asymmetric Hubbard Model

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The project aims to investigate the metal-insulator transition (MIT) in the particle-hole asymmetric Hubbard model. The study revisits this interesting problem by focusing on the behavior of the chemical potential at the critical point of the Mott transition and by employing methods such as exact diagonalization and the Density Matrix Renormalization Group (DMRG). Special attention is given to the relationship between the onsite energy and the chemical potential, with insights drawn from the literature.
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Theoretical results for the structural and electronic properties of GaN/AlN axial heterostructure in [0001] grown nanowires

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The tendency for the limit for CMOS devices is to be reduced to the dimensions of a nanowire, according to the International Roadmap for Devices and Systems (IRDS) [1]. Besides that, nanowires could be useful in the design of future nano-optoelectronic devices, such as nanoleds and nanolasers as well. For these kind of devices, the III-Nitrides are good materials to be their active media, once their bulk counterpart have excellent optical properties. In this work, we present our preliminary results for the structural and electronic properties of the axial configuration of a nanowire with the GaN/AlN interface grown in the [001] direction in both the wurtzite and zincblende phases, and the dependence of these properties on the variation of its radius and on the variation in the thickness of the materials that make up the interface. The calculations were obtained using the Tight-Binding approximation for Density Functional Theory (DFTB+ code) [2]. Our obtained results show that the interface between AlN and GaN is smooth, without large atomic distortions. However, on the lateral surfaces of all nanowires, we found that cations tend to enter the material, while anions tend to leave it, as observed for the isolated bulk nanowires, as observed in the 2D structures. Furthermore, we found that the “bandgap” due to the presence of the interface is still direct, as observed for their bulk heterostructures, and this system is useful for new optoelectronic devices. Finally, the evaluated “band offset” for this heterostructure shows that the AlN/GaN interface forms a barrier on the GaN side, which will result in type II superlattices when using these materials.

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The Role of Stone-Wales defects on the Tribological Properties of Graphene Bilayers

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Individual graphene sheets have good mechanical stiffness and high strength, approximately 1 TPa and 100 GPa, respectively [1]. However, even though individually it is a strong material, the interactions between two graphene sheets are weak [1], i.e. its coefficient of friction is low. This makes it difficult to use this material in applications that require a higher coefficient of friction [2]. One way of increasing the friction coefficient of graphene is by applying defects, for example Stone-Wales (SW) defects. Therefore, this study proposes introducing defects into graphene sheets in order to study the dependence of friction on the concentration of defects. Molecular Dynamics (MD) simulations were carried out using the LAMMPS program [3]. For these simulations, Stone-Wales defects were randomly applied to two graphene sheets placed in contact, so that one sheet was fixed and the other was free to be pulled. The results showed an increase in the friction force to separate two graphene sheets and this amount depended on the concentration of defects applied and the of the sheets. Although the introduction of Stone-Wales defects impairs the mechanical properties of an individual graphene sheet, our results indicate that for structures composed of multiple graphene sheets, the introduction of defects can improve the mechanical properties of the assembly by making it more difficult to separate the monolayers.

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Time resolved terahertz photoconductivity of photovoltaic perovskites with sub picosecond resolution

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The energy demand of humanity has been increasing steadily, making the search for renewable energy sources imperative. One of the main sources of renewable energy is solar power. Consequently, the development of photovoltaic cells has advanced significantly in the last decade, making them increasingly efficient. Currently, more than 90% of commercial solar cell technology is made of silicon. However, such cells have been approaching their theoretical efficiency limit proposed by Shockley and Queisser [1]. An alternative that has garnered significant attention from researchers is halide perovskite solar cells. These cells are much cheaper and easier to synthe, and they have achieved efficiency records in converting solar energy into electricity, evolving from 2% to 26% in just a few years [1].

Two pivotal factors significantly influence the ultimate efficiency of a solar cell: the photogeneration of charge carriers and the electronic mobility of them. The Optical Pump - Terahertz Probe (OPTP) serves as a crucial tool for investigating these parameters due to its sensitivity to both [2]. Additionally, it is contactless and offers high temporal resolution (subpicosecond), enabling the characterization of ultrafast carrier dynamics occurring in photoexcited semiconductors. This capability is fundamental for unveiling the mechanisms limiting solar cell efficiency [3]. In this study, we characterized the ultrafast photoconductivity dynamics of spin-coated synthesized halide perovskites using the OPTP technique.

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Tip-enhanced Raman mapping of strain and elastic energy in twisted graphene bilayer nano-folds

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Carbon-based materials' remarkable electronic structure and extensive properties have generated significant interest as model cases to investigate two-dimensional systems. A particularly relevant technique is the so-called Tip-Enhanced Raman spectroscopy (TERS), that allows exploration of local conditions with nanometre resolution [1]. Since graphene is usually transferred to host substrates with inherent folds and wrinkling, changes in the crystalline lattice can take place. When a crystal is subjected to compression or stretching beyond its equilibrium state, strain is induced. In this work, we performed an experimental study on the optical properties of twisted bilayer graphene. Combined with the TERS technique, spectral images with a high spatial resolution of 25 nm can be produced. The local strain variation is quantified with near-field Raman spectroscopy, assessing the Raman peak shift along a mapping grid of the sample [2]. Elastic energy is evaluated, providing an experimental indication of the resulting energies involved in a wrinkling process. A finite element model including nonuniform strain allows to understand changes in the topography and is in fair agreement with our experimental observations, indicating dominant biaxial strain in wrinkled tBLG. Such analysis in the 2D material lattice is essential for device production in twistronics and straintronics, in which optical-electronic properties can be tuned [3, 4].

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Towards $CsPbBr_3$-Based Hybrid Pixel Detectors for High-Energy X-ray Imaging

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Hybrid pixel detectors are widely employed in synchrotron X-ray imaging [1]. They directly convert photon absorption to current pulses from semiconductor sensors, which are processed by a dedicated Application Specific Integrated Circuit (ASIC). In that sense, high-energy X-ray methods demand heavy element sensors, such as CdTe, for reasonable efficiencies in absorbing up to 90 keV photons [2]. Recent experimental results with lead-based inorganic perovskites, such as $CsPbBr_3$, revealed their potential application in detecting energy ranges beyond 90 keV due to their exceptional cross-sections and noteworthy transport properties [2]. Our work assesses $CsPbBr_3$-based hybrid detectors experimentally and via simulation. We synthesized $CsPbBr_3$ crystals, studied their transport properties, and detection behavior. Furthermore, we developed a Monte-Carlo simulation approach using experimental data to calculate photo-detection current pulses via the Schokley-Ramo theorem [3]. Our measurements reveal carrier mobility around 200 cm^2/Vs, which was also used in simulating pulse duration. For 1 mm-thick $CsPbBr_3$ sensors at 800 V, 90% integration of 90 keV photons yields an 8 ns pulse duration, within Timepix4 ASICs' ~10 ns integration time [4]. Our findings suggest $CsPbBr_3$ as a promising high-energy detection alternative for hybrid pixel detectors, while estimating the operational limits these materials pose.

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Transfer-matrix method for one-dimensional quantum systems: A review

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The scientific and technological development of a society is closely related to the understanding of fundamental concepts of essential areas of knowledge. The peculiar properties of electron transmission in electric potential barriers in the context of Quantum Mechanics, for example, served as the basis for developing several devices based on heterostructures composed of semiconductors. Furthermore, multiple quantum wells and superlattices have also become important and attractive structures for applications in optical and electronic devices. Different theoretical approaches have emerged to model such structures. The transfer matrix technique, for example, is a useful and affordable method for studying a variety of one-dimensional quantum systems that are based on multiple barriers and well systems. In addition to the scope of Condensed Matter Physics, physical systems in several other areas, such as Statistical Mechanics and Optics, also use this powerful and compact formalism. The methodology used in this work will be based on the analytical development of the transfer matrix of a rectangular multi-barrier system within the context of non-relativistic quantum mechanics, using Schrödinger's equation. The solutions for an arbitrary number of symmetric barriers will be generalized and implemented in the Python programming language, with computational codes made available in a didactic and detailed way. The analyzed results start from the simple barrier structure, which is widely studied in Introduction to Modern Physics courses, to a system of infinite barriers (superlattices) where the transmission properties and energy spectrum are analyzed.

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Transport fingerprints of helical edge states in fractal landscapes

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Fractals are intriguing mathematical objects that exhibit intricate and infinitely complex patterns. Often characterized by self-similarity, the fractals possess a similar structure at different magnification levels, found in a profusion of systems and physical phenomena, like turbulence and crystal formation, among many other examples. Recent advances in the synthesis and experimental investigation of fractalized materials have attracted attention in the scientific community [1, 2], promoting a scenario with a wide range of open questions, those regarding the role of fractality in topological phases of matter, a fertile topic of discussions [3, 4], demand to understand how topological phases are affected when hosted in fractal geometries. With this aim, we develop a systematic theoretical study of the helical edge transport for different generations of Sierpinski carpets, combining the Bernevig-Hughes-Zhang model for the electronic structure and the Landauer approach. The obtained electronic conductance shows reminiscent patterns preserving the pristine quantum spin Hall conductance, resembling a miniband transport picture with fractal fingerprints. Real-space mapping of emerging resonant and antiresonant states provides an unprecedented view of helical-edge currents encoded in these intricate geometries and their multiple edges, underscoring the significance and consistency of our findings.

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Transverse-electric graphene surface plasmon polaritons on films with grating surface

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The propagation of p-polarized surface polaritons along planar and grating interfaces and films of dielectric medium characterized by isotropic and frequency-dependent constants has been extensively reported in the literature [1]. However, more recently, the propagation of s-polarized surface waves (transverse electric (TE) surface modes) was able to be observed in flat interfaces containing a monolayer of graphene [2]. It was shown that the existence of these waves is due to the existence of a 2D electron gas, which introduces a discontinuity on the electromagnetic fields at the interface owing to a non-null graphene's conductivity, which presents, beyond the Drude-like intraband contribution, an interband contribution. [3] Considering interfaces with grating surfaces, Maradudin et al. [4] have shown that s-polarized waves can also propagate perpendicularly through the grooves of a grating interface structure. In this work, we investigate the dispersion relation and the scattering problem of electromagnetic radiation incident in a two-interface system consisting of a frequency-dependent dielectric film sandwiched by two isotropic dielectric regions with a graphene sheet deposited at a flat interface and the other interface has a sinusoidal grating. Results for s-polarized surface waves using the Rayleigh method are shown and physical insights are provided in view of a two-level system originating from hybridized modes lying in the graphene sheet and in the grating. The consequences of changing the grating amplitude and period on the dispersion relation are also discussed.

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Triangular Phase of Strained Arsenene on SiC Substrate

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Two-dimensional strained arsenic allotropes have been proposed to exhibit a non-trivial topology [1,2]. Here, we experimentally grow arsenene by molecular beam epitaxy over the insulating SiC substrate [3]. The arsenene presents a flat structure with a strain field that follows the SiC surface periodicity. Our ab initio simulations, based on the density functional theory, corroborate the experimental observation. The strained structure presents a new arsenene allotrope with a triangular structure, rather than the honeycomb previously predicted for other pnictogens. This strained structure presents a Peierls-like transition leading to an indirect gap semiconducting behavior.

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Trigonal warping effect on the zitterbewegung of wave packet propagation in bilayer graphene

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Analyzing the low-energy band structure of AB-stacked bilayer graphene, one notices the presence of three Dirac mini-cones around the K and K′ valleys, whose physical reason is linked to the well known trigonal warping effect. [1,2] This effect is responsible for band structure asymmetry and implies a non-zero Berry curvature with opposite signs in the two inequivalent valleys when the time-reversal symmetry is preserved, i.e. $\Omega(K) = -\Omega(K')$, which in turn leads to a transversal anomalous velocity for the charge carrier dynamics. In this context, we theoretically investigate the time evolution of a Gaussian wavepacket in order to verify the role of the trigonal warping in the wave packet dynamics propagating in a bilayer graphene sample. Expectation values of the position (x, y) of center-of-mass and the total probability densities of the wave packet are numerically calculated by solving the time-dependent Schrödinger equation using a numerical framework based on the split-operator technique within the Dirac approach for bilayer graphene continuum Hamiltonian taking into account the effects mentioned above due to the skew interlayer hoppings. Transient spatial oscillations due to the effect known as zitterbewegung [3,4] are discussed for different initial pseudospin polarizations, wave packet widths, initial wave packet energies, and momenta.

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Tunable coupling of exciton-polaritons in bilayer graphene: electric control and cavity confinement

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The unique characteristics of microcavities hold great promise for quantum optics and atomic physics. These cavities create a confined space conducive to light-matter interactions, making them ideal for studying and manipulating the interactions between photons and matter excitations. A plethora of novel quantum phenomena have already been observed in such systems, including the formation of quantum emitters based on atoms and solid-state materials within cavities [1-3]. Conversely, two-dimensional (2D) materials have emerged as a prominent platform for light-matter interactions. Recent investigations into moiré semiconductors have revealed the presence of localized excitons that can be electrically manipulated, resulting in a tunable array of quantum emitters [4]. This work delves into the creation and tunability of exciton-polaritons in biased bilayer graphene microcavities, emphasizing their coupling dynamics. We investigate the impact of filling the microcavity with an epsilon near-zero material, such as silicon carbide, revealing a controllable modulation of exciton-polariton interactions.

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Tuning the Electronic Properties of Ternary TMD Alloys via Structural Modifications and Defects: A Combined SQS and DFT Approach

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This study investigates the impact of structural modifications and defects on the properties of the ternary transition metal dichalcogenide (TMD) alloy MoxW1−xSe2, a promising material for technological applications. We employ a robust computational approach combining Special Quasirandom Structures (SQS) and Density Functional Theory (DFT) to explore the interplay between atomic arrangement and electronic structure. SQS, coupled with Monte Carlo simulations and Short Range Order (SRO) analysis, will be used to model the disorder inherent in these alloys and identify optimized structures across a range of compositions. Subsequent DFT calculations will provide a detailed understanding of the electronic structure, density of states (DOS), and projected density of states (PDOS) of the SQS-generated structures. We will investigate the influence of various defects, including vacancies, interstitials, and antisite defects, on the electronic properties of MoxW1−xSe2. By analyzing formation energies, charge localization, and changes in the electronic structure, we aim to identify defect configurations that could lead to desirable properties such as spin-polarization, or altered band gaps. This comprehensive approach will yield valuable insights into the structure-property relationships in ternary TMD alloys, paving the way for the development of materials with tailored properties for applications in high-performance electronics, spintronics, and quantum information technology.

Tunnelling Spectorscopy in MoO3 nanowires

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Wide bandgap semiconductors are being broadly studied for their interesting characteristics such as higher working frequency [1] and temperature resilience [2]. These interesting features also turn them more applicable than narrower bandgap semiconductors. In addition, they are promising materials in the energy efficiency field [3]. This work presents the study of the electronic structure of MoO3 and phosphorus-doped MoO3 nanoribbons. The techniques employed in this work are Atomic Force Microscopy (AFM), Scanning Tunnelling Microscopy (STM) and Spectroscopy (STS), and X-Ray Photoelectron Spectroscopy (XPS). We have found that tunneling occurs at very low currents (approximately 100 picoAmps) and the band gap varies in between 1.8-2.9 Volts. These results may also prove important for the application of wide band gap semiconductors in several field, such as communication, energy storage, blue, and ultra-violet optoelectronic.

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Two-dimensional layered MA_2Z_4 van der Waals heterostructures for high-performance solar cells from first-principles calculations

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MA_2Z_4 two-dimensional (2D) monolayered materials (M = transition metals Mo, W; A = Si, Ge; Z = P, As, N) have gained a lot of attention in the past few years. After the first successful growth of $MoSi_2N_4$ and WSi_2N_4 in 2020 [1] by chemical vapour deposition, several monolayered materials from the same MA_2Z_4 family have been proposed and studied theoretically using density functional theory. They present several properties of interest, such as high mechanical strength [1], high piezoelectric coefficients [2], good thermal transport [2], high optoelectronic response [1,3], and magnetism [2]. In this work we propose and study, using density functional theory, 2D layered van der Waals (vdW) heterostructures formed by MA_2Z_4 layers as candidates for the manufacturing of solar cells. By changing the atomic composition of the MA_2Z_4 layers, it is expected that the band gaps vary significantly; therefore, we propose tandem solar cells formed by heterojunctions of these different materials. To study their stability, we performed lattice parameter optimizations, ionic position optimizations, layer distance optimizations, molecular dynamics calculations, and calculated their vibrational modes. After confirming the stability of the proposed materials, we calculated their density of states, electronic band structure, bandgap, and optoelectronic properties, such as solar energy absorption, and carrier transport properties. This class of 2D layered vdW heterostructures shows great potential to be employed as solar cells, being competitive with other high-performance materials, such as perovskites.

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Unveiling Optical Properties of Low-Dimensional Sb_2O_3

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Antimony is among the most abundant metals in the Earth's crust and It exists in various forms, including the binary oxides Sb_2O_3, Sb_2O_5, and Sb_2O_4. Antimony trioxide, in particular, has garnered attention due to its electronic properties. As a semiconductor with a band gap of 3.3 eV, Sb_2O_3 finds applications as a flame retardant, and semiconductor dopant [2]. At ambient pressure, Sb_2O_3 exhibits two crystalline phases: senarmontite (α-Sb_2O_3) and valentinite (β-Sb_2O_3). Both phases emit photoluminescence peaks in the 390 to 500 nm range, with β-Sb_2O_3 showing an extended emission up to 700 nm. Despite its prevalent use in optical glasses, studies on the vibrational properties of β-Sb2O3 remain limited. This study investigates the optical and structural properties of ultrathin β-Sb_2O_3 nanowires obtained via mechanical exfoliation.Raman spectroscopy and Synchrotron Infrared Nanospectroscopy (SINS) reveal characteristics modes of valentinite, shedding light on its vibrational properties. Additionally, cathodoluminescence data demonstrate broad emission from 390 to 770 nm, indicating the potential of β-Sb2O3 nanowires to cover a significant portion of the solar spectrum. These findings highlight the excellent room-temperature luminescence properties of these nanowires, suggesting promising applications in advanced optoelectronic nanodevices.

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Using resonant inelastic x-ray scattering to study the electronic structure of semiconductors

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Understanding the electronic structure of semiconductors is crucial for the development and optimization of electronic, spintronic, and optoelectronic devices. In its turn, resonant inelastic X-ray scattering (RIXS) is a powerful technique to probe charge-neutral electronic excitations. The possibility to study the electronic structure with element-sensitivity and high energy resolution makes RIXS an interesting tool for semiconductor research. It enables the investigation of low-energy collective excitations, such as magnons, phonons, and excitons, providing their dispersion relations. Additionally, RIXS is sensitive to local electronic excitations, including dd, ff, crystal field, and charge transfer transitions. This allows RIXS to probe structural, orbital, spin, and charge degrees of freedom in a single experiment. By providing information on fundamental energies that can validate ab initio calculations, RIXS has tremendous potential to enhance the understanding of fundamental physics. By unravelling complex electronic phenomena in semiconductors, the technique offers insights essential for advancing device functionality. In this presentation, we will demonstrate the potential of RIXS to study the electronic structure of semiconductors by discussing preliminary results obtained during the commissioning of the RIXS end station of the IPE beamline [1] for systems such as titanates and Cr-based 2D magnets.

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Vacancy in twisted bilayer graphene

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Abstract

After 20 years since the discovery of graphene, it is still considered promising for new electronic devices due to properties such as high electronic mobility (a consequence of linear dispersion near the Fermi level), high flexibility, and ease of doping. Even more relevant for electronics is bilayer graphene, whether in its most common form, AB stacking, or in AA stacking, thanks to the possibility of opening a gap, by applying an external electric field perpendicular to the layers, which is an essential characteristic for electronic devices. Following the timeline of research on graphene-based materials, twisted bilayer graphene (tBG) brings further new features to be explored, such as the influence of Moiré patterns (interference patterns that arise due to a rotation or displacement of one layer relative to the other) on the localization of states near the zero energy level [1], or its behavior as an unconventional superconductor at the so-called magic rotation angle [2]. Keeping in mind the strong localization effects of states due to vacancies in bilayer graphene [3], which have significant effects on electronic and transport properties [4], this work investigates, by means of tight-binding model, the effects of vacancies on the band structure as well as on the charge carrier localization for various rotation interlayer angles of tBG. Different point defects are explored, such as mono-, di-, and tri-vacancies, preserving or not the sublattice symmetry per layer.

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Vibrational and electronic properties of bidimensional $CsPb_2Br_5$ crystals

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Manufacturing semiconductor-based light detection requires complex and capital intensive equipment. In recent years, halide perovskites with chemical formula CsPbX 3 , where X = Br, I or Cl, have gained interest due to their easy processing and excellent properties, such as efficient light absorption and high carrier mobility. All inorganic perovskites have emerged as promising candidates for photodetection due to their favorable intermediate bandgap, thermal stability, and humidity stability. Recently, $CsPb_2Br_5$ is a two-dimensional ternary halogen-plumbate material with characteristics close to the well-reported halide perovskites, being widely used for potential applications in optoelectronics. Investigations into $CsPb_2Br_5$ are currently limited to nanostructures and powder forms of the material, which exhibit unclear and conflicting optical properties. In this study, we present the synthesis and characterization of bulky single crystals of $CsPb_2Br_5$, which allowed us to finally clarify the optical characteristics of the material. Our crystal has a two-dimensional structure composed of layers of $Pb_2Br_5^-$ spaced by Cs^+ cations. We carried out a study of the vibrational and electronic properties of this material as a function of laser energy and temperature. The single crystal exhibits a ~3.1 eV indirect bandgap with no emission in the visible spectrum.

Visualizing Twisted Bilayer Graphene inside h-BN encapsulated Samples

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With the evolution of van der Waals heterostructures, two types of structures have been highlighted. The first is sample encapsulation, capable of isolating two-dimensional Materials from interactions with the substrate and the atmosphere, thereby enhancing the electronic mobility of the sample and providing devices of the highest quality [1]. The second is twisted bilayer graphene (TBG), which exhibits a superlattice due to the formation of a Moire pattern between the crystalline networks of both graphene layers. Such structures have their electrical properties modulated by the rotation angle between the layers, leading to the existence of the magic angle, the angle at which the sample exhibits the formation of strongly interacting states, providing superconducting, insulating, and ferromagnetic states [2]. The observation of these phenomena requires encapsulated samples with accuracy in the layer rotation angle. However, the TBG fabrication process results in heterogeneous samples with various regions having different rotation angles. Since there is no characterization method for superlattices with such resolution in encapsulated samples, the device fabrication process in these samples involves a trial-and-error process until, through indirect measurements, a device in the magic angle is identified. This work demonstrates the first characterization of superlattices in TBG near the magic angle, encapsulated by a thin hBN flake, enabling the construction of samples at the magic angle precisely and quickly. The characterization was carried out using scanning Microwave Impedance Microscopy, a technique capable of sensing spatial changes in the conductivity and permittivity of a sample through a microwave reflection process [3].

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