XIX Semana da Física

Universidade Federal de São Carlos - UFSCar

Caderno de Programação do Workshop

Apresentação

A XIX SeFís, com tema "As várias faces da Física brasileira", acontecerá entre os dias 28 de outubro e 1 de novembro e contará com palestras, minicursos, oficinas, apresentações e mesas de debate com participantes ilustres.

Este ano contaremos novamente com o Workshop da graduação e pós graduação. Essa é uma oportunidade para estudantes e pesquisadores apresentarem seus trabalhos de pesquisa. Esse é um ambiente de divulgação e debate que busca promover interação entre pesquisadores e contribuir para a formação dentro de um ambiente acadêmico.

O workshop contará com com apresentações orais e sessões de pôster organizadas em dois dias, 29 e 31 de outubro, com o cronograma de sessões definido na tabela 1. Na presente edição, contaremos com 31 apresentações, sendo 15 apresentações orais e 16 apresentações de pôsteres por estudantes de graduação de pós graduação do Departamento de Física da UFSCar.

Table 1: Cronograma de Sessões do workshop da XIX SeFís - UFSCar

Horário	**Terça (29/10)**	**Quinta (31/10)**
13:00 - 14:30	Sessão de apresentação de pôsteres 1	Sessão de apresentações orais 2
14:30 - 16:00	Sessão de apresentações orais 1	Sessão de apresentação de pôsteres 3
16:00 - 16:30	Coffee Break	Coffee Break
16:30 - 18:00	Sessão de apresentação de pôsteres 2	Sessão de apresentações orais 3

Conteúdo

Terça-Feira -- 29/10 13:00 - 14:30 (Sessão de apresentação de pôsteres 1)

13:00 - 14:30
DF

Emerging 2D Materials: Exploring Monochalcogenides with Ab-Initio Methods

Marco A. M. T. Machado (Department of Physics, Federal University of São Carlos), Mateus B. P. Querne(Instituto Federal do Paraná), Ronaldo C. Prati (Center of Mathematics, Computer Science, and Cognition, Federal University of ABC), Natan M. Regis (Department of Physics, Federal University of São Carlos), Anderson Janotti (Department of Materials Science and Engineering, University of Delaware), Matheus P. Lima (Department of Physics, Federal University of São Carlos), Juarez L. F. Da Silva (São Carlos Institute of Chemistry, University of São Paulo)

Two-dimensional materials have emerged as a distinct research field in materials science since the groundbreaking study on graphene in 2004. Numerous layered materials have demonstrated that variations in composition, dimensionality, and crystalline phase result in a wide range of unique properties compared to conventional 3D materials. Despite the vast array of known 2D materials, many remain unexplored, and computational simulations offer a cost-effective approach to their investigation. In this research, we explore the optoelectronic properties of 2D monochalcogenides with the chemical formula MQ, where M represents an element from groups III, IV, or V, and Q is a chalcogen (S, Se, or Te). Our simulations consider 13 space groups: P3m1 , P3m1 , P6m2, Aem2, C2/m, P 21 /c, P4/nmm, P1 , P1 , Pbcm, Pmmn, Pmna, and Pmn21 . These space groups, associated with 27 distinct chemical compositions (MQ), totaling 351 systems. We employed ab initio simulations based on Density Functional Theory (DFT), using the Vienna Ab initio Simulation Package (VASP). Our simulations identify the lowest-energy crystalline phase for each composition and analyze their energetic and vibrational stability. Additionally, we investigated the electronic properties, focusing on the density of states (DOS), and complemented this analysis with Bader charge calculations. Vibrational instability was observed in the lowest-energy SiTe structure with the Pmna space group, leading to its replacement by the P3m1 structure. The DOS revealed that for elements in groups IV and V, the p orbitals dominate the band edge region, while the s, p, and d orbitals are observed in group III. Furthermore, the lowest-energy SbTe structure in the P1 phase exhibits metallic behavior, whereas the remaining structures are semiconductors. Our comprehensive mapping of the structural, optoelectronic properties of monochalcogenides provides valuable insights for the future development of new devices.

Keywords: Monochalcogenides; Two-dimensional materials; Electronic properties; VASP

References:

G. Henkelman, A. Arnaldsson e H. Jónsson. "A fast and robust algorithm for Bader decomposition of charge density". Em: Computational Materials Science 36 (2006), pp. 354–360. doi: 10.1016/j.commatsci.2005.04.010.

P. Hohenberg e W. Kohn. "Inhomogeneous Electron Gas". Em: Phys. Rev. 136 (3B nov. de 1964), B864–B871. doi: 10.1103/PhysRev.136.B864.

G. Kresse e J. Furthmüller. "Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set". Em: Phys. Rev. B 54 (16 ago. de 1996), pp. 11169–11186. doi: 10.1103/PhysRevB.54.11169.

G. Kresse e D. Joubert. "From ultrasoft pseudopotentials to the projector augmentedwave method". Em: Phys. Rev. B 59 (3 jan. de 1999), pp. 1758–1775. doi: 10.1103/PhysRevB.59.1758.

Kin Fai Mak et al. "Atomically Thin MoS2 : A New Direct-Gap Semiconductor". Em: Phys. Rev. Lett. 105 (13 set. de 2010), p. 136805. doi: 10.1103/PhysRevLett.105.136805.

K. S. Novoselov et al. "Electric Field Effect in Atomically Thin Carbon Films". Em: Science 306.5696 (2004), pp. 666–669. doi: 10.1126/science.1102896.

K. S. Novoselov et al. "Two-dimensional atomic crystals". Em: Proceedings of the National Academy of Sciences 102.30 (2005), pp. 10451–10453.
doi: 10.1073/pnas.0502848102.

John P. Perdew, Kieron Burke e Matthias Ernzerhof. "Generalized Gradient Approximation Made Simple". Em: Phys. Rev. Lett. 77 (18 ago. de 1996), pp. 3865–3868. doi: 10.1103/PhysRevLett.77.3865.

Mateus B. P. Querne et al. "Crystal structure and electrical and optical properties of two-dimensional group-IV monochalcogenides". Em: Phys. Rev. B 108 (8 ago. de 2023), p. 085409. doi: 10.1103/PhysRevB.108.085409.

E. Sanville et al. "An improved grid-based algorithm for Bader charge allocation". Em: Journal of Computational Chemistry 28 (2007), pp. 899–908. doi: 10.1002/jcc.20575.

W. Tang, E. Sanville e G. Henkelman. "A grid-based Bader analysis algorithm without lattice bias". Em: Journal of Physics: Condensed Matter 21 (2009), p. 084204. doi:10.1088/0953-8984/21/8/084204.

M. Yu e D. R. Trinkle. "Accurate and efficient algorithm for Bader charge integration". Em: Journal of Chemical Physics 134 (2011), p. 064111. doi: 10.1063/1.3553716.

Jun Zhou et al. "2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches". Em: Scientific Data 6.1 (jun. de 2019). issn: 2052-4463. doi: 10.1038/s41597-019-0097-3.

Analyzing Solar Cell Electrical Behavior through Cyclic Voltammetry and Impedance Spectroscopy

13:00 - 14:30
DF

Luiz Antonio Meneghetti Jr (UFSCar), Gabriel Leonardo Nogueira (UNESP-Bauru), Fabian Hartmann (University of Würzburg), Carlos Frederico de Oliveira Graeff (UNESP-Bauru), Victor Lopez Richard (UFSCar)

Hybrid organic-inorganic perovskites represent a promising advancement in solar cell technology, but significant challenges remain, particularly with stability and non-ideal electrical behavior under specific external conditions. This work introduces a conceptual framework for analyzing photovoltaic devices using impedance spectroscopy (IS) and cyclic voltammetry (CV). By adopting a multimodal, microscopic approach, the model captures the effects of memory, drift, diffusion, and displacement, providing detailed analytical models for complex admittance and current-voltage characteristics. It reveals the intrinsic link between capacitive and inductive behaviors in IS spectra and hysteresis in CV curves, demonstrating how these complementary techniques enhance understanding of the microscopic mechanisms driving device performance. The study further explores the relationship between intrinsic material properties and experimentally accessible parameters such as temperature, voltage, frequency, light intensity, and DC bias, offering new avenues for optimizing solar cell efficiency.

References:

M. A. Green, A. Ho-Baillie, and H. J. Snaith, Nature Photonics 8, 506 (2014)

L. Sun, K. Fukuda, and T. Someya, npj Flexible Electronics 6, 89 (2022)

H. Aqoma, S.-H. Lee, I. F. Imran, J.-H. Hwang, S.-H. Lee, and S.-Y. Jang, Nature Energy 9, 324 (2024)

M. A. Green, Solar Cells: Operating Principles, Technology, and System Applications, Prentice-Hall Series in Solid State Physical Electronics (Prentice-Hall, Englewood Cliffs, NJ, 1982)

R. S. W. Silva, F. Hartmann, and V. Lopez-Richard IEEE Transactions on Electron Devices 69, 5351 (2022)

A. B. de Paiva, R. S. Wengenroth Silva, M. P. F. de Godoy, L. M. Bola˜nos Vargas, M. L. Peres, D. A. W.

Soares, and V. Lopez-Richard, The Journal of Chemical Physics 157, 014704 (2022).

13:00 - 14:30
DF

Development and instrumentation of a fluorescence system with high spatial and temporal resolution

Tiago Bonicelli Gambarotto (UFSCar), Marcio Daldin Teodoro (UFSCar)

The exploration of electronic states in matter has led to a series of scientific discoveries across various research domains over time. The interaction of electromagnetic radiation with matter forms a fundamental basis for several experimental techniques that investigate the electronic structure and the time scales of dynamic processes. Specifically, fluorescence spectroscopy and time-resolved fluorescence spectroscopy play a crucial role in investigating these processes. Fluorescence spectroscopy reveals information about the electronic structure of the sample, while time-resolved fluorescence observes the temporal evolution of excited states. Due to the importance of these studies, the proposal of this work focuses on the implementation of these techniques with a tunable laser and a high temporal resolution detector (<5 ps), operating over a wide spectral and temperature range. The tunable laser allows selective exploration of different electronic states, and the high temporal resolution captures ultrafast events. This approach will advance the understanding of electronic states and dynamic processes in matter, providing a powerful experimental tool for various research groups.

13:00 - 14:30
DF

SnO2 Nanowires as Ozone Gas Sensors

Simone Macêdo Ribeiro (UFSCar), Adenilson José Chiquito (UFSCar)

T

his work involves the production, characterization and optimization of electronic devices based on SnO2 nanowires aiming at the study of electrons transport properties and detection characteristics when devices were subjected to chemical products such as ozone gas at room temperature. Different experiments showed promising and reliable results for ozone detection using single tin oxide (SnO2) devices. The detection mechanism in gas sensors based on these structures can be understood by adsorption and desorption processes between chemical species and the surface of the SnO2 nanowires. It was proposed to investigate the electronic properties of devices based on a single nanowire and nanowire films and their responses when subjected to different environments in which the exposure time to the gas of interest at room temperature was controlled. Devices with a single nanowire and with a nanowire film with different metallic contacts were also investigated in order to obtain an optimized response. Transport experiments were conducted to analyze the conduction mechanisms and their possible change when nanowires were exposed to the ozone gas. Influence of vacancies and metal-semiconductor interfaces that define electrical contacts will also be considered. Preliminary results showed that the samples/devices acting as sensors detect ozone efficiently and quickly with a detection time of 3.5 s and a cleaning time of 16 s, demonstrating high detection sensitivity. Furthermore, a comparative analysis showed that devices with a single microwire detect ozone faster than those with a nanowire film, which can be

attributed to the presence of random interface contacts between nanowires in the film architecture which, in turn, adds potential barriers to the electron conduction through the device. The response time to gas in both devices was also investigated and compared.

References:

[1] ARAÚJO, E. P.; AMORIM, C. A. de; ARANTES, A. N.; CHIQUITO, A. J. A Label-free Acetone Based SnO2 Nanowire Network Sensor at Room Temperature. Applied Physics A-Materials Science & Processing 128, 404 (2022). [2] ARAÚJO, E. P. Sensores baseados em nanofios semicondutores de SnO2: fotodetector de luz UV e sensor de gás. 2022. [3] HUANG, Jin; WAN, Qing. Gas sensors based on semiconducting metal oxide one-dimensional nanostructures. Sensors, v. 9, n. 12, p. 9903-9924, 2009. [4] WU, Y.; YANG, P. Direct observation of vapor- liquid- solid nanowire growth. Journal of the American Chemical Society, vol. 123, no. 13, pp. 3165–3166, 2001.

Terça-Feira -- 29/10 14:30 - 16:00 (Sessão de apresentações orais 1)

14:30 - 16:00
CCET

A Building Block For Universal Continuous Variables Computation In Superconducting Devices

Bruno A. Veloso (UFSCar), Ciro M. Diniz (UFSCar), Daniel Z. Rossatto (UNESP), Celso J. Villas-Bôas (UFSCar)

Using quantum properties to store and process information has garnered increasing interest as our technical abilities to control quantum systems have advanced. Traditionally, quantum computation employs the quantum analog of a bit (the qubit) to encode information. However, an alternative approach, known as Continuous Variables (CV) quantum computation, has gained significant attention, both theoretically and experimentally. Rather than using the discrete states of a qubit, this approach leverages continuous properties of quantum systems, such as mode amplitudes, to store information. To perform computations within this framework, we must be able to construct a Hamiltonian that is an arbitrary polynomial in the quadratures of the mode. Such Hamiltonians can be constructed using a finite set of interactions called the universal gate set. In this work, we propose a scalable superconducting device capable of implementing all operations required for a universal CV set. Employing Hamiltonian engineering techniques, we derive effective Hamiltonians that generate all five required interactions. Through precise control of external fluxes and device frequencies, we demonstrate high fidelity and provide the range of parameters necessary for the practical implementation of this device in superconducting circuits. Given its scalability and ability to generate all required interactions in a controlled manner, we propose this device as a building block for constructing CV quantum computers based on superconducting technology.

GROWTH AND STRUCTURAL CHARACTERIZATION OF BILAYERED KNN/CFO HETEROSTRUCTURES DEPOSITED VIA RF MAGNETRON SPUTTERING

14:30 - 16:00
CCET

R.A.R. Carvalho (Universidade Federal de São Carlos), R.P. Bonini (Universidade Federal de São Carlos), F.L. Zabotto (Universidade Federal de São Carlos), J.A. Eiras (Universidade Federal de São Carlos)

Artificial Multiferroic heterostructures combining piezoelectric and magnetostrictive materials gained attention in the early 2000s for their potential applications in electronics, including magnetic sensors and advanced memory devices based on the magnetoelectric effect. While lead-based ceramics are widely used for their exceptional piezoelectric properties, environmental concerns have driven the search for lead-free alternatives, with nanostructured (K,Na)NbO3 based systems in general emerging as promising replacements due to their excellent piezoelectric properties, high Curie temperature, and sustainable nature. In the context of this research, there is a notable gap in the literature concerning the modification of the properties of thin films of lead-free materials in the presence of a magnetic phase, most notably oxide ones. This current study aims to investigate the structural properties of K1-xNaxNbO3 /CoFe2O4 (KNN/CFO) (ferroelectric/ferrimagnetic) bilayered oxide thin films deposited on Si/SiO2/Ti/Pt(111) substrates using the RF magnetron sputtering technique under different annealing conditions – conventional thermal annealing (CTA) and rapid thermal annealing (RTA) - using x-ray diffraction and atomic force microscopy. The CFO phase shows high texturization in (111) direction while the KNN phase shows texture in (022) direction. Topography images show that the conventional oven annealed sample has higher grain size over the RTA annealed, at the same time showing higher rugosity and porosity which might compromise the physical properties of the sample.

Acknowledgments:
This work was supported by FAPESP - The São Paulo Research Foundation (2017/13769-1, 2022/04153-5 and 2023/07654-8), CNPq - National Council for Scientific and Technological Development (304200/2022-0 and 404538/2021-5) and INCT - National Institutes of Science and Technology (MATFERRCE CNPQ 406322/2022-8)

Aerodynamic performance analysis of a wingtip propeller

14:30 - 16:00
CCET

Maria Veronica Meneghetti Bomfim (Universidade Federal de São Carlos- UFSCar), Thamine Terezinha Coelho(Escola de Engenharia de São Carlos- EESC-USP), Lucas Miasiro Ciaramicoli (Escola de Engenharia de São Carlos- EESC-USP), João Paulo Eguea (Escola de Engenharia de São Carlos- EESC-USP), Fernando Martini Catalano (Escola de Engenharia de São Carlos- EESC-USP)

Due to the exponential growth of environmental problems related to climate change and air pollution in the 21st century, the aviation area has been seeking, through studies and technologies, new aircraft configurations to guarantee better performance and sustainability. This issue is of great importance and interest to the

population, industry, and academia. Based on this need, studies demonstrate that the distributed electric propulsion system, which is an electric motor system technology on the leading edge and at the tip of the wing, presents an aeropropulsive integration that allows for improved performance and reduction of CO2 emissions in aircraft, thus enabling electric and hybrid aircraft. Within this scope, the research seeks to evaluate the aerodynamic coefficients of the wing and the propulsive efficiency of the propellers, in a three-dimensional wing model, evaluating the interaction between the wing and a propeller at the wingtip rotating in the opposite direction to the wing-tip vortex. Wind tunnel tests were carried out on the model, using an aerodynamic balance, measuring drag and lift to evaluate the performance improvement provided by the propeller-wing interaction. Simultaneously, propeller thrust and torque data will be measured on a scale designed at the Experimental Aerodynamics Laboratory from the Aeronautical Engineering Department of the São Carlos School of Engineering. The results showed the propeller influence at the wing, an increase in the maximum lift, lift curve slope, and zero-lift drag coefficient, while a reduction in induced drag was obtained. As for the influence of the wing on the propeller, there was a reduction in propeller efficiency. In the end, the results showed that the aeropropulsive interaction of the wing and wing-tip propeller is efficient for take-off and climb and smaller for cruise conditions.

14:30 - 16:00
CCET

Magneto-optical effects in a twisted homo-bilayer MoS2

André Pelais (Universidade Federal de São Carlos), Frederico Barros de Sousa (Universidade Federal de São Carlos), Ivo Fernandes (Universidade Federal do Ceará), Gabriel de Oliveira (Universidade Federal do Ceará), Luciano de Almeida (Universidade Federal do Ceará), Andreij de Carvalho Gadelha (Universidade Federal de São Carlos), Márcio Daldin Teodoro (Universidade Federal de São Carlos)

Twisted bilayers of transition metal dichalcogenides (TMD) are interesting platforms for quantum information technology due to their exciton confinement imposed by the moiré potential. Recent advances in the layer engineering of 2D materials have enabled the stacking of identical or different compounds with a twist between layers, creating moiré artificial supercells depending on the angle. These structures benefit from the strong light-matter coupling of intra-layer excitons and the robust out-of-plane electric dipole interaction of inter-layer excitons. However, a polarization-sensitive study, investigating the dependency of new moiré states and multi-body phenomena with an applied magnetic field is lacking. In this context, the twisted homo-bilayer of molybdenum disulfide (MoS) plays a crucial role due to its intense photoluminescence (PL) and tunability of exciton properties. This work investigates the magneto-PL effects of excitonic complexes in a homo-bilayer of MoS twisted by 58°. The twisted bilayer MoS reveals a double PL peak in the equivalent monolayer's neutral exciton probably due to interlayer interactions and stacking order. The intensity ratio between these PL peaks depicts an oscillating behavior with the magnetic field, pointing to oscillatory resonance between Fermi and Landau levels.

Furthermore, we measured biexciton complexes whose degree of circular polarization is strongly modified by magnetic applications, revealing forbidden multibody physics. These findings shed light on moiré excitons in the twistronics field and pave the way for controlling and modifying moiré valley-spin properties for future quantum technology applications.

Terça-Feira -- 29/10 16:30 - 18:00 (Sessão de apresentação de pôsteres 2)

16:30 - 18:00
CCET

Effect of Fe/Co Codoping on the Phase Transition and Ferroelectric Properties of Bi3.25Nd0.75Ti3O12

Rafael Alves Lozano (Universidade Federal de São Carlos, Departamento de Física, SP, Brasil), José Antonio Eiras (Universidade Federal de São Carlos, Departamento de Física, SP, Brasil), Mahmoud. S. Alkathy (Universidade Federal de São Carlos, Departamento de Física, SP, Brasil), Fabio Luis Zabotto (Universidade Federal de São Carlos, Departamento de Física, SP, Brasil.)

The search for new materials for multifunctional devices has become a priority in the scientific community, driven by the growing technological demand in modern society. Among the prominent materials, those with ferroic ordering have gained special attention due to their ability to present order states controllable by external fields, being essential in areas such as sensors and functional actuators. In recent years, ferroelectrics structured in bismuth layers have aroused significant interest due to their unique properties that allow the development of more efficient and low-power memory devices. [1]. Doped ceramics of the Bi3.25Nd0.75Ti3O12 matrix, belonging to the Aurivillius family, are especially studied due to their remarkable spontaneous polarization and because they are lead-free, taking into account environmental concerns. Phase transition studies for the Bi3.25Nd0.75Ti3O12 system, a perovskite compound, focus on specific modifications aimed at improving its properties as it is doped with Fe and Co. The analysis of ferroelectric domains, regions with uniformly oriented dipoles, is fundamental to understanding the complexity of the modified BIT. Furthermore, it has been observed that Nd3+ doping reduces the Curie temperature as the symmetry of the crystal structure increases, due to the volatilization of bismuth during sintering. Therefore, the present study aims to find the phase transition temperature according to frequency through dielectric and pyroelectric characterization. Additionally, it was observed that Nd3+ doping leads to broadening and decrease in the intensity of the Curie peak, which may be related to the formation of a fine-grained microstructure and the presence of secondary phases [2]. This research plays a crucial role in the application of modified BIT in advanced electronic devices, sensors, and emerging technologies, driving the development of perovskite materials with properties tailored for specific applications.

Acknowledgements:
This work was supported by FAPESP - São Paulo State Research Support Foundation (#2017/13769-1 and 2022/04153-5) and the National Council for Scientific and

Technological Development (CNPQ/Finep/MCTIC/BRICS-STI nº 402741/2019-6 and CNPq/MCTI/BRICS-STI nº 04/2022) and INCT (MATFERRCE CNPQ 406322/2022-8).
References:] [1] Gupta, R., Kotnala, R.K. A review on current status and mechanisms of room-temperature magnetoelectric coupling in multiferroics for device applications. J Mater Sci 57, 12710–12737 (2022). Disponível em: https://doi.org/10.1007/s10853-022-07377-4. [2] ISLAM, Muhammad Aminul; ISLAM, Muhammad Saidul; GAFUR, Muhammad Abdul. Synthesis and Characterization of La and Nd Co-Doped Bismuth Titanate Ferroelectric Ceramics. International Journal of Applied Ceramic Technology, v. 12, n. S3, p. E191-E196, 2015. DOI: 10.1111/ijac.12394.

DYNAMIC FUNCTIONAL CONNECTIVITY IN PATIENTS WITH SCHIZOPHRENIA

16:30 - 18:00
DF

Belarmino, M.H.A.1 (UFSCar) e Ozelo, H.F.B.(UFSCar)

FMRI resting-state networks might be used to increase our understanding about brain disorders. In particular, higher-order networks such as the default mode network (DMN) are frequently disrupted in patients with schizophrenia. Most rs-fMRI studies have employed static connectivity methods to examine the functional organization of the brain, assuming a stationary condition throughout the scanning session. However, there is evidence that functional connectivity changes over time, showing that subjects are likely to engage in slightly different mental activities at different instances in time. We hypothesize that dynamic analysis of these networks can provide connectivity variations that may occur at different times and that would not be revealed in static methods. For this purpose, we will use the sliding time window approach, where functional connectivity (FC) is calculated for consecutive portions of the scan period and this process is repeated until the last fMRI volume. Then, the FC matrices from these windows are grouped by similarity in order to form a set of "connectivity states". Each connectivity state is formed by a set of brain regions, whose temporal pattern over time describes the functional organization of the brain. The objective of this work is to quantify variations in functional connectivity over time in order to verify whether it is possible to use them to discriminate between healthy controls and patients with schizophrenia.

16:30 - 18:00
DF

Machine learning applied to laser cooling

Vinicius Bueno Tafuri (DF/UFSCar), Gustavo Deczka Telles (IFSC/USP)

Laser-cooled samples have been around for decades and have helped to produce great science contributions. More recently, machine learning (ML) has evolved a lot and has become an efficient means to investigate empirical models of complex systems. Typically, the complex dynamics presented by many-body interaction systems preclude precise analytical optimization of cooling mechanisms and capture. In this project, we will apply fundamental machine learning methods to optimize the preparation of neutral Rubidium-87 atoms, as it is one of the fundamental stages concerning the experimental realization of Bose-Einstein condensates. More specifically, we intend to increase the number of trapped atoms in a magneto-optical trap (MOT) by establishing a connection between the physical model that describes the MOT operation and the function related to the ML algorithms' performance during the optimization (i. e. the cost function). For this purpose, we will investigate three widely known ML models: Differential Evolution, Gaussian Process and Artificial Neural Networks. The solutions found by these algorithms tend to be radically different from the adiabatic, analytic solutions currently used by researchers and will be studied and compared. Despite this, we believe that the new solutions will overcome the combination of previously known parameters optimizing the preparation of trapped atomic samples.

16:30 - 18:00
DF

A model for a leaky dielectric with memory

Igor Ricardo Filgueira e Silva (UFSCar), Ovidiu Lipan (University of Richmond), Fabian Hartmann (Universität Würzburg), Sven Höfling (Universität Würzburg) e Victor Lopez-Richard (UFSCar)

Based on a microscopic model of nonequilibrium carrier generation in a leaky dielectric, in this work we analytically derive hysteresis loops for the dielectric response of non-polar and non-ferroelectric materials. We demonstrate how complex dielectric responses can arise solely from energy and voltage polarity-dependent transport and asymmetries in the transfer rates. By combining two powerful techniques widely used in material science and nano-device characterization, Electrochemical Impedance Spectroscopy (EIS) and voltammetry, we address critical questions related to the microscopic mechanisms in poorly conductive systems dominated by displacement currents. The impedance analysis, extended to higher-order harmonics, provides deeper insights into the dynamic behavior of dielectric materials, emphasizing the need to correlate impedance spectroscopy with dielectric spectroscopy for a thorough understanding of dipole relaxation and transport phenomena. Our findings offer valuable perspectives for applications in capacitors, transistors and memory devices.

Synthesis and Characterization of the high entropy oxide (Mg,Co,Ni,Zn,Cu,Li)O

16:30 - 18:00
DF

Luan Pereira Leite (Universidade Federal de São Carlos), João Vitor Campos (Universidade Federal de São Carlos) , Isabela Reis Lavagnini (Universidade Federal de São Carlos) , Lílian Menezes de Jesus (Universidade Federal de São Carlos)

High entropy oxides (HEOs) are part of a new class of materials known as high entropy materials, in which a solid solution not predicted by the phase diagram of the constituent elements can be obtained. The first high entropy oxide was synthesized in 2015 [1]. As research on these materials progresses, intriguing electrical properties, such as a giant dielectric constant [2] and high ionic conductivity [3], have been reported for the (Mg,Co,Ni,Zn,Cu,Li)O system. However, the underlying mechanisms are still under debate. Therefore, further investigation is needed to understand the physical mechanisms that give rise to these electrical properties. In this study, we explored the synthesis of the high entropy oxide (Mg,Co,Ni,Zn,Cu,Li)O via a polymeric route to assess its electrical properties. The (micro)structural characteristics of the ceramics were evaluated using X-ray diffraction and scanning electron microscopy (SEM), while impedance spectroscopy was used to investigate their electrical properties. Based on the results obtained so far, we conclude that the polymeric synthesis is efficient in producing single-phase rock salt HEO ceramics. Additionally, conventional sintering at 1000 °C followed by quenching also yields single-phase ceramics.

Acknowledgements: CNPq (Bolsista PIBIC)

References:

[1] C.M. Rost, E. Sachet, T. Borman, A. Moballegh, E.C. Dickey, D. Hou, J.L. Jones, S. Curtarolo, J.-P. Maria, Entropy-stabilized oxides, Nat Commun 6 (2015) 8485. https://doi.org/10.1038/ncomms9485.

[2] D. Bérardan, S. Franger, D. Dragoe, A.K. Meena, N. Dragoe, Colossal dielectric constant in high entropy oxides, Physica Status Solidi - Rapid Research Letters 10 (2016) 328–333. https://doi.org/10.1002/pssr.201600043.

[3] D. Bérardan, S. Franger, A.K. Meena, N. Dragoe, Room temperature lithium superionic conductivity in high entropy oxides, J Mater Chem A Mater 4 (2016) 9536–9541. https://doi.org/10.1039/c6ta03249d.

16:30 - 18:00
DF

SnO2 nanowires based ozone sensor

Giovanni Lucas Palotta(UFSCar), Adenilson José Chiquito(UFSCar)

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.

Quinta-Feira -- 31/10 13:00 - 14:30 (Sessão de apresentações orais 2)

The role of Jahn-Teller distortion in the relative stability between the black and yellow phases of transition metal doped CsSnI3 perovskites

13:00 - 14:30
CCET

Lucas G. Chagas (UFSCar), Juarez L. F. Da Silva (IQSC-USP), Matheus P. Lima (UFSCar)

Halide perovskites show great potential as low-cost materials for efficient photovoltaic applications[1]. However, structural instabilities and lead toxicity present significant challenges for commercial applications. Specifically, these challenges are: (i) toxicity, as lead (Pb) is present in most high-efficiency devices, and (ii) inherent structural instabilities[2,3]. In particular, the CsSnI3 perovskite offers a lead-free alternative, addressing the toxicity issue, it still perpetuates the problem of instability[4]. Notably, the photo-inactive yellow phase has a lower formation enthalpy than the photo-active black phase, leading to an undesirable phase transition and inherent instability[5,6]. This work[7] employs ab initio density functional theory calculations to explore the influence of substitutional doping in CsSnI3 at the Sn-site with 3d transition metals on the relative interphase stability between the yellow and black phases. To improve the description of the Transition Metals 3d-states within the CsSnI3 compounds given their localized character, we adopted the effective Hubbard approach proposed by Dudarev et al.[8] with Uef f = 0 eV, 3 eV and 6.0 eV. Our investigation shows that doping with Co, Cu, and Zn transforms the photo-active phase into the lowest formation enthalpy phase. This stability exchange is attributed to Jahn-Teller distortions within the doped octahedra, taking into account the distinctive octahedral connections in the black and yellow phases. In the black phase, the octahedra are corner-shared, whereas in the yellow phase, they are edge-shared. Of particular note is the impact of Zn ion doping, which not only alters the relative stability but also preserves a pristine bandgap region, free of defect states. These findings have substantial implications for the development of stable, non-toxic photovoltaic materials with enhanced performance.

References:

[1] Chen, Z.; Turedi, B.; Alsalloum, A. Y.; Yang, C.; Zheng, X.; Gereige, I.; AlSaggaf, A.; Mo-hammed, O. F.; Bakr, O. M. ACS Energy Letter 2019,4, 1258–1259.

[2] Torres, Israel S.; Da Silva, Juarez L. F.; Lima, Matheus P. The Journal of Physical Chemistry C 2023, 127, 1713-1721.

[3] dos Santos, Ramiro M.; Ornelas Cruz, Iván.; Dias, Alexandre C.; Lima, Matheus P.; Da Silva, Juarez L. F. ACS Applied Energy Materials 2023, 6, 5259-5273.

[4] Dias, A. C.; Lima, Matheus P.; Da Silva, Juarez L. F. The Journal of Physical Chemistry C 2021, 125, 19142-19155.
[5] Ma, J.-Y.; Yan, H.-J.; Li, M.-H.; Sun, J.-K.; Chen, Y.-X.; Wang, D.; Hu, J.-S. Nanoscale 2020,12, 7759–7765.
[6] Akbulatov, A. F.; Tsarev, S. A.; Elshobaki, M.; Luchkin, S. Y.; Zhidkov, I. S.; Kurmaev, E.Z.;Aldoshin, S. M.; Stevenson, K. J.; Troshin, P. A. The Journal of Physical Chemistry C 2019,123, 26862–26869.
[7] Chagas, Lucas G. and Da Silva, Juarez L. F. and Lima, Matheus P. Physical Review B 2024, 109, 014106.
[8] S. L. Dudarev, G. A. Botton, S. Y. Savrasov, C. J. Humphreys, and A. P. Sutton; Physical Review B 1998,57, 1505.

13:00 - 14:30
CCET

Magnetoabsorption and spin polarization inversion in quantum wells

G. M. Jacobsen (Universidade Federal de São Carlos), V. Lopes-Oliveira (Universidade Estadual de Mato Grosso do Sul), V. Laurindo Jr. (Universidade Federal de São Carlos), Yu. I. Mazur (University of Arkansas), M. E. Ware (University of Arkansas), G. J. Salamo (University of Arkansas), B. L. Liang (University of California), G. E. Marques (Universidade Federal de São Carlos), E. Marega Jr. (Universidade de São Paulo), V. Lopez-Richard (Universidade Federal de São Carlos) e M. D. Teodoro (Universidade Federal de São Carlos)

The spin dynamics in GaAs/AlGaAs and GaAs 1-x Sb x /GaAs quantum wells (QWs) featuring distinct growth surfaces, composition and well thicknesses were investigated by means of magneto-photoluminescence measurements. The GaAs/AlGaAs specimens, grown on (100) and (311)A GaAs-surfaces, manifested oscillations in the intensity emission at elevated magnetic fields, indicative of magnetoabsorption due to inter-band transitions between Landau levels under near-resonant excitation. Analogous spin dependent characteristics were also observed in the low-Sb-content (5.0%) GaAs 1-x Sb x /GaAs QWs, shedding insights on the correlation between spin flip rates and coherence mechanisms. Furthermore, uncommon optical responses were also found in both quantum well samples, such as an inversion in the circular polarization degree with the external magnetic field, modulated by excitation power and temperature. To elucidate the experimental findings, an eight-level theoretical model, including electron and hole ground and excited states was developed, proving thermalization as the leading and sufficient factor governing the spin inversion phenomena under external parameter variations.

Collective effects in chiral systems

13:00 - 14:30
CCET

Marcella Loyola Xavier (UFSCar), Romain P. M. Bachelard (UFSCar)

Since the pioneering work on collective effects in the 1950's, many advances have been made on the study of these effects in the optical domain. The quantum many-body problem of N atoms interacting with a common external field can be treated classically when dealing with weak-driving probes, using the assumption of only one excitation. Each atom can be described by a dipole submitted to the external field and the field radiated by the other N -1dipoles; this approach is called Coupled-Dipole Model (CDM). When the system is chiral, a different optical response is expected for an incident light with right-handed circular polarization (RCP) and for a left-handed circular polarization (LCP). This is due to the enantioselective character of these systems, which leads to the definition of a chirality parameter, the g-factor, given by a relation between the transmission coefficient for each direction. This work aims to study the interplay between chirality and collective effects, such as super- and subradiance, characterizing a relation of the g-factor with the enhancement (or not) of such effects.

Optimization of Synthesis Conditions and Structural Properties in $Bi_5Ti_4FeO_{15}$ Aurivillius-Type Multiferroic Ceramics

13:00 - 14:30
CCET

Vitor Melo Frata Barbosa (UFSCar), José Antonio Eiras (UFSCar), Mahmoud.S. Alkathy (UFSCar), Fabio Luis Zabotto (UFSCar)

The progress of contemporary society has led to an escalating set of technological challenges, particularly in terms of speed and computational processing capabilities. Within this context, there's been a growing interest in devices based on multiferroism, denoting systems that exhibit two or more ferroic orders concurrently at the same temperature. An additional noteworthy effect is the capacity to manipulate polarization through a magnetic field and magnetization through an electric field, achieved via magneto-electric (ME) coupling. Within this framework, layered perovskites of the Aurivillius type, especially those based on the $Bi_5Ti_4FeO_{15}$ system, have emerged as a promising system, with reported multiferroic behavior and ME coupling with values of up to 25 $mV.Oe^(-1).cm^(-1)$. Nevertheless, there are gaps in the literature regarding the optimal conditions for the chemical and structural optimization of this compound when synthesized through a solid-state reaction. Therefore, the present study aims to identify the conditions that maximize the formation of the desired phase of the $Bi_5Ti_4FeO_{15}$ system, as well as its ferroic properties. This will be achieved through investigations, X-ray diffraction, density and scanning electron microscope.

Acknowledgements:
This work was supported by FAPESP- Fundação de Amparo à Pesquisa do Estado de São Paulo (#2017/13769-1 and 2022/04153-5, by Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPQ/Finep/MCTIC/BRICS-STI nº 402741/2019-6 e CNPq/MCTI/BRICS-STI No 04/2022) e INCT (MATFERRCE CNPQ 406322/2022-8) and CPES (08887.912727/2023-00)

Keywords: Multiferroic, magnetoelectic, single-phase, Aurivillius system.

13:00 - 14:30
CCET

Anderson localization for light in 2D systems at low density

Alexandre Fuzita (UFSCar), Romain Bachelard (UFSCar)

Anderson localization [1] is a physical phenomenon that occurs when waves propagate in disordered media. However, there is no conclusive observation of the existence of electromagnetic wave localization, most likely due to its vectorial nature [2]. This property has been discussed in both three-dimensional [2] and two-dimensional systems [3]. Interestingly, in two-dimensional media, which allow for a direct comparison of the scalar and vector scattering channels for light, polarization effects must be taken into account in the latter. One characteristic of Anderson localization is the decay of the dimensionless conductance (also called Thouless number) with the system size. For example, in a 2D system, the vector channel has a conductance nearly constant with respect to the size of the system, whereas the scalar channel presents an exponential decay. This work is devoted to studying the influence of the near-field and polarization coupling terms in 2D systems in the limit of low density and large size. Indeed, the polarization-coupling term which prevents light localization in the vector channel is expected to be very weak, so localization may occur in this limit. We consider a two-dimensional circular cloud of point-like scatterers in a two-dimensional vacuum. Numerical simulations are carried out to study the conductance as the system size increases, tuning the scatterers' density. We present preliminary results on the scaling of the dimensionless conductance in the limit of decreasing densities, giving hints about the behavior of localization in low-density 2D systems.

References:

[1] ANDERSON, P. W. Absence of diffusion in certain random lattices. Physical review, APS, v. 109, n. 5, p. 1492, 1958.

[2] SKIPETROV, S. E.; SOKOLOV, I. M. Absence of anderson localization of light in a random ensemble of point scatterers. Physical review letters, APS, v. 112, n. 2, p. 023905, 2014.

[3] MAXIMO, C. E. et al. Spatial and temporal localization of light in two dimensions. Physical Review A, APS, v. 92, n. 6, p. 062702, 2015.

Quinta-Feira -- 31/10 14:30 - 16:00 (Sessão de apresentação de pôsteres 3)

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

14:30 - 16:00
DF

José Romário de Sousa Lima (UFSCar;CNPEM), Francisco C. B. Maia (CNPEM), Adenilson J. Chiquito (UFSCar), Ingrid D. Barcelos (CNPEM)

Phonon polaritons (PhPs) result from the coupling of electromagnetic fields and crystal lattice vibrations, creating bosonic quasi-particles analogous to photons confined at crystal lattice interfaces with opposite signs of permittivity. They exist from THz to mid-infrared spectral frequencies within Reststrahlen bands (RBs), between transverse (w_{TO}) and longitudinal (w_{LO}) phonon optical frequencies. In nanostructured polar dielectric materials, PhPs allow light confinement beyond the diffraction limit, enabling super-resolution imaging, thermal emission, and data storage, and offer several advantages, mainly related to the usual higher quality factors and significantly lower optical losses of PhPs compared to plasmon polaritons. In the mid-infrared, strongly confined phonon polaritons (HPhPs) in h-BN[1], α-MoO3[2], and SnO2[3] have gained much attention as they exhibit natural hyperbolicity and enhanced waveguiding properties. In the scope of photonics, Sn3O4 shows negative permittivity in specific spectral ranges from far- to mid-infrared where different polaritons coexist. Here, we present low-dimensional Sn3O4 nanowires as a lithography-free nanophotonic platform suitable for infrared radiation cavity confinement. After sample growth, a mechanical exfoliation process was performed (van der Waals-type material). After discrete nanowires were obtained, characterizations were performed by optical microscopy, in addition to characterization of the nanowires via SEM to obtain high-resolution images of the nanowire surface, EDS for the chemical composition and to show that there is no contamination of the material. Statistics of the nanowire dimensions were prepared by AFM and Raman spectroscopy. Thus, we can obtain the main optical and vibrational characteristics of the material. Aided by near-field scattering scanning optical microscopy (s-SNOM) coupled to sources based on synchrotron infrared accelerators, we used broadband infrared nanospectroscopy (SINS) to access the cavity modes of PhPs experimentally.

14:30 - 16:00
DF

Control of the classical dynamics of a particle in the Morse-soft-Coulomb potential

Gabriel Albertin Amici (Universidade Federal de São Carlos), Emanuel Fernandes de Lima (Universidade Federal de São Carlos)

We introduce the one-dimensional Morse-soft-Coulomb (MsC) potential consisting of a Morse repulsive barrier smoothly connected with a soft-core Coulomb potential at the origin. This new potential is differentiable up to second order and possesses a single parameter that controls the softness of the repulsive barrier and the well depth. When this softening-depth parameter tends to zero, the MsC potential approaches the Coulomb potential with an infinite repulsive barrier, which is a known successful model for the hydrogen atom. We investigate the classical chaotic dynamics of the MsC potential subjected to time-dependent external fields, comparing the results with the Coulomb potential. We show that the MsC potential reproduces the dynamics and the ionization probabilities of the Coulomb potential for sufficiently small values of the softening parameter. We also investigate the role of the softening parameter in the phase-space structure, showing that the increasing of its value leads to the increasing of the chaotic sea and consequently to the rise of the ionization probability. Finally, we address the problem of controlling the dynamics of a particle in the MsC potential by means of optimal control theory, which cannot be directly applied to the Coulomb potential due to the singularity at the origin. Our results show that the MsC potential can be a useful simple model for investigating the hydrogen atom.

References:

[1] M. A. Carrillo-Bernal, R. P. M. y Romero, H. N. Núñez-Yépez, A. L. Salas-Brito, D. A. Solis, European Journal of Physics 41, 065405 (2020).
[2] J. G. Leopold, D. Richards, Journal of Physics B: Atomic and Molecular Physics 18, 3369 (1985).
[3] D. E. Kirk, Optimal Control Theory An Introduction (Prentice-Hall, 1970)

14:30 - 16:00
DF

Experimental evidences of light-induced interactions between atoms

Pablo Dias (DF-UFScar), Marcia Frometa (Istituto Nazionale di Ottica), Matheus Martins (DF-UFSCar), Ana Cipris (IFSC-USP), Philippe Courteille (IFSC-USP), Raul Celistrino (DF-UFSCar)

Atomic systems with high spatial density often present complex challenges, particularly in accounting for interactions between atoms, including those induced by light. Such interactions can lead to phenomena like the saturation of the refractive index, increased transmission in dense systems, and the absence of light localization. Probing high-density samples is particularly challenging because most of the light becomes trapped within them. Nonetheless, the light that escapes can still provide valuable insights into the interactions occurring within the sample. In our investigation, we focus on a dense cloud of strontium atoms confined in an Optical Dipole Trap (ODT). This setup enables us to achieve atomic densities as high

as $10^{14} atoms/cm^3$, where near-field interactions significantly impact the scattering cross-section. Our experiments have revealed saturation effects in the optical density of the sample. Specifically, we observed that as the atomic density increased, the optical density reached a point of saturation, where further increases in density did not lead to corresponding increases in the measured optical depth. This saturation effect highlights the complex interplay between light and atoms in high-density regimes. To probe such a small amount of light, we require specialized equipment, very long integration times, and a specific detection scheme to account for fluctuations due to uncontrolled experimental parameters such as the number of atoms, the cloud's temperature, and varying laser powers. Simulations of these experiments are ongoing to reproduce the observed behavior.

Optical Memory Effect in 2D Materials

14:30 - 16:00
DF

Gabriel Albuquerque Dias Souza (UFSCar), Alessandra Ames (UFSCar), Marcio Daldin Teodoro (UFSCar), Alisson R. Cadore (LNNano), Ingrid D. Barcelos (LNLS), Raphaela de Oliveira (LNLS), Victor López-Richard (UFSCar)

Transition metal dichalcogenides (TMDs), comprising materials known as lamellars, are widely explored as building blocks for van der Waals heterostructures (vdWHs) due to the intense luminescence exhibited by their monolayers. The light emission process from these materials can be modulated by charge transfer and roughness presented by the substrates on which they are deposited. Therefore, improving 2D devices formed by vdWHs using substrates with flat surfaces, wide bandgaps, and lamellar characteristics is the focus of many studies. In this context, synthetic materials used as substrates, such as hexagonal boron nitride (hBN), despite being the current standard, are not cost effective. An intriguing alternative gaining attention is the use of lamellar insulating materials of natural occurrence, including clinochlore, which exhibits promising characteristics such as a flat surface, a 4.35 eV bandgap, and significantly lower acquisition costs compared to hBN. The aim of this work is to study the magneto-optical properties of van der Waals heterostructures containing a monolayer of TMD (MoSe2) deposited on clinochlore, and to explore the memory effects that arise in optical responses under an applied electric field, thanks to interface effects and natural doping of clinochlore.

14:30 - 16:00
DF

Diffusing Wave Spectroscopy in a Cloud of Cold Atoms

Daniel Siqueira Coelho (Universidade Federal de São Carlos), Raul Celistrino Teixeira (Universidade Federal de São Carlos), Philippe Wilhelm Courteille (Universidade de São Paulo)

In the research field of light-matter interaction using a dense cloud of cold atoms, this project aims to apply diffusing wave spectroscopy (DWS) techniques based on the coupled dipole model to understand the relevance of short-range terms ($1/r^2$ and $1/r^3$) in the dipolar interatomic interaction of light scattering. This project will be studied through numerical simulation using MATLAB software, starting with the creation of the cold atom cloud and analyzing the temporal autocorrelation function. The simulation will be performed with the dependence of the optical depth (b0) and spatial density (^{3}) parameters. This will allow for progress in understanding the phenomena associated with light scattering and may be applied in the future to the 88Sr laboratory experiment. The analysis of the simulation results will be compared with existing theoretical models to validate and improve the understanding of dipole interactions in atomic clouds.

References:

W. Guerin, M.T. Rouabah, and R. Kaiser. Light interacting with atomic ensembles: collective, cooperative and mesoscopic effects. Journal of Modern Optics, 64(9):895–907, August 2016.

Marcia Frometa Fernandez, Pablo Gabriel Santos Dias, Pedro Henrique Nantes Magnani, Raul Celistrino Teixeira, and Philippe Wilhelm Courteille. Coherent transmission of light through a dense cloud of cold atoms. In Young Atom Opticians conference - YAO. Institute of Photonic Sciences - ICFO, 2023.

D. J. Pine, D. A. Weitz, P. M. Chaikin, and E. Herbolzheimer. Diffusing wave spectroscopy. Phys. Rev. Lett., 60:1134–1137, Mar 1988.

14:30 - 16:00
DF

A study of the life cycle of stars and its influence on the creation of Heavy Elements

Gabriel Barone (Universidade Federal de São Carlos), Raphael Santarelli (Universidade Federal de São Carlos), Javier Ramos-Caro (Universidade Federal de São Carlos)

The study of astronomy and stellar astrophysics dates back to ancient civilizations such as the Greeks, Babylonians, and Incas, with their observations of the night sky and maps stellar . However, it was during the 19th and 20th centuries that the physics of stars actually improved, with the development of techniques of stellar classification, such as the “H-R Diagrams”, by E. Hertzsprung and H. Russel; of investigation of the interior of stars, with the analysis of possible thermonuclear reactions, such as the ”CNO-cycle” and the ”Proton-Proton chains”, by H. Bethe; and, mainly, with the development of the ”differential equations of stellar structure”, mathematical models that describe the physical evolution of these celestial bodies. Thus, this project proposes to carry out a general theoretical and introductory study

about the physical processes and structural equations responsible for the stellar life cycle, achieving, until now, the development of all four main equations that govern the stars, including the construction and understanding of the main parameters used on those equations and in the study of stellar astrophysics.

References:

[1] BETHE, H. A. Energy production in stars. Physical Review 55, 5 (1939), 434.
[2] CARROLL, B. W., AND OSTLIE, D. A. An introduction to modern astrophysics. Cambridge University Press, 2017.
[3] MARTINS, R. A. O Universo: teorias sobre sua origem e evolução. Livraria da Física, 2012.

Quinta-Feira -- 31/10 16:30 - 18:00 (Sessão de apresentações orais 3)

16:30 - 18:00
DF

2D Anderson Localization of light in cold atoms

João Ferreira (Universidade Federal de São Carlos), Noel Araújo (Universidade de São Paulo), Robin Kaiser (Universit´e Cote d'azur), Romain Bachelard (Universidade Federal de São Carlos)

Although Anderson localization of light had been reported experimentally, near field terms, absent from scalar waves such as matter and acoustic waves, were identified to prevent the localization transition. This result, reported both in 3D[1] and 2D[2] is at odds from the scaling theory proposed in[3], where the details of the interaction are not taken into account. With the initial experimental reports of light localization reinterpreted, a major challenge for the observation of the transition is the identification of unambiguous signatures, to rule out parasitic effects such as absorption. In this context, two-dimensional samples are particularly interesting, because they possess both scalar (without near-field terms and with localization) and vectorial (with near-field and without localization) scattering channels. It is thus an ideal platform to explore the role of near-field effects on localization. In this work we show how the statistics of the scattered light can be used as signatures of Anderson localization, exploiting the transmission profile of the intensity[4,5] characterized by the phenomenon of "transverse localization", and the deviations from Rayleigh law for diffusion[6]. More precisily, we show how the evolution of the beam width[5] and the transmission coefficient differ in the scalar and vectorial channels, witnessing the different regimes explored. Indeed, while the diffusion, in the vectorial channel, is a scale-free process, the localization, in the scalar channel, sets a characteristic spatial scale for the scattered light in space-yet another way to access the localization length.

References:

[1] S. E. Skipetrov and I. M. Sokolov, 2014.
[2] C. E. Máximo, N. Piovella, P. W. Courteille, R. Kaiser, and R. Bachelard, 2015.
[3] E. Abrahams, P. Anderson, D. Licciardello, and T. Ramakrishnan, 1979.
[4] H. De Raedt, A. Lagendijk, and P. de Vries,1989.
[5] N. Cherroret, S. Skipetrov, 2010.
[6] F. Cottier, A. Cipris, R. Bachelard, and R. Kaiser, 2019.

Work and heat definitions in Quantum Thermodynamics

16:30 - 18:00
DF

Sinara Santos Dourado (Universidade Federal de São Carlos), Celso J. Villas-Boas (Universidade Federal de São Carlos)

Quantum Thermodynamics is a relatively recent field of study that has attracted significant interest in both fundamental and technological research. It aims to describe the microscopic dynamics of systems with a reduced number of degrees of freedom. In other words, this occurs when the number of constituents is sufficiently small for environmental fluctuations to play a significant role in the characterization of thermodynamic quantities. Despite the growing body of research in this area, establishing definitions of heat and work that account for coherences and correlations remains a challenge. Our objective is to compile various proposals for distinguishing heat and work and to compare their outcomes in a simple two-qubit system. We hope this analysis will guide future research on the definitions of heat and work in quantum systems.

References:

R. Alicki, The quantum open system as a model of the heat engine. Journal of Physics A: Mathematical and General, vol. 12, L103–L107 (1979);
Borhan Ahmadi, and Sina Salimi, and A. Khorashad. On the contribution of work or heat in exchanged energy via interaction in open bipartite quantum systems. Sci Rep. 13, vol. 160 (2023);
Roie Dann and Ronnie Kosloff. Unification of the first law of quantum thermodynamics. New Journal of Physics, vol. 25, 043019 (2023);
Bertúlio de Lima Bernardo. Unraveling the role of coherence in the first law of quantum thermodynamics. Physical Review E, vol. 102 (2020);
S. Alipour, A. T. Rezakhani, A. Chenu, A. del Campo, and T. Ala-Nissila. Entropy-based formulation of thermodynamics in arbitrary quantum evolution. American Physical Society, vol. 105 (2022);
Sai Vinjanampathy and Janet Anders. Quantum thermodynamics. Informa UK Limited, vol. 57, 545–579 (2016).

Growth of high-quality YBa2Cu3O7−d thin films by PLD for electromigration studies

16:30 - 18:00
DF

Caio C. Quaglio (Universidade Federal de São Carlos), Davi A. D. Chaves (Universidade Federal de São Carlos/KU Leuven), Pedro Schio (CNPEM),Tom H. Johansen (University of Oslo), Wilson A. Ortiz (Universidade Federal de São Carlos), Maycon Motta (Universidade Federal de São Carlos)

The compound YBa2Cu3O7-d (YBCO) was the first material to exhibit superconductivity at temperatures higher than that of liquid nitrogen. This remarkable behavior is closely tied to its oxygen vacancy concentration, represented by d, which plays a key role in determining its superconducting properties. For $d < 0.65$, YBCO exhibits a superconducting orthorhombic phase, with critical temperatures strongly affected by its oxygen content. In the range $0.65 < d < 1.0$, YBCO transitions to

a tetragonal structure and loses its superconducting properties. We are currently developing an experimental setup for electromigrating YBCO nanostructures, which will allow us to locally adjust the oxygen concentration by inducing atomic displacement through high electrical current densities. To achieve this, high-quality YBCO films are needed, with a preferential orientation along the crystallographic c-axis due to the material's anisotropic properties. Thus, we investigated the growth of YBCO thin films by pulsed laser deposition (PLD) on SrTiO3 (001) substrates. In our experiments, we systematically adjusted parameters such as laser fluence and energy, substrate temperature, the number of pulses, and oxygenation procedures with the goal of achieving epitaxial film growth and maximizing the critical temperature. The structural properties of the films have been examined using X-ray diffraction and scanning electron microscopy. Furthermore, the superconducting properties of the fabricated YBCO films have been evaluated through temperature-dependent electrical resistance measurements and by magneto-optical imaging. We will report on our progress in the deposition of YBCO films by PLD and in the lithography of structures suitable for the proposed experiments.

Acknowledgements:
This research used facilities of the Brazilian Nanotechnology National Laboratory (LNNano), part of the Brazilian Center for Research in Energy and Materials (CNPEM), a private non-profit organization under the supervision of the Brazilian Ministry for Science, Technology, and Innovations (MCTI). The In-Situ Growth Laboratory (LCIS) and the Micro and Nanofabrication Laboratory (MNF) staff are acknowledged for the assistance during the experiments LCIS-20232334 and MNF-20233770. The authors thank CNPq and FAPESP (Grants No. 2022/03124-1 and 2023/11915-1) for financial support.

16:30 - 18:00
DF

Two-Dimensional Transition Metal Halides for Optical Applications: Impact of Excitons

Natan M. Regis (Department of Physics, Federal University of São Carlos), Juarez L. F. Da Silva (São Carlos Institute of Chemistry, University of São Paulo), Matheus P. Lima (Department of Physics, Federal University of São Carlos)

The synthesis of graphene in 2004 marked a breakthrough in two-dimensional (2D) materials research, motivating studies on other families of atomically thin materials. Quantum confinement of electrons in a planar structure gives rise to uncommon effects, such as large exciton binding energies, observed in monolayers of Transition Metal Dichalcogenides (TMDs). Additionally, Transition Metal Halides (TMHs), which consist of a transition metal layer sandwiched between halide atom layers and belong to the van der Waals (vdW) crystal family, have gained interest as a new class of 2D materials. In this work, we explore excitonic effects in TMHs, selected from the Computational 2D Materials Database (C2DB). We focused on materials with stoichiometry AB, AB2, and AB3, where A is a transition metal and B is a halide (Cl, Br, or I), identifying 24 materials suitable for photovoltaics. These systems were studied using advanced theoretical methods, including ground-state description via Density Functional Theory (DFT) and excited-state analysis

through the Bethe-Salpeter Equation (BSE). By comparing the optical properties of the ground and excited states, we observed changes in the optical bandgap due to exciton levels above the electronic bandgap. In one system, we found evidence of an excitonic insulator, where the exciton binding energy exceeded the material's bandgap, making excited states more energetically favorable. We also observed changes in the light absorption spectrum, where exciton calculations showed a lower maximum absorption spectrum and changes in the spectrum region of maximum light absorption. We evaluated the systems' optoelectronic potential applications by calculating possible heterojunction types, noting that excitons are fundamental for accurately describing the heterojunction type.

References:

[1] Haastrup, S. et al. The Computational 2D Materials Database: High-Throughput Modeling and Discovery of Atomically Thin Crystals. 2D Mater. 2018, 5 (4), 042002.

[2] Gjerding, M. N. et al. Recent Progress of the Computational 2D Materials Database (C2DB). 2D Mater. 2021, 8 (4), 044002.

[3] Hohenberg, P.; Kohn, W. Inhomogeneous Electron Gas. Phys. Rev. 1964, 136 (3B), B864.

[4] Kohn, W.; Sham, L. J. Self-Consistent Equations Including Exchange and Correlation Effects. Phys. Rev. 1965, 140 (4A), A1133.

[5] Salpeter, E. E.; Bethe, H. A. A Relativistic Equation for Bound-State Problems. Phys. Rev. 1951, 84 (6), 1232–1242.

[6] Dias, A. C.; Silveira, J. F. R. V.; Qu, F. WanTiBEXOS: A Wannier Based Tight Binding Code for Electronic Band Structure, Excitonic and Optoelectronic Properties of Solids. Computer Physics Communications 2023, 285, 108636.

Nanostructures of WO3: Synthesis and Investigation of gas sensing performance

16:30 - 18:00
DF

Mayron S. Castro (Universidade Federal de São Carlos), João V. Almas (Universidade Federal de São Carlos) , Luís F. da Silva (Universidade Federal de São Carlos)

The tungsten trioxide (WO3) is a n-type semiconducting metal oxide (MOx) which can be found in different crystalline structures, being monoclinic the most stable. WO3 compound has been employed, for example, as a (photo)catalyst, photoelectrode for energy generation, and gas sensor [1]. Resistive gas sensors based on MOxs occurs through the surface reaction between the material and gas molecules present in the atmosphere [2]. Thus, the alteration of particle size generated during the synthesis process may influence the sensing performance. Herein, an investigation was conducted on the effect of calcination rate on the microstructural and gas sensing properties of WO3 compound synthesized via the polymeric precursors method [3,4]. For that, the precursors WO3 powders were annealed at 700°C for 2 hours, while the furnace heating rate was varied (1°C/min and 50°C/min). The as-obtained powders were characterized by Raman spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM) techniques. The results revealed the formation of the

monoclinic phase of WO3, without the presence of secondary phases. SEM images showed that annealing treatment at high heating rates allowed obtaining smallest particles. The average size obtained were approximately 0,9 m (1°C/min) and 0,6 m (50°C/min). Regarding the evaluation of the sensing performance , we found that the samples were sensitive to different levels of ozone gas (O3) when operated at room temperature and under continuous photostimulation.

References:

[1] YAO, Y. et al. A Review on the Properties and Applications of WO3 Nanostructure-Based Optical and Electronic Devices. Nanomaterials, v. 11, n. 8, p. 2136, 22 ago. 2021.

[2] - WANG, Ze et al. One-dimensional nanomaterials in resistive gas sensor: From material design to application. Chemosensors, v. 9, n. 8, p. 198, 2021.

[3] SILVA et al. An Understanding of the Photocatalytic Properties and Pollutant Degradation Mechanism of SrTiO3 Nanoparticles. Photochemistry and photobiology, v. 92, n. 3, p. 371–378, 22 abr. 2016.

[4] Y. GUHEL et al. Rapid thermal annealing of cerium dioxide thin films sputtered onto silicon (111) substrates: Influence of heating rate on microstructure and electrical properties. Materials science in semiconductor processing, v. 30, p. 352–360, 1 fev. 2015.