20th Brazilian Workshop On Semiconductor Physics

Rapport sur les contributions

https://indico.in2p3.fr/e/20bwsp

ID de Contribution: **3** Type: **Oral**

Yara Gobato

ID de Contribution: **4** Type: **Non spécifié**

Anisotropic vortex squeezing and supercurrent diode effect in non-centrosymmetric Rashba superconductors

Orateur: Prof. KOCHAN, Denis (Institute for Theoretical Physics/University of Regensburg)

Classification de Session: Short Talk 1

ID de Contribution: **5** Type: **Non spécifié**

Crystal growth mechanism of zinc selenide semiconductor: Molecular dynamics simulations and theoretical calculations

Orateur: Prof. SEPARDAR, Leila (Federal University of São Carlos)

Classification de Session: Short Talk 1

ID de Contribution: **6** Type: **Non spécifié**

g-factor physics in 2D materials and van der Waals heterostructures

Orateur: Prof. DE FARIA JUNIOR, Paulo Eduardo (Institute for Theoretical Physics / University of Regensburg)

Classification de Session: Short Talk 1

ID de Contribution: **7** Type: **Non spécifié**

WanTiBEXOS: a Wannier based Tight-Binding code for excitonic and optoelectronic properties of solids

Orateur: Prof. CAVALHEIRO DIAS, Alexandre (Universidade de Brasília)

Classification de Session: Short Talk 1

ID de Contribution: **9** Type: **Non spécifié**

Natural 2D Insulating Materials in van der Waals Heterostructures: and Experimental and Theoretical study

Orateur: Prof. RONIERI CADORE, Alisson (School of Engineering/Mackenzie Presbyterian University)

Classification de Session: Short Talk 1

ID de Contribution: **10** Type: **Non spécifié**

Acoustic Manipulation of Excitons in 2D Semiconductors

Orateur: Prof. D. D. COUTO JR., Odilon (State University of Campinas (UNICAMP))

Classification de Session: Short Talk 1

ID de Contribution: **11** Type: **Non spécifié**

First-principles investigation of the electronic structure of the α-Al2O3-graphene interface

Orateur: Prof. P. MACIEL, Renan (Uppsala University)

Classification de Session: Short Talk 1

ID de Contribution: **12** Type: **Non spécifié**

Phyllosilicates: an emerging class of naturally abundant layered materials

Orateur: Prof. DE OLIVEIRA, Raphaela (Physics Department/ Federal University of Minas Gerais (UFMG))

Classification de Session: Short Talk 1

ID de Contribution: **13** Type: **Non spécifié**

Using terahertz spectroscopy to investigate optical phonons in PbTe thin films

mercredi 14 septembre 2022 15:00 (5 minutes)

Orateur: MASSARICO KAWAHALA, Nicolas

Classification de Session: Lightning Talk

ID de Contribution: **14** Type: **Non spécifié**

Electronic study of the doped carbon nanotube

mercredi 14 septembre 2022 15:05 (5 minutes)

Orateur: AMORIM GONÇALVES, Vanessa

Classification de Session: Lightning Talk

ID de Contribution: **15** Type: **Non spécifié**

Sublinear drag regime at mesoscopic scales in viscoelastic materials

mercredi 14 septembre 2022 15:10 (5 minutes)

Orateur: S. DE SOUSA, Jeanlex

Classification de Session: Lightning Talk

ID de Contribution: **16** Type: **Non spécifié**

Stark many-body localization in spin-chains with single-ion anisotropy

mercredi 14 septembre 2022 15:15 (5 minutes)

Orateur: GUIMARÃES SOUSA, Márcio

Classification de Session: Lightning Talk

ID de Contribution: **17** Type: **Non spécifié**

Obtaining realistic parameters for effective Hamiltonians from ab initio fitting

mercredi 14 septembre 2022 15:20 (5 minutes)

Orateur: BARROS WANDERLEY, Adilson

Classification de Session: Lightning Talk

ID de Contribution: **18** Type: **Non spécifié**

Stark many-body localization in the J1-J2 Heisenberg model

vendredi 16 septembre 2022 14:30 (20 minutes)

Abstract

Stark many-body localization (SMBL) is a phenomenon observed in interacting systems with a nearly uniform spatial gradient applied field. Contrasting to the traditional many-body localization phenomenon, SMBL does not require disorder [1]. We have investigated SMBL in a spin-1/2 described by a Heisenberg model including a next-nearest-neighbor exchange coupling [2]. By employing an exact diagonalization approach and time evolution calculation we analyze both level spacing ratio (LSR) statistics of the Hamiltonian model as well as the dynamics of the system from a given initial state. Our results reveals that for zero field in our finite system, LSR statistics suggest localization while the dynamics shows thermalization, which has been attributed to a finite size effect. Slightly nonuniform field gradient, LSR statistic predictions agree very well with the dynamics of the physical quantities indicating delocalization and localization for small and large field gradient, respectively. More interestingly, we find that localization is robust in the presence of next-nearest-neighbor coupling in the Hamiltonian. Moreover, this coupling can be tuned to enhance SMBL in the system, meaning that localized regimes can be obtained for smaller field gradient as compared to the traditional nearest-neighbor isotropic Heisenberg model [3].

References

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Orateur: Prof. VERNEK, Edson (Instituto de Física - Universidade Federal de Uberlândia)

Classification de Session: Oral

ID de Contribution: **19** Type: **Non spécifié**

Tunable properties of excitons in double monolayer heterostructures

mercredi 14 septembre 2022 12:10 (20 minutes)

Abstract

Nowadays, the so-called van der Waals heterostructures represent a prominent research area within optoelectronics in semiconductor 2D materials. The layered structures are related to the fact that they support the formation of excitons –bound electron-hole pairs –and excitonic complexes with binding energies more than an order of magnitude greater than conventional semiconductors, i.e. on the order of hundreds of meV, and small Bohr radii in the range of several nanometers [1-6]. In this work, we study the exciton properties of double layers of transition metal dichalcogenides (TMDs), where between the layers we have a dielectric spacer. We used an expansion of Chebyshev polynomials to solve the Wannier equation for the exciton. We systematically study both homo and hetero double layer systems for MX2, showing the dependence of the inter and intralayer excitons binding energy as functions of the spacer width and dielectric constant. We also show how the exciton energy, that includes the effects of the changing band gap, depends on those geometric properties.

References
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Orateur: Prof. A. S. PEREIRA, Teldo (Instituto de Física - Universidade Federal de Mato Grosso)

Classification de Session: Oral

ID de Contribution: **20** Type: **Non spécifié**

Effective kp Hamiltonians calculated from ab initio data

Abstract

In this talk we will present a new code, called QE2KP, which calculates the effective kp Hamiltonian using the ab initio wave-functions as basis functions to calculate the matrix elements of the kp theory within the Löwdin perturbation approach. The kp method is widely used to obtain effective Hamiltonians to describe a chosen set of bands of crystalline materials. The derivation of these Hamiltonians start by identifying the symmetry group of the crystal, and irreducible representations of the bands at the central k point for the perturbative expansion. Then, combining the kp method with fundamentals of group theory [1] (theory of invariants), one is able to obtain the functional form of the Hamiltonian. For instance, for graphene, and up to linear powers in k, one obtains H = $\hbar$vF σ.k, which leads to the cone Dirac. However, the kp and group theory approaches can only tell us that the coefficient $\hbar$vF is finite (selection rules), but it cannot give it a numerical value. Currently, the python packages IrRep [2] and Qsymm [3] are quite useful to help us obtain these functional forms of H. Therefore, the goal of our new code QE2KP is to take a step further and calculate the numerical values of these parameters (e.g. $\hbar$vF, Kane and Luttinger parameters). In this talk, we'll show preliminary results (see Fig. 1) of our code and describe the methodology we are using to combine the QE data with the python packages IrRep and Qsymm to fully describe both the functional form and the numerical values for the effective Hamiltonians of any crystal.

References

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Orateur: Prof. J. FERREIRA, G. (Instituto de Física - Universidade Federal de Uberlândia)

Classification de Session: Oral

ID de Contribution: **21** Type: **Non spécifié**

Growth of Al2O3 thin films using plasma-activated deionized water as a new oxidant in thermal atomic layer deposition process

jeudi 15 septembre 2022 09:30 (20 minutes)

Abstract

The atomic layer deposition (ALD) of metallic oxides, mainly alumina (Al2O3), when performed in thermal mode uses deionized water (DI) as oxidant source and trimethylaluminum (TMA) as a metal reactant. However, growth per cycle (GPC) of Al2O3 thin films for the reactant and co-reactant mentioned above is limited to 0.1 nm/cycle [1]. This barrier in the GPC is overcome by using plasma technology as an oxygen source. This technique is commonly called energy-enhanced ALD because the plasma oxygen source provides tremendous activation energy during the co-reactant step, which allows for greater efficiency in generating active sites on the substrate surface, promoting thus more reactions between the surface and the metal reactant. This process, called plasma-enhanced ALD (PEALD), is commonly used to replace DI water with O2 plasma as an oxygen source. It is reported in the literature that for the TMA reactant, this replacement of the vapor phase oxygen source (thermal ALD) by a plasma oxygen source (PEALD) generates an increase in the alumina GPC to 0.12 nm/cycle, i.e., a gain of 20% [2]. However, this gain in the GPC has a high cost, as the PEALD uses a sophisticated plasma source. The present work presents a cheap alternative to increase the GPC of alumina by 17%. An atmospheric gliding arc plasma jet and compressed air were used to activate DI water. Plasma-activated water (PAW) was prepared by a forward vortex flow reactor (FVFR) type with air at atmospheric pressure. The activation times were 10, 30, and 60 min, and the following pH of 3.5, 3.0, and 2.5 were obtained. PAWs were characterized by UV-vis spectrophotometry in order to obtain the reactive oxygen and nitrogen species (RONS), namely, H2O2, HNO2, NO2-, and NO3-. After activation, plasma-activated water (PAW) is carried out into a recipient and introduced in the line of oxygen source in thermal ALD. The ALD pulse times were 0.15-4-0.3-4 s, TMA, N2 purge, PAW, and another N2 purge. The number of cycles was fixed at 1000 cycles, and Si(100) was used as substrate. Alumina thin films growth was characterized by in-situ mass spectrometry and ex-situ by optical profilometry, FT-IR and FEG-SEM. According to the characterizations mentioned above, the existing RONS in PAW probably contributed to the activation of sites in the Si(100) substrate, thus increasing the GPC of the alumina.

References

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Orateur: Prof. S. PESSOA , R. (Plasma and Processes Laboratory - Aeronautics Institute of Technology)

Classification de Session: Oral

ID de Contribution: **22** Type: **Non spécifié**

Optical Properties of Moiré excitons in WS2 -MoSe2 heterostructures

lundi 12 septembre 2022 09:50 (20 minutes)

Abstract

Twisted van der Waals (vdW) heterostructures exhibit periodic variations, leading to a new type of in-plane superlattice known as moiré superlattice/pattern which modifies considerably the optical properties of excitons in transition metal dichalcogenides (TMD) vdW heterostructures. The period of these moiré superlattices is determined by the lattice constant mismatch and the twist angle between the two layers [1]. In most of the cases, the vdW heterostructures have a type-II band alignment [1]. The strong Coulomb interaction in
TMD materials gives rise in the formation of interlayer moiré excitons (IEs) with electrons and holes located in different TMD layers [1]. Furthermore, there are also vdW heterostructures where the electron (or hole) wavefunction is distributed over both layers and these excitons
are referred to as hybrid excitons [1-3].

Here, we report on the impact of the moiré pattern on the magneto-optical properties of a WS2/MoSe2 heterobilayer with twist angles of approximately 0◦ and 60◦ under perpendicular
magnetic fields up to 20 T. We observed two neutral exciton peaks in the PL spectra: the lower energy one exhibits a reduced g-factor relative to that of the higher energy peak, and much lower than the recently reported values for interlayer excitons in other vdW heterostructures such as WSe2-MoSe2 [4]. In addition, similar values of g-factors are obtained for samples with twist angles of approximately 0◦ and 60◦ which indicates a weak hybridization between the intralayer and interlayer excitons for this heterostructure. In general, our results provide evidence that such a discernible g-factor stems from the spatial confinement of the exciton in the potential landscape created by the moiré pattern, due to lattice mismatch and/or inter-layer twist in heterobilayers [4].

References

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Orateur: Prof. GALVÃO GOBATO, Yara (Physics Department - Federal University of São Carlos)

Classification de Session: Oral

ID de Contribution: **23** Type: **Non spécifié**

To be defined

Abstract

We carried out first-principles density functional theory calculations of hydrogen and oxygen adsorption and diffusion on subnanometer MoS nanowires. The nanowires are robust against adsorption of hydrogen. On the other hand, interaction with oxygen shows that the nanowires can oxidize with a small barrier. Our results open the path for understanding the behavior of MoS nanowires under realistic environment.

References

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Orateur: Prof. LUISA DA ROSA, Andreia (Universidade Federal de Goiás)

Classification de Session: Oral

ID de Contribution: **24** Type: **Non spécifié**

Pd-based dichalcogenides: the 1T and the novel 1OT regular and Janus structures: from electronic to thermal properties

Abstract

The discovery of two dimensional (2D) graphene has opened the doors to investigate a myriad of new 2D materials that have better characteristics. Out of these are the transition metal dichalcogenides (TMDs). In this talk, I will shine light on the electronic, optical and thermal properties of the 1T [1] Pd-based dichalcogenides, namely PdS2, PdSe2, PdSSe, PdSTe, and PdSeTe systems, that do not have a fair share of research like the Mo or W-based TMDs. Our results show that the thermal electronic conductivity (⊠e), the electronic conductivity (σe), the Seebeck effect (S), and the figure of merit (ZT) along the x and y directions register the largest values in the case of electron doping for the PdSe2 and PdSeTe 2D crystals [1]. Additionally, ZT of the Janus structures are larger than their corresponding pristine PdX2 (X = S, Se) structures [1]. Once synthesized, such information is crucial for the implementation of the PdXY (Y = Se, Te) structures in industrial applications.

I will also discuss the electronic and optical properties for the novel 1OT [2] metastable (with monoclinic symmetry) structures that we have modelled in our group. Our calculations reveal that, without the inclusion of spin-orbit coupling, all structures considered have a semi-metallic behavior with a non-zero (DOS) at the Fermi level. Furthermore, they demonstrate a wider range of absorption spectra than 1T systems, and can emit or absorb within the infrared (IR) regime. They are dynamically stable and their thermal lattice conductivities should be lower than their 1T analogs, making them suitable candidates for thermoelectric devices. The Born-Oppenheimer Molecular Dynamics (MD) simulations [3] show that the 1OT PdS2 and PdSe2 structures are thermally stable at temperatures above 300 K, while the Janus PdSSe system remains stable up to temperatures close to 600 K and is completely destroyed at 900K [2].

References

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Orateur: Prof. A. MOUJAESS, Elie (Physics department - Federal University of Rôndonia)

Classification de Session: Oral

ID de Contribution: **25** Type: **Non spécifié**

Structural and electronic properties of III-Nitrides, MoS2 and MoSe2: From bulk polytypes to 2D structures

While it is well known that the III-Nitrides are the materials for the highly efficient light-emitting diodes, among other optoelectronic devices, the transition metal dichalcogenides (TMDC) also offer a great potential use in the field of 2D materials with interesting electronic and optoelectronic properties. In the case of III-Nitrides, the interest on these materials was renewed, now as a 2D material, when Tsipas and collaborators [1] found that it is possible to grow hexagonal AlN nanolayers on surfaces of Ag (111) and Al Balushi and colleagues found that hexagonal GaN can be obtained via encapsulation of graphene [2]. Moreover, in the case of TMDC, their bulk counterparts were less studied than the 2D ones, and the knowledge of their structural and vibrational properties could help to obtain better 2D samples. It is well known that the bulk structure of these materials presents polytypism, which is not yet well understood by the scientific community. The same holds in the case of III-Nitrides, which the zincblende, wurtzite and the rocksalt forms were extensively studied, and not their hexagonal closed-packed (hcp) structure. So, in this work, we report our theoretical results (with van der Waals corrections included) for the structural and vibrational properties of the bulk polytypes of MoS2 and MoSe2, as well as for the hcp form of III-Nitrides, extending our study to the 2D structures of these materials. For the 2H polytype of MoS2, we have found that, the experimental measured bulk modulus is underestimated once, from our theoretical data, these measurements show a combination of hydrostatic and axial strains, which preserves the symmetry of the unit cell, due to its lubricant properties. We have also shown that, in the case of III-Nitrides, an axial strain applied to the wurtzite structure can transform it to the hexagonal closed-packed one. Going to the III-Nitrides 2D structures, we have studied the graphene-like, the square lattice and the haeckelite 8-4 ones. Our results show that the graphene-like structure is more stable one and their electronic structures show an indirect bandgap. Finally, we show our results for the structural and electronic properties of MoS2/MoSe2 lateral interfaces in both zig-zag and armchair configurations. Band offsets and alignment of these interfaces were also obtained. Our results have shown that the band offsets 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.

Orateur: Prof. W. LEITE ALVES, Horacio (Departamento de Ciências Naturais - Universidade Federal de São João del Rei)

Classification de Session: Oral

ID de Contribution: **26** Type: **Non spécifié**

Experimental studies on epitaxial films of three-dimensional (Bi2Te3) and crystalline (Pb1-xSnxTe) topological insulators

mardi 13 septembre 2022 09:50 (20 minutes)

Abstract

Bismuth telluride (Bi2Te3) is an archetype of a three-dimensional topological insulator, which presents topological surface sates (TSS) with a linear dispersion like in a Dirac cone positioned between the valence and conduction bands. The Dirac fermions on the surface are protected against scattering by the time inversion symmetry [1]. On the other hand, Pb1-xSnxTe is a topological crystalline insulator, in which the topological nature of the electronic structure arises from the crystalline symmetry. In this case, the TSS appear only for samples with Sn compositions where the band inversion occurs [2]. Details about the molecular beam epitaxial growth of Bi2Te3 and Pb1-xSnxTe thin films on (111) BaF2 substrates and their structural characterization will be presented here. Angle resolved photoemission spectroscopy (ARPES) revealed metallic surface states in the form of a Dirac cone within the energy gap of the Bi2Te3 films with the Fermi level crossing only the TSS, demonstrating a bulk insulating behavior [3]. We will also show results on the investigation of our Bi2Te3 epitaxial films doped with europium [4]. Experiments on the electronic transport of our Pb1-xSnxTe films at intense magnetic fields up to 30 T and temperatures varying from 4.2 to 300 K will be presented in detail. Pronounced Shubnikov - de Haas oscillations were detected on SnTe film up to 80 K. Our analysis showed that the observed beating pattern on these quantum oscillations originates from the Rashba splitting of the bulk longitudinal ellipsoid in SnTe [5]. Preliminary results on extrinsic n-type doping of Pb1-xSnxTe with bismuth will be also exhibited here [6].

References

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Orateur: Prof. ABRAMOF, Eduardo (Grupo de Pesquisa e Desenvolvimento de Materiais e Plasma - Instituto Nacional de Pesquisas Espaciais)

Classification de Session: Oral

ID de Contribution: **27** Type: **Non spécifié**

Magnetotransport measurements for detection of Dirac fermions in topological insulators

Abstract

Topological insulators (TIs) are materials that are insulating in their bulk but present metallic states on their surface. This is the simplest definition for a complex quantum effect that results from strong spin-orbit coupling that changes the topological order of the material. The metallic states host spin-polarized currents composed of Dirac fermions flowing on the topological surface states (TSS). The TSS of TIs are protected by time-reversal symmetry (their physics is independent of whether time is flowing backward or forward). 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. In the particular case of TIs and TCIs, the potential to application in quantum computation and spintronic is enormous. Prior to the application in development of new technologies, however, the detection of Dirac Fermions via electrical transport measurements is mandatory [1].

The detection of Dirac fermions in TIs via transport measurements represents a big challenge for experimentalist. 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. In this talk, the results of magnetotransport measurements performed on Bi2Te3 and SnTe nano-structures will be presented. The investigation will involve the analysis of Shubnikov-de Haas oscillations in SnTe structures [2] and weak anti-localization effect in Bi2Te2 nano films providing a full description of the important parameters that characterize the electrical transport in these materials.

References

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Orateur: Prof. L. PERES, Marcelos (Instituto de Física e Química - Universidade Federal de Itajubá)

Classification de Session: Oral

ID de Contribution: **28** Type: **Non spécifié**

From Majoranas to parafermions: topological zero modes in condensed matter systems

Abstract

The so-called "search for Majoranas"has mobilized several groups over the last decade with the goal of achieving the "holy grail"of topological quantum computation in condensed matter systems [1-2]. In spite of the advances, particularly in devices of semiconductor nanowires with proximity induced superconductivity, many unanswered questions and challenges remain, as highlighted the recent events that shook the community [3]. This begs the question of whether other platforms hosting Majorana zero modes or other topological excitations which could be used as non-Abelian anyons can
be viewed in a different light.

In this talk, I will discuss some of the scenarios for what's next in the Majorana saga. I will present some of the works in our group involving Majoranas in alternative platforms such as vortex cores in 2D topological superconductors [4]. I will also discuss our recent proposals for modeling parafermionic zero modes, Majoranas' Z_n symmetric cousins, in strongly interacting electronic systems [5,6]. We also propose a way to detect these rather exotic quasiparticles using quantum dots [5].

References

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Orateur: Prof. G. DIAS DA SILVA, Luis (Instituto de Física - Universidade de São Paulo)

Classification de Session: O28

ID de Contribution: **29** Type: **Non spécifié**

Structure of Energized Microlamps in Micrometric Scale

vendredi 16 septembre 2022 09:50 (20 minutes)

Abstract

This work presents a study about the structure of thin films, deposited to be a protection layer against oxidation of microlamps, as well as chemical and structural modifications induced by their heating under operation. The studied microlamps (fig. 1) were produced by Plasma Enhanced Chemical Vapor Deposition (PECVD) and sputtering, over silicon substrates, and have applications in microelectromechanical systems. The analyzed protection layer is a film on top of a small Cr filament. Four different materials were used as protection layer: a-SiC, a-SiOxNy, AlN and TiO2. The intensity and time interval of the electric current applied in the device were varied (up to 50 mA and during 10 s to 1,0 h). The beamline LUCIA of the SOLEIL
synchrotron (France), that was used in this work, has a microfocus beam (3 x 3 μm²), allowing the evaluation of the micro region thermally affected, exactly on top of the filament, using X-ray absorption spectroscopy (XANES). The results demonstrated that the a-SiOxNy and TiO2 (rutile) films are the indicated ones for this application, because, besides their thermal stability, they dissipate less heat. The AlN and a-SiC (fig. 1) protective films showed structural changes caused by the heating related to the device operation. To improve the studies of these materials additional thin films samples, deposited over ordinary large flat substrates, were produced and analyzed by X-Ray Absorption Spectroscopy (XANES and EXAFS region), Grazing Incidence X-Ray Fluorescence (GIXRF) and Rutherford Backscattering Spectroscopy
(RBS). The a-SiC films showed an intense and increasing oxidation as the intensity and duration of the applied current in the microlamps were raised. In addition, structural differences in the a-SiC film were observed in the micro area over the filament, compared with a reference film deposited over Si (fig. 1). The results achieved with the additional thin films revealed the diffusion of Cr and O into the a-SiC. Theoretical XANES spectra of a-SiC structures, constructed by molecular dynamics, were calculated by the Finite Difference Method Near Edge Structure (FDMNES) code, aiming to study the modifications induced by the presence of Cr and O into the material. The conclusion was that the microlamp design
induced the growth of a PECVD silicon carbide far from the best conditions, probably due to the presence of a cavity under the filament that reduced the substrate temperature during the deposition.

Orateur: Prof. R. S. CASSIMIRO, Vinicius (Faculdade de Tecnologia do Tatuapé (FATEC))

Classification de Session: Oral

ID de Contribution: **30** Type: **Non spécifié**

2D Materials for Photovoltaic Energy Harvesting

vendredi 16 septembre 2022 11:50 (20 minutes)

Abstract

Two-dimensional (2D) semiconducting materials as active layers in photovoltaic devices is a subject that has attracted a lot of attention in the last years [1]. Nowadays, the most employed materials for this kind of application are transition metal dichalcogenides (TMDCs), which are semiconductors with chemical configuration MX2 [2], where M is a transition metal such as Mo, W, and X is a chalcogen atom such as S, Se, or Te. However, many other 2D materials have also been proposed.

As far as TMDCs are concerned, while significant attention has been given to single layer TMDCs, a limited number of works have addressed the few layer case which is particularly relevant for photovoltaic devices. Herein, we studied the electronic and optical properties of few layer TMDCs composed of Mo, W, S, and Se within the G0W0 and Bethe-Salpeter approach. First-principles calculations based on density functional theory were carried out using the Quantum ESPRESSO package [3]. The many-body perturbation theory and Bethe-Salpeter calculations were performed using YAMBO code [4]. We address the photovoltaic performance of these TMDCs estimating the spectroscopic limited maximal efficiency (SLME) [5] as a function of the thickness of the semiconductor. We compared the different TMDCs to known materials used in photovoltaics paving the way for efficient nanoscopically thin solar cells.

We have also employed the same methodology described above to study a polymorph of h-BN that has been theoretically proposed recently [6]. This material, named as orthorhombic diboron dinitride (o-B 2 N 2), is a direct band gap semiconductor. We show that the band gap energy of o-B 2 N 2 varies strongly with number of layers and consequently it has potential to be employed in photovoltaic devices.

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Orateur: Prof. VENEZUELA, Pedro (Universidade Federal Fluminense)

Classification de Session: Oral

ID de Contribution: **31** Type: **Non spécifié**

Controlling the Nonlinear Optical Response of Semiconductor Nanomaterials by Heterostructure Engineering

vendredi 16 septembre 2022 11:30 (20 minutes)

Abstract

The possibility of controlling the optical and electronic structure in semiconductor by quantum confinement has turn semiconductor colloidal nanocrystals (NCs) one of the most investigates class of materials for optoelectronics applications. In the last two decades, much effort has been devoted to gain further control over those properties by electronic wavefunction engineering via core/shell heterostructuring. Despite all the advances in this field, very little is known about the influence of these heterostructures on the nonlinear optical response of NCs. Particularly, two-photon absorption, in the so-called quasi-continuum spectral range, has been shown to be linearly dependent on the NCs volume, on a quasi-universal scaling rule. [1] As a result, the most common method to increase the nonlinear absorption response in NCs is to make the nanomaterial larger, resulting on a red shift of their size-dependent bandgap. Here, we discuss how bandgap engineering by core/shell heterostructuring can be used to enhance the nonlinear optical response of NCs without drastically changing the emission energy. It will be shown that by wisely choosing the core and shell dimensions one can enhance the two-photon absorption cross section by one order of magnitude while maintaining the same emission energy. An alternative approach to further control the nonlinear optical response is to explore non-spherical shell as it is the case for dot-in-rod heterostructures. [2] With this type of NCs one can explore extra degrees of freedom in order to control the electronic properties and, ultimately, the nonlinear optical response.

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Orateur: Prof. A. PADILHA, Lazaro (Instituto de Física Gleb Wataghin - Universidade Estadual de Campinas)

Classification de Session: Oral

ID de Contribution: **32** Type: **Non spécifié**

Exploring field-effect transistors based on graphene for the ultrasensitive detection of biomarkers

vendredi 16 septembre 2022 09:30 (20 minutes)

Abstract

Biosensors based on graphene field-effect transistors (GFETs) are highly attractive technology, as they allow real-time label-free electrical detection, scalability, inexpensive mass production, miniaturization, the use of a low volume of sample, and the possibility of on-chip integration of both sensor and measurement systems. Besides that, graphene possesses unique properties such as: i) high charge carrier mobilities and electrical conductivity, ii) flexibility, iii) biocompatibility, iv) facile chemical functionalization, and v) large specific surface area, allowing the immobilization of high density of bioreceptors, leading to increased sensitivity [1]. This presentation will provide an overview of the fundamentals and applications of GFETs, highlighting the use of these in the ultrasensitive detection of breast cancer biomarkers (HER-2 protein) and the Spike (S) proteins of the SARS-CoV-2 virus. Furthermore, we will show how the decoration of graphene by gold nanoparticles and aptamers improved the limited detection of these devices to fM levels. Our results have shown that the GFETs exhibited a high electrical sensitivity in the detection of HER-2 proteins and the S protein, allowing us to explore this technology to detect the breast cancer biomarkers and SARS-CoV-2 virus in real samples, such as blood and saliva, respectively.

Reference

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Orateur: Prof. CASTRO SILVA, CECILIA DE CARVALHO (Mackenzie Institute for Research in Graphene and Nanotechnologies)

Classification de Session: Oral

ID de Contribution: **33** Type: **Non spécifié**

A Database of Spin Splittings in 2D Materials

mardi 13 septembre 2022 14:30 (20 minutes)

Abstract

The development of spintronic devices demands the existence of materials with some kind of spin splitting (SS). With de the advance in the development of 2D materials in the last two decades, this family of compounds brought great opportunities for applications in spintronic devices. Finding the best materials for this assignment, however, is a challenging task. To advance the understanding of this subject, we build a database of ab initio calculated SS in 2D materials. More than that, we propose a workflow for materials design integrating an inverse design approach and a Bayesian inference optimization. We use the prediction of SS prototypes for spintronic applications as an illustrative example of the proposed workflow. The prediction process starts with the establishment of the design principles (the physical mechanism behind the target properties), that are used as filters for materials screening, followed by density functional theory (DFT) calculations. Applying this process to the C2DB database, we identify and classify 358 2D materials according to SS type at the valence and/or conduction bands. The SS type can be either Rashba, Dresselhaus, Zeeman, or high order. The Bayesian optimization captures trends that are used for the rationalized design of 2D materials with the ideal conditions of band gap and SS for potential spintronics applications. Our workflow can be applied to any other material properties. In this talk, we will explain the construction process for the database and illustrate how it can be used for further studies.

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Orateur: Prof. M. DALPIAN, Gustavo (Center for Natural and Human Sciences - Federal University of ABC)

Classification de Session: Plenary

ID de Contribution: **34** Type: **Non spécifié**

Stability of subnanometer MoS wires under realistic environment

lundi 12 septembre 2022 10:10 (20 minutes)

Abstract

We carried out first-principles density functional theory calculations of hydrogen and oxygen adsorption and diffusion on subnanometer MoS nanowires. The nanowires are robust against adsorption of hydrogen. On the other hand, interaction with oxygen shows that the nanowires can oxidize with a small barrier. Our results open the path for understanding the behavior of MoS nanowires under realistic environment.

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Orateur: Prof. LUISA DA ROSA, Andreia (Universidade Federal de Goiás)

Classification de Session: Oral

ID de Contribution: **35** Type: **Non spécifié**

Topological Properties at Fractal Dimensions

lundi 12 septembre 2022 11:00 (30 minutes)

Abstract

Fractals have been used since long as decorative art, but only in the last century they have be
Last year, we unveiled the quantum dynamics in fractals using photonics experiments. By injec

References

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Orateur: Prof. MORAIS SMITH, Cristiane (Utrecht University)

Classification de Session: Plenary

ID de Contribution: **36** Type: **Non spécifié**

Pd-based dichalcogenides: the 1T and the novel 1OT regular and Janus structures: from electronic to thermal properties

lundi 12 septembre 2022 11:30 (20 minutes)

Abstract

The discovery of two dimensional (2D) graphene has opened the doors to investigate a myriad of new 2D materials that have better characteristics. Out of these are the transition metal dichalcogenides (TMDs). In this talk, I will shine light on the electronic, optical and thermal properties of the 1T [1] Pd-based dichalcogenides, namely PdS2, PdSe2, PdSSe, PdSTe, and PdSeTe systems, that do not have a fair share of research like the Mo or W-based TMDs. Our results show that the thermal electronic conductivity (⊠e), the electronic conductivity (σe), the Seebeck effect (S), and the figure of merit (ZT) along the x and y directions register the largest values in the case of electron doping for the PdSe2 and PdSeTe 2D crystals [1]. Additionally, ZT of the Janus structures are larger than their corresponding pristine PdX2 (X = S, Se) structures [1]. Once synthesized, such information is crucial for the implementation of the PdXY (Y = Se, Te) structures in industrial applications.

I will also discuss the electronic and optical properties for the novel 1OT [2] metastable (with monoclinic symmetry) structures that we have modelled in our group. Our calculations reveal that, without the inclusion of spin-orbit coupling, all structures considered have a semi-metallic behavior with a non-zero (DOS) at the Fermi level. Furthermore, they demonstrate a wider range of absorption spectra than 1T systems, and can emit or absorb within the infrared (IR) regime. They are dynamically stable and their thermal lattice conductivities should be lower than their 1T analogs, making them suitable candidates for thermoelectric devices. The Born-Oppenheimer Molecular Dynamics (MD) simulations [3] show that the 1OT PdS2 and PdSe2 structures are thermally stable at temperatures above 300 K, while the Janus PdSSe system remains stable up to temperatures close to 600 K and is completely destroyed at 900K [2].

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Orateur: Prof. A. MOUJAESS, Elie (Physics department - Federal University of Rôndonia)

Classification de Session: Oral

ID de Contribution: **37** Type: **Non spécifié**

Structural and electronic properties of III-Nitrides, MoS2 and MoSe2: From bulk polytypes to 2D structures

lundi 12 septembre 2022 11:50 (20 minutes)

While it is well known that the III-Nitrides are the materials for the highly efficient light-emitting diodes, among other optoelectronic devices, the transition metal dichalcogenides (TMDC) also offer a great potential use in the field of 2D materials with interesting electronic and optoelectronic properties. In the case of III-Nitrides, the interest on these materials was renewed, now as a 2D material, when Tsipas and collaborators [1] found that it is possible to grow hexagonal AlN nanolayers on surfaces of Ag (111) and Al Balushi and colleagues found that hexagonal GaN can be obtained via encapsulation of graphene [2]. Moreover, in the case of TMDC, their bulk counterparts were less studied than the 2D ones, and the knowledge of their structural and vibrational properties could help to obtain better 2D samples. It is well known that the bulk structure of these materials presents polytypism, which is not yet well understood by the scientific community. The same holds in the case of III-Nitrides, which the zincblende, wurtzite and the rocksalt forms were extensively studied, and not their hexagonal closed-packed (hcp) structure. So, in this work, we report our theoretical results (with van der Waals corrections included) for the structural and vibrational properties of the bulk polytypes of MoS2 and MoSe2, as well as for the hcp form of III-Nitrides, extending our study to the 2D structures of these materials. For the 2H polytype of MoS2, we have found that, the experimental measured bulk modulus is underestimated once, from our theoretical data, these measurements show a combination of hydrostatic and axial strains, which preserves the symmetry of the unit cell, due to its lubricant properties. We have also shown that, in the case of III-Nitrides, an axial strain applied to the wurtzite structure can transform it to the hexagonal closed-packed one. Going to the III-Nitrides 2D structures, we have studied the graphene-like, the square lattice and the haeckelite 8-4 ones. Our results show that the graphene-like structure is more stable one and their electronic structures show an indirect bandgap. Finally, we show our results for the structural and electronic properties of MoS2/MoSe2 lateral interfaces in both zig-zag and armchair configurations. Band offsets and alignment of these interfaces were also obtained. Our results have shown that the band offsets 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.

Orateur: Prof. W. LEITE ALVES, Horacio (Departamento de Ciências Naturais - Universidade Federal de São João del Rei)

Classification de Session: Oral

ID de Contribution: **40** Type: **Non spécifié**

Strain and crystal field splitting inversion in III-Nitrides

mardi 13 septembre 2022 09:30 (20 minutes)

The wurtzite phase group III-Nitrides (AlN, GaN, InN) have attracted great interest due to their successful applications in the optoelectronics since the 90's. In this paper we perform a comprehensive study of AlN, GaN and InN structural elastic and electronic properties using hybrid and conventional Density Functional Theory, presenting a comparison of the features of the three compounds. We perform a direct comparison of the features of their electronic structures, including the inversion of the top valence band associated with a negative crystal field splitting and its relation to the challenges of acceptor-doping on AlN systems. With the determination of elastic constants and the Young modulus we provide a simple model to connect a deformation energy associated with the parameter u and the effective crystal-field splitting, showing a direct relation among internal strain and the crystal-field splitting.

Orateur: Prof. M. SIPAHI, Guilherme (Instituto de Física de São Carlos - Universidade de São Paulo)

Classification de Session: Oral

ID de Contribution: **41** Type: **Non spécifié**

Polariton Engineering with Quantum Materials

mercredi 14 septembre 2022 09:30 (20 minutes)

Abstract

Polaritons, which are quasiparticles composed of a photon coupled to an electric or magnetic dipole, are a major focus in nanophotonic research of low-dimensional materials. Polaritons can be active in a broad range of the electromagnetic spectrum (meVs to eVs) and exhibit momenta much higher than the corresponding free-space radiation. Hence, the use of high momentum broadband sources or probes is imperative to excite those quasiparticles and measure the frequency-momentum dispersion relations, which provide insights into polariton dynamics. Synchrotron infrared nanospectroscopy[1] (SINS) is a technique that combines the nanoscale spatial resolution of scattering-type scanning near-field optical microscopy with synchrotron infrared radiation, making it highly suitable to probe and characterize a variety of polaritons. Here, the advances enabled by SINS on the study of key different types of polaritons from the THZ to mid-infrared will be described. In this talk, I will explore low-dimensional materials [2,3] as the polaritonic materials and their remarkable optical properties. I will present recent studies in the field of polaritons in contact with different interfaces dielectric/air(metal) and heterostructures using SINS. Furthermore, I will show that these experimental observations provide an attractive platform for understanding light-matter interaction and, therefore, could be harnessed in compact nanophotonic devices and applications involving subdiffractional light traffic.

Acknowledgments

FAPESP, CNPq, Brazilian Nanocarbon Institute of Science and Technology (INCT/Nanocarbono) and CNPEM.

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Orateur: Prof. DAVID BARCELOS, Ingrid (Brazilian Synchrotron Light Laboratory (LNLS) - Brazilian Center for Research in Energy and Materials (CNPEM))

Classification de Session: Oral

ID de Contribution: **42** Type: **Non spécifié**

To be announced

mercredi 14 septembre 2022 09:50 (20 minutes)

Orateur: Prof. PEREIRA JÚNIOR, João Milton (Universidade Federal do Ceará)

Classification de Session: Oral

ID de Contribution: **43** Type: **Non spécifié**

Combined experimental and ab-initio studies of Ca3Ti2O7 local structure

Abstract

Techniques for studying short-range interactions have been successfully used to evaluate local parameters of crystals with high precision. In particular, experiments using perturbed angular correlation (PAC) spectroscopy were able to track the high-temperature phase transitions of hybrid improper ferroelectrics. Here, we continued such works by combining PAC spectroscopy with electronic structure calculations based on the density functional theory to study the evolution of the electric field gradient at the Ca sites of Ca 3Ti2O7. Our results show a structural phase transition from the low-temperature A21am structure to a second phase above 1050 K. This second environment found above the critical temperature is characterized by an electric field gradient distribution with high axial asymmetry. In agreement with the probing of a locally distorted environment, the high-temperature results are compatible with the Acaa structural symmetry. These results contradict previous reports on a direct structural transition from the polar A21am to the aristotype I4/mmm symmetry.

Orateur: Prof. VITORIA CREDIDIO ASSALI, Lucy (Instituto de Fisica da Universidade de São Paulo)

Classification de Session: Plenary

ID de Contribution: **45** Type: **Non spécifié**

Constructing realistic low-energy effective models of materials

jeudi 15 septembre 2022 11:30 (20 minutes)

Abstract

Model hamiltonians are a useful tool to approach the many-body problem in materials. They often provide valuable physical insight and enable larger length-scale studies. However, since model parameters are invariably unknown, this approach often lacks predictive power, an issue that turns more significant in materials with strong electronic correlations. Being able to controllably construct accurate effective models of materials is thus highly desirable. I will present a methodology that uses highly accurate many-body simulations to inform the construction of model hamiltonians that accurately approximate a material's low-energy physics. I will show results on low-dimensional materials.

Orateur: Prof. RODRIGUES BARBOSA, João Nuno (Universidade Federal do ABC - UFABC)

Classification de Session: Oral

ID de Contribution: **47** Type: **Non spécifié**

Effective kp Hamiltonians calculated from ab initio data

jeudi 15 septembre 2022 12:10 (20 minutes)

Abstract

In this talk we will present a new code, called QE2KP, which calculates the effective kp Hamiltonian using the ab initio wave-functions as basis functions to calculate the matrix elements of the kp theory within the Löwdin perturbation approach. The kp method is widely used to obtain effective Hamiltonians to describe a chosen set of bands of crystalline materials. The derivation of these Hamiltonians start by identifying the symmetry group of the crystal, and irreducible representations of the bands at the central k point for the perturbative expansion. Then, combining the kp method with fundamentals of group theory [1] (theory of invariants), one is able to obtain the functional form of the Hamiltonian. For instance, for graphene, and up to linear powers in k, one obtains H = $\hbar$vF σ.k, which leads to the cone Dirac. However, the kp and group theory approaches can only tell us that the coefficient $\hbar$vF is finite (selection rules), but it cannot give it a numerical value. Currently, the python packages IrRep [2] and Qsymm [3] are quite useful to help us obtain these functional forms of H. Therefore, the goal of our new code QE2KP is to take a step further and calculate the numerical values of these parameters (e.g. $\hbar$vF, Kane and Luttinger parameters). In this talk, we'll show preliminary results (see Fig. 1) of our code and describe the methodology we are using to combine the QE data with the python packages IrRep and Qsymm to fully describe both the functional form and the numerical values for the effective Hamiltonians of any crystal.

References

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Orateur: Prof. J. FERREIRA, Gerson (Instituto de Física - Universidade Federal de Uberlândia)

Classification de Session: Oral

ID de Contribution: **48** Type: **Non spécifié**

Magnetotransport measurements for detection of Dirac fermions in topological insulators

vendredi 16 septembre 2022 12:10 (20 minutes)

Abstract

Topological insulators (TIs) are materials that are insulating in their bulk but present metallic states on their surface. This is the simplest definition for a complex quantum effect that results from strong spin-orbit coupling that changes the topological order of the material. The metallic states host spin-polarized currents composed of Dirac fermions flowing on the topological surface states (TSS). The TSS of TIs are protected by time-reversal symmetry (their physics is independent of whether time is flowing backward or forward). 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. In the particular case of TIs and TCIs, the potential to application in quantum computation and spintronic is enormous. Prior to the application in development of new technologies, however, the detection of Dirac Fermions via electrical transport measurements is mandatory [1].

The detection of Dirac fermions in TIs via transport measurements represents a big challenge for experimentalist. 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. In this talk, the results of magnetotransport measurements performed on Bi2Te3 and SnTe nano-structures will be presented. The investigation will involve the analysis of Shubnikov-de Haas oscillations in SnTe structures [2] and weak anti-localization effect in Bi2Te2 nano films providing a full description of the important parameters that characterize the electrical transport in these materials.

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Orateur: Prof. L. PERES, Marcelos (Instituto de Física e Química - Universidade Federal de Itajubá)

Classification de Session: Oral

ID de Contribution: **49** Type: **Non spécifié**

Effective g-factors of excitons in van der Waals semiconductors

lundi 12 septembre 2022 09:30 (20 minutes)

Abstract

The future application of few-layer semiconductors, such as transition metal dichalcogenides (TMDCs), as building blocks for opto-electronic devices relies on a full understanding of the light-induced strongly bound electron-hole pairs (excitons) in these materials. Through the investigation of Zeeman and diamagnetic shifts in the excitonic peaks under high magnetic fields, magneto-photoluminescence has been proven an important experimental tool for unravelling the angular momentum character of electron and hole states in few-layer materials. However, unexpected values for the g-factors of these states have been consistently observed in monolayer and heterobilayers of TMDCs, which motivates us to develop accurate theoretical models for explaining these experimental observations.
In this talk, I will present a theoretical approach for predicting the angular momentum (and, consequently, the g-factor) of excitonic states in monolayer and bilayer semiconductors within a multiscale approach, involving a combination of ab initio and continuum model tools. [1] As we will discuss in details, this model has been successfully used to explain experimentally observed Zeeman shifts (i) of ground and excited exciton states in monolayer WSe2, [2] (ii) of hybrid exciton states, with k-space direct and indirect components, in monolayer WS2, [3] and (iii) of excitons confined by moiré patterns in a MoSe2/WS2 van der Waals bilayer.

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Orateur: Prof. CHAVES, Andrey (Universidade Federal do Ceará)

Classification de Session: Oral

ID de Contribution: **50** Type: **Non spécifié**

The DFT-1/2 method for gap correction

lundi 12 septembre 2022 15:00 (1 heure)

Abstract

For the past 40 years density functional theory (DFT) has been the dominant method for the quantum mechanical simulation of periodic systems, predicting the ground state properties of metals, semiconductors, and insulators with great success. This success not only encompasses standard bulk materials but also complex materials such as proteins, polymers, solids, nanostructures and DNA. Practical applications of DFT are based on approximations for the so-called exchange-correlation potential. Common approximations are the so-called Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA), which produce semiconductor band gaps significantly smaller than experiment. This fact raises the issue of how to obtain reliable excited-state properties. We addressed this question by proposing the DFT-1/2 method in 2008 and provide general form to calculate one-particle excitations in solids [1,2]. The method consists of calculating the self-energy as the quantum mechanical average of a "self-energy potential", which is added to the local part of the pseudopotential or to the -2Z/r part of the all-electron potential. We obtained band gaps of several semiconductors that compare very well with experiment, with the precision of the GW method, but at negligible computational cost. This great advantage of the method allows approximate quasiparticle correction for more complex systems as alloys, interfaces, perovskites, etc. The method was also applied to 34 different 2D materials showing results in their majority superior to the HSE06. Moreover, based on the knowledge of the method and chemical information of the material, we can predict the small number of cases in which the method is not so effective and provide the best recipe for an optimized DFT-1/2 method based on the electronegativity difference of the bonding atoms. The method is nowadays used in several codes by several groups around the world.
In this tutorial, we will provide a basic theoretical overview and perform a few hands-on practices.

References

[1] L. G. Ferreira, M. Marques and L. K. Teles, Phys. Rev. B 78, 125116 (2008).

[2] L. G. Fereira, M. Marques and L. K. Teles, AIP Adv. 1032119 (2011).

Orateur: Prof. GUILHON, Ivan (Instituto Tecnológico de Aeronáutica)

Classification de Session: Tutorial

ID de Contribution: **51** Type: **Non spécifié**

The DFT-1/2 method for gap correction

lundi 12 septembre 2022 16:30 (1 heure)

Abstract

For the past 40 years density functional theory (DFT) has been the dominant method for the quantum mechanical simulation of periodic systems, predicting the ground state properties of metals, semiconductors, and insulators with great success. This success not only encompasses standard bulk materials but also complex materials such as proteins, polymers, solids, nanostructures and DNA. Practical applications of DFT are based on approximations for the so-called exchange-correlation potential. Common approximations are the so-called Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA), which produce semiconductor band gaps significantly smaller than experiment. This fact raises the issue of how to obtain reliable excited-state properties. We addressed this question by proposing the DFT-1/2 method in 2008 and provide general form to calculate one-particle excitations in solids [1,2]. The method consists of calculating the self-energy as the quantum mechanical average of a "self-energy potential", which is added to the local part of the pseudopotential or to the -2Z/r part of the all-electron potential. We obtained band gaps of several semiconductors that compare very well with experiment, with the precision of the GW method, but at negligible computational cost. This great advantage of the method allows approximate quasiparticle correction for more complex systems as alloys, interfaces, perovskites etc. The method was also applied to 34 different 2D materials showing results in their majority superior to the HSE06. Moreover, based on the knowledge of the method and chemical information of the material, we can predict the small number of cases in which the method is not so effective and provide the best recipe for an optimized DFT-1/2 method based on the electronegativity difference of the bonding atoms. The method is nowadays used in several codes by several groups around the world.
In this tutorial, we will provide a basic theoretical overview and perform a few hands-on practices.

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[2] L. G. Fereira, M. Marques and L. K. Teles, AIP Adv. 1032119 (2011).

Orateur: Prof. GUILHON, Ivan (Instituto Tecnológico de Aeronáutica)

Classification de Session: Tutorial

ID de Contribution: **52** Type: **Non spécifié**

Electron Transport in Gated Nanodevices

mardi 13 septembre 2022 12:10 (20 minutes)

Abstract

Atomically-thin materials and systems have provided theorists with new perspectives to exploit the electronic structure under direct and indirect interactions. For example, the electron response to static electric field, bias voltage, or even by including the spin-orbit coupling may lead to the discovery of new phenomena, as well as interesting electronic properties at low dimensions [1,2]. As is well known in condensed matter, conduction properties are sensitive to the material extension and can be controlled by an external electric or magnetic field. Furthermore, electron and spin transport properties can be tuned as a function of the size for a characteristic dimension of the material. In this direction, we have investigated how these interactions exhibit close relationships with several electronic properties in different systems and devices. In this communication, we explore the electronic properties of gated quasi-one-dimensional devices and two-dimensional materials. Our computational methodology is based on density functional theory combined with the finite-field approach and the Keldysh nonequilibrium Green's function technique.

Acknowledgment

This work has been funded by Brazilian agencies FAPESB and CNPq.

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[1] C. P. de Castro et al., J. Vac. Sci. Technol. B 39, 060601 (2021).

[2] R Rivelino et al., ACS Appl. Electron. Mater. 2, 3242 (2020).

Orateur: Prof. RIVELINO, Roberto (Universidade Federal da Bahia - Instituto de Física)

Classification de Session: Oral

ID de Contribution: **53** Type: **Non spécifié**

Buckling induced flat bands: Giant nanoscale periodic strain

lundi 12 septembre 2022 09:00 (30 minutes)

Abstract

Two-dimensional atomic crystals can radically change their properties in response to external i
The strain fields induced by periodically buckling graphene result in a periodic pseudo-magn
Using scanning tunneling microscopy and spectroscopy, together with numerical simulations, w
From the geometry, amplitude, and period of the periodic pseudo-magnetic field, we determine

References

[1] J. Mao, S. P. Milovanovic, M. Anđelković, X. Lai, Y. Cao, K. Watanabe, T. Taniguchi, L. Covaci, F. M. Peeters, A. K. Geim, Y. Jiang, and E. Y. Andrei: "Evidence of Flat Bands and Correlated States in Buckled Graphene Superlattices", Nature 584, 215 (2020).

Orateur: Prof. M. PEETERS, François (Condensed Matter Theory, Universiteit Antwerpen, B-2020 Antwerpen, Belgium)

Classification de Session: Plenary

ID de Contribution: **54** Type: **Non spécifié**

Mechanical and electronic properties of hybrid graphene-hBN monolayers under strain

mercredi 14 septembre 2022 10:10 (20 minutes)

Abstract

Hybrid graphene-hexagonal boron nitride (hBN) monolayers have already been synthesized, but most investigations on their properties have only considered relaxed structures. In this talk, I will discuss the mechanical and electronic properties of two types of monolayers: in (i), we have a graphene sheet with hBN domains; in (ii), we have an hBN sheet with graphene domains. The results were obtained by combining density functional theory and molecular dynamics simulations. Regarding the mechanical properties, we find that we can control the Young´s modulus by adjusting the fraction of graphene and hBN in the hybrid monolayer, whereas the ultimate strength and strain are limited by the strength of the hybrid C-B and C-N bonds. Furthermore, the results show that the mechanical properties do not depend on the size of the considered structure. Concerning the electronic properties, we find that by combining composition and strain, we can produce hybrid sheets with band gaps spanning an extensive range of values (between 1.0 eV and 3.5 eV). Our results also show that the band gap depends more on the composition than on the external strain, particularly for structures with low carbon concentration.

Orateur: Prof. D. MACHADO, Leonardo (Departamento de Física - Universidade Federal do Rio Grande do Norte)

Classification de Session: Oral

ID de Contribution: **55** Type: **Non spécifié**

Optical properties and giant valley polarization of interlayer excitons in van der Waals heterostructures

mercredi 14 septembre 2022 11:00 (30 minutes)

Abstract

The 2D materials, such as monolayer transition metal dichalcogenides (TMDs) 1-4, can form van der Waals (vdWs) heterostructures held together by weak van der Waals forces, providing an unprecedented platform to engineer quantum materials with exotic physical properties. Among the different vdWs heterostructures, the most interesting ones for optical applications are those characterized by a type II band alignment where the valence band maximum and the conduction band minimum lie in different layers. This configuration energetically promotes ultrafast charge separation, prompting the photoexcited electrons to reside on one TMD layer and the holes to be on the other, forming interlayer excitons (IXs). The IXs possess the recombination times and valley lifetimes several orders of magnitude longer than that of the monolayer excitons, making them ideally suited for some spintronics and valleytronic device applications. A weak interlayer vdW interaction, however, inhibits interlayer charge transfer across vdW heterostructures, significantly constraining the population of the IXs. In addition, the reduced oscillator strength of IXs renders them further darkish. The small population together with the darkness of the IXs substantially limit their experimental probing and potential applications. In this work, firstly, we will present our computational packet–WanTiBEXOS which is a parallel computational FORTRAN code, constituted of a maximally localized Wannier functions based tight-binding model in conjunction with the Bethe–Salpeter equation framework. Our packet can be used to study optical properties of excitons including IXs in conventional semiconductors, 2D magnetic and non-magnetic materials, TMD vdW heterostructures and perovskite, etc.. After that, we will move to magnetic proximity effect on IX dynamics in the TMD vdWs heterostructures grown on magnetic substrate5, focusing on optical properties and giant valley polarization of interlayer excitons.

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[1] Fanyao Qu, et. al. 2D Materials, 6, 045014 (2019).

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Orateur: Prof. QU, Fanyao (Universidade de Brasília)

Classification de Session: Plenary

ID de Contribution: **56** Type: **Non spécifié**

Advances and prospects of 2D ferromagnetic semiconductors

jeudi 15 septembre 2022 11:00 (30 minutes)

The intrinsic ferromagnetism in two-dimensional (2D) materials has been a long-term concern and pursuit. Only few years ago it has been realized, after thinning CrGeTe 3 and CrX3 (X = Cl, Br, I) from bulk down to a monolayer. These materials were not only ferromagnetic, but also semiconducting - which stimulated intensive research on novel emergent phenomena and creative concepts. In this talk I will summarize the recent progress of 2D ferromagnetic semiconductors and discuss ongoing (theoretical) strategies proposed to enhance ferromagnetism, tailoring the very mechanisms of magnetic exchange interaction and magnetic anisotropy. Moreover, I will discuss the multifunctionality of such materials and their promise towards advanced van de Waals heterostructures in magnetoelectric, multiferroic, and nondissipative electronic technology –tailored practically at will.

Orateur: Prof. V. MILOŠEVIĆ, Milorad (University of Antwep)

Classification de Session: Plenary

ID de Contribution: **57** Type: **Non spécifié**

Pentaoctite Phase of Group-V Nanostructures

mercredi 14 septembre 2022 11:30 (20 minutes)

Abstract

Recently, the existence of an allotrope phase of bismuthene called pentaoctite, in which all hexagonal rings are replaced by either pentagons or octagons, has been proposed.[1,2] These structures show a sizeable bandgap, can be stable under strain, and have topological insulator behavior with protected surface nontrivial Dirac states. From this information, we extend our investigations of this allotrope phase to phosphorene,[3]arsenene,[4,5] and antimonene.[6,7] Our first-principles calculations show that these 2D structures are metastable against their respective hexagonal phases, but have relatively low formation energies. In particular, group-V pentaoctite can become a direct gap material under tensile or compressive strain. Our calculated dielectric function shows that all structures have absorption edges in the visible region, making these materials suitable for optoelectronic applications.
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Orateur: Prof. NASCIMENTO LIMA, Erika (Universidade Federal de Rondonópolis)

Classification de Session: Oral

ID de Contribution: **58** Type: **Non spécifié**

Analyze of non-ideal charge transport in QWIPs and infrared phtotodiodes

jeudi 15 septembre 2022 10:10 (20 minutes)

Abstract

Infrared sensors have many important applications both in civilian and military sectors. Due to the military application, the commercialization of such devices are controlled by the governors of the countries that fabricate such devices, specifying the types and the performance of the devices that can be sold to each country, even to civilian applications. This situation asks for an autonomous development of the technology for fabricating then. A group of Brazilian researchers, grouped in the INCT-DISSE (Instituto Nacional de Ciência e Tecnologia em nanoDispositivos Semicondutores), has dedicated to such development. Part of the knowledge accumulated will be shared in this talk. The sources of non-ideal behavior of dark current in QWIPs and InGaAs photodiodes are analyzed improving the existing models. The talk summarizes and links the work presented in 5 papers from students of the lecturer, adding additional material. Part of the results presented here was obtained or comes from samples generated during a research abroad funding by FAPESP (grant 2016/05516-3).

Orateur: Prof. SOARES VIEIRA, Gustavo (Divisão de Física Aplicada, Instituto de Estudos Avançados)

Classification de Session: Oral

ID de Contribution: **59** Type: **Non spécifié**

Superconducting quantum devices for quantum computing

mardi 13 septembre 2022 15:00 (1 heure)

Abstract

Superconducting quantum computing is a burgeoning field that seeks to develop Josephson-junction-based qubits and superconducting circuitry as a scalable architecture for quantum information processing. In particular, advancements in qubits design and fabrication techniques have led to the development of the building blocks necessary for the development of one of the leading technologies for quantum computing. This lecture series will give an overview of this rapidly developing field. We will provide the students, researchers, and other attendees with a broad introduction to the basic physics of superconducting circuits and a review of the field, avenues of investigation, and applications of research in the field. The lectures will be structured to provide the fundamentals of this cutting-edge technology and the relevant up-and-coming technologies such as quantum processing, communication, and simulation. Moreover, the lectures will provide the relevant information to seek additional resources for a more in-depth study and research involvement in the future.

Orateur: Prof. ROUXINOL, Francisco (University of Campinas)

Classification de Session: Tutorial

ID de Contribution: **60** Type: **Non spécifié**

Superconducting quantum devices for quantum computing

mardi 13 septembre 2022 16:30 (1 heure)

Abstract

Superconducting quantum computing is a burgeoning field that seeks to develop Josephson-junction-based qubits and superconducting circuitry as a scalable architecture for quantum information processing. In particular, advancements in qubits design and fabrication techniques have led to the development of the building blocks necessary for the development of one of the leading technologies for quantum computing. This lecture series will give an overview of this rapidly developing field. We will provide the students, researchers, and other attendees with a broad introduction to the basic physics of superconducting circuits and a review of the field, avenues of investigation, and applications of research in the field. The lectures will be structured to provide the fundamentals of this cutting-edge technology and the relevant up-and-coming technologies such as quantum processing, communication, and simulation. Moreover, the lectures will provide the relevant information to seek additional resources for a more in-depth study and research involvement in the future.

Orateur: Prof. ROUXINOL, Francisco (University of Campinas)

Classification de Session: Tutorial

ID de Contribution: **61** Type: **Non spécifié**

Stability and Rupture of Ultrathin Ionic Wires

jeudi 15 septembre 2022 14:30 (30 minutes)

Using a combination of in situ high-resolution transmission electron microscopy (Fig. 1) and density functional theory (Fig. 2), we report the formation and rupture of ZrO2 atomic ionic wires. Near rupture, under tensile stress, the system favors the spontaneous formation of oxygen vacancies, a critical step in the formation of the monatomic bridge. In this length scale, vacancies provide ductile-like behavior, an unexpected mechanical behavior for ionic systems. Our results add an ionic compound to the very selective list of materials that can form monatomic wires and they contribute to the fundamental understanding of the mechanical properties of ceramic materials at the nanoscale.

Orateur: Prof. B. CAPAZ, Rodrigo (Brazilian Nanotechnology National Laborator)

Classification de Session: Plenary

ID de Contribution: **62** Type: **Non spécifié**

Guima, the theoretical pioneer in semiconductors in Brazil

vendredi 16 septembre 2022 15:40 (30 minutes)

Professor Luiz Guimarães Ferreira, Guima as he was called by his friends, passed away last year. He was born in Rio de Janeiro in January 1937, he attended Santo Inácio College, graduating at the top of his class. He Joined ITA in 1955 in first place in the entrance exam and was most brilliant undergraduate student at ITA. He majored in Electronic Engineering in 1959, and soon joined MIT where he obtained his Ph.D. in 1964 under the guidance of Professor George W Pratt Jr.in Professor Slater's group. Professor Guimarães, was the first theoretical physicist in Semiconductors in Brazil and pioneered the intensive use of computers to understand the electronic structures of solids, molecules, and atoms. Full Professor at the Institute of Physics at University of São Paulo,SP, where he worked from 1965 to 1990. After retiring he was a visiting professor at the State University of Campinas. He was the Director of the Institute of Physics at USP from 1982 to 1986 and was a full member of the Brazilian Academy of Sciences. One of the pioneers in the field of Solid State Physics in Brazil, he exerted a great influence on the formation of the research community in the area of Electronic Structure. I will talk a little bit about his contribution to condensed matter physics and his important contribution to the training of our researchers.

Orateur: Prof. FAZZIO, Adalberto (Ilum School of Science - Brazilian Center for Research in Energy and Materials (CNPEM))

Classification de Session: Closing

ID de Contribution: **63** Type: **Non spécifié**

Development of Advanced Semiconductor Materials and Devices For Next Generation Photovoltaics: Opportunities And Challenges

jeudi 15 septembre 2022 09:00 (30 minutes)

Renewable energy production is a key component in the drive towards a safe, secure energy supply for future low-carbon economies. Using energy from the sun to generate electricity provides a sustainable source of free, abundant, safe, clean energy, without use of any fossil fuels and without waste or pollution.

Solar cells (photovoltaic cells) are made of semiconductor materials that convert energy from the sun directly into electrical energy. Sunlight consists of a spectrum of different wavelengths (colours) of light, each corresponding to a different energy level. Semiconductor materials can only convert sunlight of specific wavelengths and energy into electrical energy. Remaining energy from the sun is lost. Existing semiconductors cannot utilise the entire spectrum distribution of sunlight. The strategy to increase the efficiency of solar cells is to use semiconductors optimised for different wavelength ranges of the spectrum.

Existing 'three junction'solar cells, which utilise three different semiconductors, are capable of converting sunlight from three regions of the spectrum into electrical energy. The drawback is that state of the art solar cells currently only convert 33% of solar energy into electricity. There is a great interest worldwide into developing innovative semiconductor materials capable of converting sunlight from a fourth specific portion of the solar spectrum into electrical energy. Retrofitting this fourth generation material onto current solar cells should significantly improve solar cell efficiency to >60%.

Currently a wide range of semiconductors is explored for their potential use in photovoltaic applications. However, solar cells are already an important part of our lives. The simplest systems power many of the small calculators and wristwatches. The complicated systems provide electricity for pumping water, powering communications equipment, and even lighting our homes and running our appliances. With the growth of the satellite industry and the increase of power requirements, larger solar arrays are needed to produce the required power. The familiar wings of most modern satellites are made of solar arrays.

In this talk, I will give an overview of the principles of solar cells, the properties of semiconductors suitable for solar cells, and some selected recent achievements in III-V solar cells.

Orateur: Prof. HENINI, Mohamed (School of Physics and Astronomy - University of Nottingham)

Classification de Session: Plenary

ID de Contribution: **64** Type: **Non spécifié**

Magnetic van der Waals membranes in motion

mercredi 14 septembre 2022 16:45 (30 minutes)

Atomically thin membranes are ideal building blocks for nanoelectromechanical systems (NEMS) because of their unique mechanical properties and their low mass. We make membranes by transferring atomically thin layers on top of silicon oxide substrates that are pre-patterned with (circular) holes. The suspended membranes are characterized by a laser interferometer set-up that gives access to information on the dynamics in the frequency- and time-domain. The interferometer setup is equipped with a moveable x-y stage so that the membrane motion can be visualized with a lateral resolution of 140 nm and a displacement resolution of 11 fm/√Hz; additionally, the nonlinear response of the motion can be used to extract the mechanical parameters such as the Young' s modulus. Recently, it has become clear that nanomechanics can probe thermodynamic properties such as thermal conductivity, specific heat, and thermal expansion [Dynamics of 2D material membranes, 2D Materials 8 (2021) 042001]. Specifically, we have detected the Néel temperature of antiferromagnetic FePS3 membranes as (magnetic) phase transitions are typically accompanied by abrupt changes in the specific heat, resulting in accompanying changes in the strain of the material. This strain change modifies the resonances frequencies which together with the Q-factor of the resonance are detected as a function of temperature. In this way, the free-hanging van der Waals materials are probed without the need of electrical contacts and without the interaction with substrate, purely by mechanical means.

Orateur: Prof. S. J. VAN DER ZANT, Herre (Kavli Institute of Nanoscience)

Classification de Session: Plenary

ID de Contribution: **65** Type: **Non spécifié**

Uncovering Singlet Fission in TIPS-tetracene Crystals

lundi 12 septembre 2022 14:30 (30 minutes)

Abstract

Singlet fission in organic semiconductors is a promising concept that can be used to increase the efficiency of solar photovoltaic cells. Upon light absorption a singlet exciton (S = 0) is created, which splits into two triplet excitons (S = 1), via an intermediate triplet-pair state (S = 1 ⊗ S = 1). This carrier-multiplication process potentially reduces the thermalization losses hampering solar power conversion efficiency.

We identify several sharp triplet-pair peaks in the low temperature (1.4 K) photoluminescence (PL) spectrum of high-quality TIPS-tetracene (5,12-bis(triisopropylsilylethynyl)tetracene) single crystals. Using magnetic fields up to 30 T, we are able to tune the S = 1 and S = 2 triplet-pair states into resonance with the S = 0 triplet-pairs, resulting in a drastic reduction of the PL intensity at resonant magnetic fields [1]. The position of the resonances permits the determination of the exchange coupling constant of the triplet-pair state J = 0.44 meV. The triplet-pair emission displays a characteristic vibrational spectrum and is found to disappear above 2.4 K, which is attributed to the thermal activation of triplet-pair dissociation via the triplet-pair quintet states (S =2) [2]. Most remarkably, we find that the 1.4 K triplet-pair PL decay time exceeds 10 ms, indicating that in the absence of thermal dissociation the triplet-pairs can have a very long lifetime [2]. Finally, the PL reduction at the resonant magnetic fields can be as large as 90%, much more than the maximum of 50% anticipated before [1]. PL decay time measurements in an applied magnetic field show that this is a dynamic effect, as the decay time decreases at the resonant field strengths. Our results pave the way for a detailed (time-resolved) study of the properties of triplet-pairs and the singlet fission process.

Acknowledgment

V.S. Bechai, K. van den Hoven, K. Mukhuti, H. Engelkamp. This work was supported by HFML-RU/NWO-I, member of the European Magnetic Field Laboratory (EMFL).

References

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Orateur: Prof. C. M. CHRISTIANEN, Peter (High Field Magnet Laboratory - HFML-EMFL - Radboud University)

Classification de Session: Plenary

ID de Contribution: **66** Type: **Non spécifié**

Characterization of CdTe/CdMnTe quantum wells grown on Si(111)

mardi 13 septembre 2022 11:30 (20 minutes)

The II-VI semiconductor compound CdMnTe have been studied for a long time due to its opto-electronic properties and application as solar cells, x-ray detectors and other devices. The great majority of these studies have used GaAs(001) as substrates since II-VI substrates with good quality are rare and very expensive. This work describes the characterization of CdTe/CdMnTe quantum wells grown directly on Silicon(111) substrate by molecular beam epitaxy. The growth parameters were adjusted to produce a 20 nm CdTe QW between 120 nm thick CdMnTe barriers, with 11% Mn content. High resolution x-ray diffraction, atomic force microscopy and micro-photoluminescence were used for sample characterization. Despite a lattice mismatch of almost 19% between the II-VI heterostructure and the Si substrate, the samples studied showed a remarkably intense photoluminescence signal. The PL spectrum is composed by a main peak, which can be assigned to QW confined state and low intensity shoulder near 1.47 eV, attributed to Cd vacancy defects. The main PL peak has a FWHM of about 0.02 eV but shows a fine structure composed by a series of very narrow lines with FWHM ten times smaller. The position and intensity of these lines change when the incident laser beam moves to different positions. These narrow lines are probably caused by 3D confined structures which can be formed during the QW growth, due to the sample surface roughness. This work has been supported by CAPES (88881.068506/2014-1), CNPq and FAPEMIG funding agencies.

Orateur: Prof. OLAVO FERREIRA, Sukarno (Department of Physics - Universidade Federal de Viçosa)

Classification de Session: Oral

ID de Contribution: **67** Type: **Non spécifié**

Excited states, stability and polyradicaloid character of periacenes and modified periacenes

vendredi 16 septembre 2022 10:10 (20 minutes)

Abstract

The n-acenes are a class of polyaromatic hydrocarbons (PAHs) composed of linearly condensed benzene rings, resembling a quasi-1D graphene strip with zigzag boundaries. The two-dimensional structures are known as periacenes. The acenes with more than five linear benzene rings, are characterized by having a singlet open shell wave function in the ground state, showing that these systems endue an elevated radical nature. Because of their small band gaps and high charge-carrier mobilities these PAHs have attracted strong interest since they can be used in many applications such as organic semiconductors, in organic light-emitting diodes (OLEDs), in singlet fission processes, in nonlinear optics and as energy storage devices. The characterization of the ground and excited states electronic properties of the pristine and modified structures by means of quantum chemistry methods provide important information to build new materials. However, due to their radicaloid character at least two main conclusions are well-known from the literature: (1) the multireference character of the ground state electronic configuration increases with increasing number of fused benzene rings and (2) doubly excited configurations contribute to the wave functions of the low-lying excited states. Therefore, for a completely satisfactory treatment of the ground and excited states of these systems multireference methodology are preferentially requested. In this presentation, the results of the ground and excited states using multireference methods are reported for different sets of acenes and periacenes, as well as for the modified systems with B/N substitution to carbons, which proved to be a powerful tool to tune the polyradical character of PAHs. As descriptors for the biradicaloid character natural orbital occupations, number of unpaired electrons and singlet/triplet splitting are used. These benchmark data are compared with density functional theory (DFT) results in terms of spin contamination and the fractional occupation number weighted density (FOD). Examples for B/N modification of acenes to find optimal singlet fission compounds will be given.

Acknowledgment

Acknowledgment to FAPESP, CNPq, and CAPES

Orateur: Prof. B. C. MACHADO, Francisco (Instituto Tecnológico de Aeronáutica)

Classification de Session: Oral

ID de Contribution: **68** Type: **Non spécifié**

Electronic devices based on thin films of conjugated polymers and carbon nanostructures

vendredi 16 septembre 2022 09:00 (30 minutes)

Organic eletronics based on thin films as electrodes or active layers offer some processing advantages and new possibilities in the manufacture of these devices, such as flexibility and large areas. Interest in this area of research has grown significantly in last decade, presenting many innovations, whether in the synthesis of new materials, in the understanding of optoelectronic properties or in new device geometries allowing the increase of their efficiencies. The combination of conjugated polymers and carbon nanostructures can be an interesting way of organizing the nanostruture of thin film. In this work some examples of this property will be presented in the fabrication of electronic devices based on thin films obtained by: simple mixture in a common solvent; generated by interfacial synthesis; and by miniemulsion technique. The solution processed devices can take the advantage of nanostructured inks to allow their fabrication using spin coating or slot die coating in flexible substrates. Examples of gas sensors, active layers of solar cells, COVID optical sensors and electrodes obtained with this approach will be presented and discussed.

Orateur: Prof. STOLZ ROMAN, Lucimara (Departamento de Física - Universidade Federal do Paraná)

Classification de Session: Plenary

ID de Contribution: **69** Type: **Non spécifié**

Mean-field interaction effects on the topological phases of Kagome-graphene systems

jeudi 15 septembre 2022 16:45 (30 minutes)

The improving ability to synthesize new materials has intensified the interest in describing properties of systems modeled by more complex lattices. The 2D super-honeycomb lattices, including the Kagomé-graphene lattice, have been explored recently in metallic organic frameworks. They have been revealed as an essential route to achieving localized electronic responses, manifested as flat bands in their electronic structure with topological insulating behavior. Therefore, a natural inquiry for these systems is a complete analysis of their topological phases in the presence of electronic correlation effects. In this work, we use the tight-binding model to reveal a careful analysis of the impact of the electron-electron correlation effects via Hubbard mean-field approximation on the topological phases of Kagomé-graphene lattices. The spin conductivity phase's diagrams describe metallic, trivial Mott insulator and topological insulating behaviors, considering different intrinsic spin-orbit couplings, Hubbard mean-field intra-site energy intensities, and electronic occupations. This study can contribute to advances in tunable nanostructured devices prospection with relevant application potential in spintronics and transport responses.

Orateur: Prof. LATGÉ, Andrea (Universidade Federal Fluminense)

Classification de Session: Plenary

ID de Contribution: **70** Type: **Non spécifié**

Simulating hot carrier relaxation in materials: from bulk to low dimensional systems

mardi 13 septembre 2022 11:50 (20 minutes)

Abstract

Light matter interaction is of utmost importance in a number of technological applications. In photovoltaics, the excitation of carriers is a key ingredient. It leads to the formation of excitons, which are strongly bound in low dimensional systems, and the dynamics of carriers upon excitations if energy harvesting is possible.
In this talk I will discuss some recent developments in our group regarding optical excitations and the dynamics of hot carriers in several scenarios. I will discuss the formation of strongly bound excitons in van der Waals materials with possible applications in photovoltaics. Furthermore, for the case of Tellurene I will present work on ab initio calculated hot carrier lifetimes [2]. This is done using a combination of density functional theory, density functional perturbation theory, GW simulations and the inclusion of electron-hole correlations via the Bethe-Salpeter equation.
In the case of photocatalytic metals such as palladium and platinum I will discuss how direct optical transitions of photoexcited carriers in these metals are mainly generated in the near-infrared range. We also find that the electron-phonon mass enhancement parameter for Pt is 16% higher than Pd, a result that helps explain several experimental results. Finally, I will discuss how efficient hot electron generation and extraction can be achieved in nanofilms of Pd and Pd cleaved in specific directions.

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Orateur: Prof. REILY ROCHA, Alexandre (São Paulo State University)

Classification de Session: Oral

ID de Contribution: **71** Type: **Non spécifié**

Robustness of topological insulators and the fragility of trivial insulators

vendredi 16 septembre 2022 15:10 (30 minutes)

Abstract

Vacancies in materials structure, lowering its atomic density, take the system closer to the atomic limit, to which all systems are topologically trivial. Here we show a mechanism of mediated interaction between vacancies inducing a topologically nontrivial phase. We explore topological transition dependence with the vacancy density in transition metal dichalcogenides. As a case of study, we focus on the PtSe2. On the other side, the topological properties of materials are, until now, associated with the features of their crystalline structure, although translational symmetry is not an explicit requirement of the topological phases. We show that two-dimensional amorphous materials can also display topological insulator properties. More specifically, we present a realistic state-of-the-art study of the electronic and transport properties of amorphous bismuthene systems, showing that these materials are topological insulators. All calculation were done using ab initio DFT calculations.

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Orateur: Prof. FAZZIO, Adalberto (Ilum School of Science, Brazilian Center for Research in Energy and Material)

Classification de Session: Plenary

ID de Contribution: **72** Type: **Non spécifié**

Quantum devices in graphene

mardi 13 septembre 2022 11:00 (30 minutes)

Abstract

Electrostatically defined quantum dots in bilayer graphene offer a promising platform for spin qubits with presumably long coherence times due to low spin-orbit coupling and low nuclear spin density. We employ a capacitively coupled charge sensor to study the time dynamics of the excited state using the Elzerman technique. We find that the relaxation time of the excited state is of the order of milliseconds. We perform single-shot readout of our two-level system which is an important step for developing a quantum information processor in graphene.

We also present quantum devices fabricated on magic-angle-twisted bilayer graphene and demonstrate operation of a Josephson junction and a SQUID.

Acknowledgment

This work was done in collaboration with Lisa Maria Gächter, Rebekka Garreis, Chuyao Tong, Max Josef Ruckriegel, Folkert Kornelis de Vries, Annika Kurzmann, Wister Wei Huang, Elias Portoles, Giulia Zheng, Peter Rickhaus, Shuichi Iwakiri, Takashi Taniguchi, Kenji Watanabe, and Thomas Ihn.

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Orateur: Prof. ENSSLIN, Klaus (Solid State Physics Laboratory - ETH Zurich)

Classification de Session: Plenary

ID de Contribution: **73** Type: **Non spécifié**

Few-body Physics in 2D materials

lundi 12 septembre 2022 12:10 (20 minutes)

We briefly review the rich aspects of the three-body physics in two dimensions with attractive short-range potentials and contrast it with the three-dimensional case. Then we address the interesting case of two attractive and one repulsive potential appropriate to describe trions in 2D materials. The emergent property is the frustration of the trion binding with respect to the exciton, which is a distinctive feature dominating the structure of the e-e-h bound system, exemplified in the non-realistic case of a short-range potential acting between the charge carriers. The negative trion in a layer of MoS2 computed with Rytova-Keldysh potentials is shown to exhibit the same characteristic in its structure, albeit the interaction is long-ranged. This model-independent behavior is traced back to the frustration of binding the trion resulting in a weakly bound system. Based on these considerations, some prospects for future directions will be discussed.

Orateur: Prof. FREDERICO, Tobias (Instituto Tecnológico de Aeronáutica)

Classification de Session: Oral

ID de Contribution: **74** Type: **Non spécifié**

Anisotropic vortex squeezing and supercurrent diode effect in non-centrosymmetric Rashba superconductors

lundi 12 septembre 2022 17:30 (15 minutes)

Abstract

Most of 2D superconductors are of type II, i.e., they are penetrated by quantized vortices when exposed to out-of-plane magnetic fields. In a presence of a supercurrent, a Lorentz-like force acts on the vortices, leading to drift and dissipation. The current-induced vortex motion is impeded by pinning at defects. Usually, the pinning strength decreases upon any type of pair-breaking interaction perturbs a system.

In the talk I will discuss surprising experimental evidences showing an unexpected enhancement of pinning in synthetic Rashba 2D superconductors when applying an in-plane magnetic field. When rotating the in-plane component of the field with respect to the driving current, the vortex inductance turns out to be highly anisotropic. We explain this phenomenon as a direct manifestation of Lifshitz invariant that is allowed in the Ginzburg-Landau free energy when space-inversion and time-reversal symmetries are broken. As demonstrated in our experiment [1], elliptic squeezing of vortices—an inherent property of the non-centrosymmetric superconducting condensate—provides an access to fundamentally new property of Rashba superconductors, and offers an entirely novel approach to vortex manipulation.

Another interesting feature of the non-centrosymmetric superconductors in the applied magnetic field is the supercurrent diode effect—the critical current in one direction exceeds its counterpart in the opposite one—what stems from the Cooper pairs with finite centre of mass momentum. In the pioneering experiment [2] we demonstrated the emergence of the supercurrent diode effect in the Josephson junctions based on synthetic Rashba superconductors made of Al-InAs quantum wells. In the talk, I will discuss novel experimental method—measurements of the Josephson inductance—and the semiquantitative microscopic model capturing all the essential features as observed in experiment.

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Orateur: Prof. KOCHAN, Denis (University of Regensburg - Slovak Academy of Sciences)

Classification de Session: Short Talk 1

ID de Contribution: **75** Type: **Non spécifié**

Crystal growth mechanism of zinc selenide semiconductor: Molecular dynamics simulations and theoretical calculations

lundi 12 septembre 2022 17:45 (15 minutes)

Abstract

Crystal nucleation and growth are fundamental natural processes and central phenomena in several technologies. Crystal nucleation relies on the emergence of a critical nucleus from an SCL that enables other atoms or molecules to join the system, starting crystal growth. According to classical theories, the crystal growth rate can be separated into thermodynamic and kinetic terms. Two main theoretical models have been proposed to describe the crystal growth mechanism and dynamics. In the first model, proposed by Wilson [1] and Frenkel [2] (WF), the addition rate of atoms or molecules to a crystal is proportional to the atomic diffusion coefficient; whereas in the second scenario, which Broughton-Gilmer-Jackson proposed (BGJ) [3], called collision-controlled crystal growth, the ordering kinetics are controlled by the thermal velocity of the particles. For each theoretical setting, two main growth models exist: one is the "Continuous"or "Normal"growth model (N-model), and the second is the "Screw Dislocation"model (SD-model). In the N-model, the crystal surface is atomically rough, and the degree of roughness is independent of temperature. In the SD model, the crystal/SCL interface is smooth on the atomic scale, and atomic or molecular addition to a growing crystal occur preferentially on screw dislocations. In this work, we applied molecular dynamics (MD) simulations of spontaneous and seeded growth to infer the crystallization kinetics in supercooled zinc selenide (ZnSe) liquid used as a model material for which an excellent interatomic potential already exists, which was proposed by one of us (J.P. Rino). ZnSe is a type II-VI semiconductor, which is very important in optics. Experimental attempts have been made to understand its structural evolution and crystallization from vapor and melt. Hence, knowledge about its crystal growth mechanism is significant for technology applications. In MD simulations, ZnSe can nucleate spontaneously on the MD time scale only at deep supercoolings, T < 0.75 Tmelt. Hence, using the seeding method, we determined growth velocities at shallow supercooling and then, according to WF and BGJ theories, extrapolated them towards deep supercooling where MD could detect spontaneous nucleation and growth. The results showed that the Normal Growth model is the most probable growth mechanism in this material. Although the inserted seed had a zinc-blende structure, which is the most stable polymorph of ZnSe, during the growth process, layers with wurtzite structure also form, demonstrating that seeding with the desired crystalline structure (here, the ZB structure) does not always lead to the same crystalline structure. The final crystal structure in both approaches, seeded and spontaneous growth, at different supercoolings, was a mixture of the two most stable phases of this material, i.e., zinc blende and wurtzite, with a predominance of the latter. This double-crystal formation probably occurs because the difference in the thermodynamic stability of the two phases is relatively small. This work sheds light on the mechanism and structural details of crystal growth in this important semiconductor.

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Orateur: Mlle SEPARDAR, Leila (Federal University of São Carlos)

Classification de Session: Short Talk 2

ID de Contribution: **76** Type: **Non spécifié**

g-factor physics in 2D materials and van der Waals heterostructures

mardi 13 septembre 2022 17:30 (15 minutes)

Abstract

The interplay of the spin and the orbital angular momenta of electrons in semiconductors governs the Zeeman splitting, often described by the g-factors. In this talk, I will cover the basic physics behind the Zeeman splitting and g-factors, with recent examples involving two-dimensional materials and related van der Waals heterostructures. Particularly, I will show that in monolayer phosphorene[1], the g-factors are driven by spin-orbit coupling, thus acquiring small corrections. In transition metal dichalcogenides (TMDCs) monolayers, I will discuss a full ab initio approach for the g-factors[2] that nicely reproduces the experimental values, demystifying the so-called valley-Zeeman physics in TMDCs and connecting it to the longstanding knowledge of g-factors in III-V materials. Using this full ab initio approach, I will discuss the effect of mechanical strain in the g-factors of monolayer TMDCs in close connection to experiments[3,4].
Beyond monolayers, I will discuss TMDC-based van der Waals heterostructures, particularly MoSe 2/WSe2 [2]and WS2/graphene systems, in which the spin-valley physics and g-factors encode valuable information about the interlayer coupling. Reaching the bulk limit of TMDCs, I will address the origin of ultrafast oscillations for in-plane magnetic fields in bulk MoSe2 and WSe2[5].

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Orateur: Dr E. FARIA JUNIOR, Paulo (University of Regensburg)

Classification de Session: Short Talk 3

ID de Contribution: **77** Type: **Non spécifié**

WanTiBEXOS: a Wannier based Tight Binding code for excitonic and optoelectronic properties of solids

mardi 13 septembre 2022 17:45 (15 minutes)

Abstract

The GW plus the Bethe-Salpeter (BSE) equation approach becomes a methodology commonly used for computing the quasiparticle and optical properties of condensed-matter systems. However, GW approach requires a fine k-point sampling of the Brillouin zone, and GW plus BSE (GW-BSE) demands an even finer k-point sampling. Hence it is rather easy to reach the limits of what can be practically computed. In order to overcome this challenge, we have developed WanTiBEXOS, a parallel computational FORTRAN code, constituted of an effective tight-binding (TB) model in conjunction with BSE framework. The former is constructed by means of maximally localized Wannier functions. The WanTiBEXOS package can be executed via any density functional theory package interfaced with Wannier90 code[1] with computational time being reduced up to one or more orders of magnitude in comparison with that of GW-BSE. In order to demonstrate its the reliability, flexibility, efficiency and versatility of WanTiBEXOS, we provide the input files to perform electronic and optical property calculations for the representative materials, including conventional bulk semiconductors, CsGeCl3 super cubic,[2] nano-monolayer materials and van der Waals heterostructures. The results are also presented accordingly.

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Orateur: Prof. C. DIAS, Alexandre (Universidade de Brasília)

Classification de Session: Short Talk 4

ID de Contribution: **78** Type: **Non spécifié**

Natural 2D Insulating Materials in van der Waals Heterostructures: an Experimental and Theoretical study

mercredi 14 septembre 2022 17:15 (15 minutes)

Abstract

Naturally occurring van der Waals crystals have brought unprecedented interest to nanomaterial researchers in recent years. So far, more than 1800 layered materials (LMs) have been identified but only a few insulating and naturally occurring LMs were deeply investigated [1,2]. Thus, as soon as a new LM is identified, the investigation of its optical, mechanical, and electrical properties is promptly examined. Moreover, with the advent of techniques able to stack LMs precisely one on top of another creating the so-called van der Waals heterostructures (vdWHs) [3], new applications and studies are envisioned. Consequently, individual LMs and their vdWHs are often considered building blocks for future optoelectronic devices. Here, I will present a high throughput characterization of some naturally occurring LMs found in Brazilian mines by employing several experimental techniques and will demonstrate that these LMs can be mechanically exfoliated down to their monolayer limit. I will then corroborate the major findings with first-principles calculations, as well as demonstrate their use in vdWHs for optoelectronic devices [4-6]. Our studies show that naturally occurring LMs should be regarded as good and interesting candidates as substrates for LM-based applications.

Acknowledgments: Fundo Mackenzie de Pesquisa e Inovação, CAPES, CNPq, and FAPESP.

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Orateur: Prof. R. CADORE, Alisson (Mackenzie Presbyterian University)

Classification de Session: Short Talk 5

ID de Contribution: **79** Type: **Non spécifié**

Acoustic Manipulation of Excitons in 2D Semiconductors

mercredi 14 septembre 2022 17:30 (15 minutes)

Abstract

The Stark effect is one of the most efficient mechanisms to manipulate many-body states in semiconductor nanostructures. In mono- and few-layer transition metal dichalcogenides, it is usually induced by optical and electric field means. In this contribution [1], we address the tunability of the optical emission energies of excitonic states in MoSe2 monolayers employing the 220 MHz in-plane piezoelectric field carried by surface acoustic waves (SAWs). We transfer the monolayers to high dielectric constant piezoelectric substrates, where the neutral exciton binding energy is significantly reduced. In this way, we are able to dissociate the excitonic complexes (neutral exciton and trions) and quench their photoluminescence emission by more than 90 %. The SAW in-plane piezoelectric field also redshifts the excitonic optical emissions. A model for the acoustically-induced Stark effect yields neutral exciton and trion in-plane polarizabilities of approximately 530 and 630 x 10-5 meV/(kV/cm)2, respectively, which are considerably larger than those reported for monolayers encapsulated in hexagonal boron nitride. Our findings contribute to create alternative routes to manipulate and modulate multi-exciton interactions in two-dimensional semiconductor systems for optoelectronic applications.

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Orateur: Prof. D. D. COUTO JR., Odilon (Universidade Estadual de Campinas)

Classification de Session: Short Talk 6

ID de Contribution: **80** Type: **Non spécifié**

First-principles investigation of the electronic structure of the α-Al2O3-graphene interface

mercredi 14 septembre 2022 17:45 (15 minutes)

Abstract

First-principles calculations reported here illuminate the effects of the interface properties of Al2O3 and graphene, with emphasis on the structural and electrical properties. Various contact interfaces and with different alpha-Al 2O3 surface terminations are considered with on and slightly-off stoichiometric aluminum oxide. We show that depending on whether aluminum or oxygen is near graphene, a sp 3 structural deformation and spontaneous spin-polarization may occur next to the interface contact [1,2] (see Fig. 1). Interestingly, when the oxygen atoms near graphene do not cause such deformation, and for specific stoichiometries of the alumina layer, the Dirac cone of the graphene band structure shifts to lie above the Fermi level. This Such shifts suggest p-type doping, which primarily has its origin from the oxygen atoms, for situations when hybridization between O and the graphene is weak. We also show that our analysis supports the observation done in recent experiments [3]

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Orateur: Prof. P. MACIEL, Renan (Uppsala University)

Classification de Session: Short Talk 7

ID de Contribution: **81** Type: **Non spécifié**

Phyllosilicates: an emerging class of naturally abundant layered materials

jeudi 15 septembre 2022 17:15 (15 minutes)

Abstract

Beyond graphene, most of the attempts in finding interesting layered materials (LMs) that are capable of being reduced to mono and few-layers have been made in synthesized materials such as hexagonal boron nitride and transition metal dichalcogenides. In an effort to increase the list of naturally occurring LMs that are abundant in nature and could become an alternative low-cost source of two dimensional (2D) materials over its synthetic counterparts, recent research has been carried out in the group of phyllosilicate minerals which are wide band gap insulators that can be mechanically exfoliated to monolayers [1]. We present here this emerging class of naturally abundant LMs, which include talc and muscovite mica as the most studied materials. We also performed a systematic characterization of two barely explored phyllosilicate specimens –clinochlore and phlogopite - by several experimental techniques followed by a theoretical study by first-principles calculations. We provide a complete description of their 2D structures and fundamental properties from their bulk 3D form. Our results identify that the impurities present in the samples play a fundamental role in determining their macroscopic properties and demonstrate that ultrathin layers with atomically flat surface can be obtained for both materials [2,3]. Specifically, we shown that clinochlore maintain its vibrational assignment and insulating properties when reduced to a few layers [2] and, exploring phlogopite in van der Waals heterostructures, we demonstrated an enhancement on the 1L-WS2/phlogopite optical quality similarly to that obtained on 1L-WS2/hexagonal boron nitride heterostructures [3].

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Orateur: Mlle DE OLIVEIRA, Raphaela (Federal University of Minas Gerai -Brazilian Synchrotron Light Laboratory)

Classification de Session: Short Talk

ID de Contribution: **82** Type: **Non spécifié**

Tuning Desirable Properties in Molecular Electronics

mardi 13 septembre 2022 10:10 (20 minutes)

Abstract

Molecular electronics has attracted attention due application in nanoscale electronic devices. Feynman was the first scientist to propose that a molecular machine could be built, in which atoms would work the same role as the bricks of a regular size structure, composing a nanometer appliance. These nanostructures can present features which are sometimes similar to well-known devices as Zener diodes, resonant tunnel diode, field-effect transistors,
thyristors, capacitors, electrochromic devices and so on. However, it offers a viable alternative to overcome difficulties associated with the continuing shrinking of electronic devices in the silicon-based technology. In this presentation we discuss recent finds in the
field, focusing on one- and two-dimensional organic systems working as usual and non-usual devices and addressing important effects related with electronic transport, such as push-pull molecules, Coulomb blockage, negative differential resistance, strong and weak coupling, quantum interference, topological insulator behavior, edge passivation, coherent and incoherent transport, tunnelling regime, semiconductor-metal transition ,switches, and a few applications will be addressed. Also, as example, we have investigated by means of
nonequilibrium Green's functions method coupled to Density Functional Theory, the electronic transport properties of molecular heterojunctions attached to metallic organic electrodes. We are going to show how tuning electronic properties as current and conductance and how they are strongly correlated to Fowler-Nordheim and Millikan-Lauritsen signatures for several systems.

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[10] The author thanks to Brazilian CNPq funding agency (305064/2020-7) and PROPESP/UFPA.

Orateur: Prof. DEL NERO, Jordan (Universidade Federal do Pará)

Classification de Session: Oral

ID de Contribution: **83** Type: **Non spécifié**

Nanostructured materials for applications in photonics and food science

mercredi 14 septembre 2022 11:50 (20 minutes)

Abstract

In this seminar, some applications of optical spectroscopy in materials and food science will be presented. The first subject consists of quantum cutting luminescence for solar cells application. In the quantum-cut optical phenomenon, two lower-energy photons are obtained by the energy partition of a high-energy photon. As a consequence, this process opens the possibility of its application in solar cells technology in order to enhance the efficiency of the latter via thermal loss prevention without structural change. In the present case we studied the influence of Yb3+ ions on near infrared quantum cutting luminescence (~1.0 and 2.0 μm) in Pr3+/Yb3+ codoped glasses through 443 nm excitation. Then we move for multilayered and nanostructured doped silica fiber for Second Harmonic Generation (SHG). In the former, the doped core consists of alternating germanium layers (or phosphorous). Through poling process, doped layers trap positive charges that migrate due to strong eletric potential difference. This breaks the translational invariance of the fiber producing second harmonic light after the input of pulsed infrared laser.The second approach was the adoption of multi-composition core fiber. In this approach metal nanoparticles were incorporated into fiber core. In our case, WO3−x nanoparticles were incorporated along with aluminum via MCVD coupled with solution doping technique. These fiber samples have shown high SHG intensity as obtained by optical spectrum analyzer. The last subject concern two applications in Food Science Technology.

The first method consists of a device to determine protein concentration in milk based on the detection of the integral current generated by a quantum dot infrared photodetector fabricated with III-V semiconductors by researchs of DISSE –National Institute of Science and Technology in Semiconductor Nanodevices. The second example consists of a methodology, time-resolved phtoluminescence, to determine the amount of milk fat and therefore the type of milk: skimmed milk, whole milk and semi-skimmed milk.

Acknowledgment

The author like to acknowledge Brazilian Funding Agencies: CNPq, CAPES and FAPEMIG.

Orateur: Prof. VIRGILIO DE CARVALHO DOS ANJOS, Virgilio (Universidade Federal de Juiz de Fora)

Classification de Session: Oral

ID de Contribution: **84** Type: **Non spécifié**

Recent progress in generating femtosecond pulses using 2D materials

mercredi 14 septembre 2022 09:00 (30 minutes)

2D materials have been studied in basic research and used in technological applications in many areas of physics and related fields because they have extraordinary properties and are relatively easy to obtain and friendly to work with. In laser physics and technology, 2D materials simplify the way to obtain femtosecond pulses and have become a powerful tool in the ultra-fast field. In this talk we will show the latest results on the generation of femtosecond pulses using various 2D materials.

Orateur: Prof. ANTONIO THOROH DE SOUZA, Eunézio (MackGraphe - Graphene and Nanotechnology Research Center, Mackenzie Presbyterian Institute)

Classification de Session: Plenary

ID de Contribution: **85** Type: **Non spécifié**

Evidence of type-I to type-II band alignment evolution in InAsP/GaAs self-assembled quantum dots

jeudi 15 septembre 2022 09:50 (20 minutes)

In this work we studied the shape anisotropy and its relation with the band alignment in the InAsP/GaAs quantum dots by means of three technics: polarized photoluminescence, time resolved photoluminescence and magneto photoluminescence. For comparison, InAs/GaAs and InP/GaAs quantum dots were also analyzed, as not only their recombination energy sets a lower and an upper limit to the InAsP/GaAs quantum dots, but also they present different band offsets - type I and type II, respectively. Polarized photoluminescence results showed a larger in-plane shape anisotropy for the InAsP/GaAs sample with higher phosphorous contents and time resolved photoluminescence pointed towards higher time decay for this same sample in comparison with the one richer in arsenic, indicating a type I/type II transition in the alloy. Magneto photoluminescence provided additional evidence by revealing an Aharonov-Bohm type oscillation when the hole ground state changes its angular momentum from lh =0 to lh =1 and 2, which is only possible in type II heterostructures. In this way, we were able to identify a type-I to type-II progressive evolution for the band alignment of InAsP/GaAs quantum dots.

Orateur: Prof. RIBEIRO, Evaldo (Federal University of Paraná)

Classification de Session: Oral

ID de Contribution: **86** Type: **Non spécifié**

Spin phenomena in van der Waals heterostructures

mardi 13 septembre 2022 09:00 (30 minutes)

Abstract

Graphene has weak spin-orbit coupling and no magnetic order. But when placed in contact with a strong spin-orbit coupling material, such as a TMDC, or a ferromagnet, such as Cr2Ge2Te6, Dirac electrons acquire strong spin-orbit or exchange coupling, respectively. Such proximity effects render graphene suitable for spintronic applications that require spin manipulation [1]. In addition, graphene with strong proximity spin interactions can host novel topological states [2]. Fascinating new phenomena appear when bilayer graphene gets encapsulated by a TMDC from one side, and a ferromagnet from another. The resulting, so called ex-so-tic structure [3], offers spin swap functionality: switching spin-orbit and exchange coupling on demand by gate. In this talk I will review the recent developments in the proximity phenomena in graphene, and present some recent theoretical results on the control of the proximity spin-orbit and exchange coupling by twisting the van der Waals layers. I will show that the signature proximity spin-orbit coupling in graphene—valley Zeeman coupling—can be efficiently tuned by the twist angle [4], and that proximity exchange coupling can be switched by the twist angle, and even morph from ferromagnetic to antiferromagnetic [5], see Fig. 1. Support from DFG SPP1244, SFB 1277, and EU Graphene Flagship is acknowledged.

References

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[5] K. Zollner and J. Fabian, Phys. Rev. Lett. 128, 106401 (2022)

Orateur: Prof. FABIAN, Jaroslav (University of Regensburg)

Classification de Session: Plenary

ID de Contribution: **87** Type: **Non spécifié**

Effects of surface acoustic waves in the photoluminescence of WSe2 monolayers

mercredi 14 septembre 2022 15:25 (5 minutes)

Orateur: LUIZ FERREIRA GOMES, Marcos

Classification de Session: Lightning Talk

ID de Contribution: **88** Type: **Non spécifié**

Type-II induced quantum confinement in type-I heterostructured semiconductor nanowires

mercredi 14 septembre 2022 15:30 (5 minutes)

Orateur: FERNANDO OLIVEIRA LARA, Temerson

Classification de Session: Lightning Talk

ID de Contribution: **89** Type: **Non spécifié**

Magneto Optical properties of monolayer MoWSe2

mercredi 14 septembre 2022 15:35 (5 minutes)

Orateur: RICARDO RABAHI, César

Classification de Session: Lightning Talk

ID de Contribution: **90** Type: **Non spécifié**

Defect activated optical Raman modes in single layer MoSe2

mercredi 14 septembre 2022 15:40 (5 minutes)

Orateur: OFREDI CARDOSO FÁBIO, Maia

Classification de Session: Lightning Talk

ID de Contribution: **91** Type: **Non spécifié**

Exchange interaction mediated by Weyl Fermi arcs

mercredi 14 septembre 2022 15:45 (5 minutes)

Orateur: FERREIRA ALVES, João Victor

Classification de Session: Lightning Talk

ID de Contribution: **92** Type: **Non spécifié**

Hyperbolic surface exciton-polaritons at superlattices of 2D materials

jeudi 15 septembre 2022 15:00 (5 minutes)

Orateur: RODRIGUES ANDRADE, Michel (Universidade Federal do Ceará)

Classification de Session: Lightning Talk

ID de Contribution: **93** Type: **Non spécifié**

Kondo effect in a quantum dot embedded between topological superconductors

jeudi 15 septembre 2022 15:05 (5 minutes)

Orateur: RAMOS-ANDRADE, Juan Pablo (Univerisdad de Antofagasta)

Classification de Session: Lightning Talk

ID de Contribution: **94** Type: **Non spécifié**

Investigation of electrically controlled charge Qubit in van der Waals

jeudi 15 septembre 2022 15:10 (5 minutes)

Orateur: BRIZOLLA, Gusthavo

Classification de Session: Lightning Talk

ID de Contribution: **95** Type: **Non spécifié**

Ultrafast Excitation Dynamics of Spin Polarons

jeudi 15 septembre 2022 15:15 (5 minutes)

Orateur: C. P. VAN KOOTEN, Sjoerd

Classification de Session: Lightning Talk

ID de Contribution: **96** Type: **Non spécifié**

Development and optimization of the anti-reflective layer for SWIR devices

jeudi 15 septembre 2022 15:20 (5 minutes)

Orateur: GOMES RUA, Marcelo

Classification de Session: Lightning Talk

ID de Contribution: **97** Type: **Non spécifié**

High-energy Landau levels in graphene beyond first nearest-hopping processes: Corrections to the effective Dirac Hamiltonian

jeudi 15 septembre 2022 15:25 (5 minutes)

Orateur: JOHNMAR URCIA VIDARTE, Kevin

Classification de Session: Lightning Talk

ID de Contribution: **98** Type: **Non spécifié**

Anisotropic excitonic effects on 2D black phosphorus: an ab initio approach considering the DFT-1/2 method

jeudi 15 septembre 2022 15:30 (5 minutes)

Orateur: M. N. THOMEN, Diana

Classification de Session: Lightning Talk

ID de Contribution: **99** Type: **Non spécifié**

Quantum emitters in monolayer WSe2 on nano-roughness glass substrates

jeudi 15 septembre 2022 15:35 (5 minutes)

Orateur: CAVALINI, Camila

Classification de Session: Lightning Talk

ID de Contribution: **100** Type: **Non spécifié**

Efficient and extensible tight-binding model for twisted bilayer graphene

jeudi 15 septembre 2022 15:40 (5 minutes)

Orateur: MORELE DUARTE, Victor Gabriel

Classification de Session: Lightning Talk

ID de Contribution: **101** Type: **Non spécifié**

Valley-current filter in bilayer graphene based on Magnus Hall effect

jeudi 15 septembre 2022 15:45 (5 minutes)

Orateur: NOBRE DOS SANTOS, Sergio Levy

Classification de Session: Lightning Talk

ID de Contribution: **102** Type: **Non spécifié**

From Majoranas to parafermions: topological zero modes in condensed matter systems

vendredi 16 septembre 2022 14:50 (20 minutes)

Abstract

The so-called "search for Majoranas"has mobilized several groups over the last decade with the goal of achieving the "holy grail"of topological quantum computation in condensed matter systems [1-2]. In spite of the advances, particularly in devices of semiconductor nanowires with proximity induced superconductivity, many unanswered questions and challenges remain, as highlighted the recent events that shook the community [3]. This begs the question of whether other platforms hosting Majorana zero modes or other topological excitations which could be used as non-Abelian anyons can be viewed in a different light.

In this talk, I will discuss some of the scenarios for what's next in the Majorana saga. I will present some of the works in our group involving Majoranas in alternative platforms such as vortex cores in 2D topological superconductors [4]. I will also discuss our recent proposals for modeling parafermionic zero modes, Majoranas' Z_n symmetric cousins, in strongly interacting electronic systems [5,6]. We also propose a way to detect these rather exotic quasiparticles using quantum dots [5].

References

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Orateur: Prof. DIAS DA SILVA, Luis G. (Universidade de São Paulo)

Classification de Session: Oral