Condensed Matter Theory in the Metropolis

Book of Abstracts

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Talks

Jimena A. Olmos-Asar - Cordoba

On the search of new lightweight materials for the automotive technology: a computational approach

One of the most serious problems of mankind is global warming. Despite all the efforts to raise awareness in society and implement politics related to atmospheric pollution and emission of greenhouse gases, CO_2 values continue to increase [1]. 35% of this amount is due to electricity production while 32% comes from to transports. It is estimated that the world energy consumption will double by 2050 [2].

With the aim of reducing the environmental impact of transport, some countries intend to regulate the fabrication of new vehicles. The toxic trash generation is trying to be prohibited. The reduction in the weight of the vehicles is another alternative to avoid excessive CO_2 emanations. Also, the replacement of traditional carbon based fuels by alternative clean energies, such as hydrogen, is pursued. However, the use of H_2 is complex because of its low energy density and its flammability. A promising option is to store hydrogen in novel materials.

Mg seems to be the key to improve the vehicle technology. With a weight of only 24 kg/mol, it is the lightest structural metal, and its abundance makes it a sustainable resource [3]. However, due to its low corrosion resistant and limited ductility, several alloys have been developed to improve its mechanical properties.

For hydrogen storage, magnesium hydride has low cost and possesses a reasonably high gravimetric and volumetric hydrogen storage capacity [4]. However, MgH_2 also has a high enthalpy of decomposition resulting in desorption temperatures too high for most practical applications [5]. For this reason, nanomaterials and novel alloys are proposed as well to improve Mg performance.

In this work, new lightweight materials for automotive applications are studied by means of computer simulations. The prediction of materials using computer simulations represents a powerful way to save time, effort and money from industry. After a hypothetical material is demonstrated to be suitable, experimental effort will be put through to try to synthesize it.

[1] http://www.eia.gov
[2] C. Frei, et al., World Energy Scenarios: Composing Energy Futures to 2050 - World Energy Council: Project Partner Paul Scherrer Institute (PSI), Switzerland, 2013
[3] Y. Sun, C. Shen, Q. Lai, W. Liu, Da-Wei Wang, Kondo-Francois Aguey-Zinsou - Energy Storage Materials 10 (2018) 168
[4] L. Schlapbach, A. Züttel - Nature 414 (2001) 353
[5] J.-C. Crivello, B. Dam, et.al - App. Phys. A 122 (2016) 97

André Vieira - USP

Emergent dimerization and localization in disordered quantum chains

We uncover a novel mechanism for inducing a gapful phase in interacting many-body quantum chains. The mechanism is nonperturbative, being triggered only in the presence of both strong interactions and strong aperiodic (disordered) modulation. In the context of the critical antiferromagnetic spin-1/2 XXZ chain, we identify an emerging dimerization, which removes the system from criticality and stabilizes the novel phase. This mechanism is shown to be quite general in strongly interacting quantum chains in the presence of strongly modulated quasiperiodic disorder, which is, surprisingly, perturbatively irrelevant. Finally, we also characterize the associated quantum phase transition via the corresponding critical exponents and thermodynamic properties.

Eduardo Miranda - UNICAMP

Abandoned by Bloch: the dominance of disorder

Among the pillars of solid state physics is Bloch's theorem and its consequences: itinerant excitations, quasi-particles, quasi-homogeneity, unique physical properties and responses, etc. We are so accustomed to these concepts that we often do not inquire about their applicability range. Often, small amounts of disorder can be accommodated through small modifications of clean theories, but this need not always be the case. Sixty years ago, Anderson showed that single-particle states can go from extended to localized with increasing disorder. Since then, many examples have been found in which disorder has to be treated on its own terms. I will show results from recent years which illustrate this point of view. Emphasis will be given to instances where typical values of physical quantities differ by many orders of magnitude from their average values.

Luis Gregorio Dias - USP

Título: Detection and manipulation of Majorana zero modes in mesoscopic systems.

Abstract: The realization of Majorana bound states (MBS) in condensed matter systems has been a very active research topic, with possible applications to topological quantum computation. In this talk I will present the work done in our group for MBS formed in two different systems: semiconductor quantum wires coupled to quantum dots and magnetic chains on 2D honeycomb materials with induced superconductivity. In the first case, we show that quantum dots can be used as as interesting tool to both detection and manipulation of MBS by tuning gate voltages. In the second case, we establish chemical potential vs Zeeman splitting phase diagrams showing that the topological regions are strongly dependent on the spiral angle along the magnetic chain. Moreover, we show that the energy oscillations with magnetic field strength due to MBS splitting can show very different behaviors depending on the parameters. In some regimes, we find oscillations with increasing amplitudes and decreasing periods, while in the other regimes the complete opposite behavior is found.

This talk will be an overview of the work done by members of our group at IFUSP in this topic and, if time allows, other related subjects. The idea is to present the techniques and ongoing work to stimulate discussion and future collaborations.

Tobias Micklitz - CBPF

On localization in Fock-space

In the talk we discuss recent field theory efforts to address many-body localization.

Francisco Rouxinol - UNICAMP

Quantum Information and Quantum Sensing Applications using Macroscopic Scale Elements

Techniques to observe non-classical behavior of micro- and nano- scale mechanical structures, which are normally well described by classical laws of physics, has received considerable attention in recent years because of the potential to use these systems as elements in quantum computing and quantum communication architectures, and for fundamental studies of the quantum-classical boundary. One important route for observing such behavior is the coupling of micro- and nanomechanical resonators to optical and microwave cavities and superconducting qubits. In this talk, we will give an overview of the field, and discuss our efforts, at UNICAMP, toward devising an electromechanical circuit to strongly couple a nanomechanical resonator to a superconducting qubit and a microwave cavity. It is expected that such hybrid systems could be an import platform to enable the production and measurement of a diversity of non-classical states of nanoscale structures; making then a potentially important element for quantum processing architectures and testing quantum behavior in new limits.

Juarez L. F. Da Silva - USP

First-Principles Investigation of Chalcogenides Materials: From Nanoflakes to 2D Solids.

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Two-dimensional chalcogenides have attracted great attention due to their unique properties and several promising applications along a wide range of fields, e.g., thin-film solar cells, CO_2 reduction, biomedicine, etc. In our group, Quantum Theory of Nanomateriais - QTNano (https://www.facebook.com/QTNano/), we have focused on the study of 2D dichalcogenides [1,2,3,4], which spread from nanoflakes to 2D solids, as well as quaternary chalcogenides with the aim to tune the electronic properties. In this talk, we will report our recent highlights, which spread from the formation of 2D nanoflakes [3,4] to the stability mechanism in quaternary chalcogenides [1,2].

[1] R. Besse, F. P. Sabino, and J. L. F. Da Silva, Phys. Rev. B 93, 165205 (2016).
[2] R. Besse and J. L. F. Da Silva, J. Phys.: Condens. Matter. 29, 035402 (2017).
[3] R. Besse, N. A. M. S. Caturello, C. M. O. Bastos, D. Guedes-Sobrinho, M. P. Lima, G. M. Sipahi, J. L. F. Da Silva, J. Phys. Chem. C 122, 20483, (2018).
[4] N. A. M. S. Caturello, R. Besse, A. C. H. Da Silva, D. Guedes-Sobrinho, M. P. Lima, and J. L. F. Da Silva, J. Phys. Chem. C xxx, xxxx (2018).

Luana Sucupira Pedroza - UFABC

Water-solid interfaces

The properties of water at the interface of solid surfaces are crucial in many processes, like electrocatalysts for fuel cells, corrosion-resistant surfaces among other systems. These interfaces are interesting due to the complex ways in which the hydrogen bonding network of water adapts to the presence of a symmetry-breaking interface. However, our atomic level understanding of water adsorption remains unclear and basic questions on the bonding pattern on various surfaces remain unanswered. Therefore, first principles simulations can provide valuable information about water-solid interfaces. In this work we analyze the structural, dynamic and energetic properties water interacting with solid surfaces using first principles molecular dynamics, both in the presence and absence of an external bias potential applied to the solid.

Cedric Leao - UFABC
Title: Homojunctions and heterojunctions in 2D materials

2D materials often come from 3D materiasl in which atomically thin layers are held together through Van der Waals interactions. The isolation of graphene in 2004 open a path for the production of several other 2D materials, which present properties markedly different from their bulk counterparts. Combining the features of 2D layers of different materials has become a new possibility in materials engineering to tailor them for specific technological applications. In this talk we use parameter free computer simulations to exemplify how the combination of the outstanding properties of two different 2D materials result in optimal properties for optoelectronic devices. We analyze experimental data about defects in the interface of bilayer graphene material and show how these defects can present different characteristics from the monolayer. We show that the study of defects in homo and heterojunctions of 2 D materials is an important area of research.

Caetano Miranda - USP

Nano-confined water in interfaces: a fresh and sonic molecular look

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Water-mineral interfaces play a central role in geological and physical-chemical processes such as biomineralization, oil exploration and durability of concrete structures. At nanoscale, the fluids properties may considerable change due to the surface and spatial confinement effects. In this work, we investigate the water and brine confinement on nanopores within different sizes (1 to 6 nm) and materials (silica, calcite and cement). The distinct chemical nature of those surfaces can modify the fluid-solid interaction and the fluid properties under spatial confinement, as well it can also influence the adsorption of other chemical species. To properly investigate the Nano-confined water in those interfaces, molecular dynamics simulations were employed to analyze the hydrogen bond network (HBN) and to calculate NMR relaxation times. Here, we provide new insights with additional atomistically detailed analysis by relating the topology of the hydrogen bond network with the dynamical properties in nanoconfinement interfaces. In complement, the data generated by molecular dynamics over the HBN dynamics was converted in sound to compare and cross correlated the properties over distinct thermodynamic conditions, interfaces and spatial confinement of molecules. Not only, the sonification technique allows us to improve our perception of the molecular behavior of fluids under confinement, but also it can be used as a material for music composition.

Leandro Seixas - Mackenzie

Phase transitions and covalent functionalization in two-dimensional transition metal dichalcogenides

In this talk, we will present recent results on phase transition of two-dimensional transition metal dichalcogenides (TMD), and how covalent functionalization with organic groups (methane, acetic acid and acetamide) can change the stability and energy barrier for phase transitions.

Edison Z. da Silva - UNICAMP

Double Rainbow and the Physics of Clusters: Computer Simulations Meets Experiments

A novel process, the formation and growth of metallic Ag nanowires (NWs) and nanoparticles (NPs) on a-Ag2WO4 upon electron beam irradiation has been discovered and was extensively investigated by different experimental techniques including transmission electron microscopy (TEM) [1-3]. Nucleation and formation of metallic Ag initiates when Ag atoms diffuse from the bulk to the surface. Ag metallic NWs grow on a-Ag2WO4, further observation showed also the formation of Ag NPs during exposition to the electron beam [4]. The present work concentrates in the study and the understanding of physical processes that occur with these new Ag NPs and their interaction. The experiments found the formation of Ag NPs of sizes from 2 to 10 nm. These NPs produced in vacuum, show very interesting behavior displaying coalescence effects [5] where two nearby NPs meet forming other large particles. Mie theory that explains the formation of the Double Rainbow is also responsible for surface plasmon resonance (SPR) effects which explains observed coalescence processes with the NPs. Associating theory and computer simulations we model this evolution process that is driven by SPR due to the electron beam, presenting new and interesting results that help the understanding of the experiments.

References
[1] E. Longo, L. S. Cavalcante, D. P. Volanti, A. F. Gouveia, V. M. Longo, J. A. Varela, M. O. Orlandi and J. Andres, Sci. Rep., 3, 1676 (2013).
[2] J. Andrés, L. Gracia, P. Gonzalez-Navarrete, V. M. Longo, W. Avansi Jr., D. P. Volanti, M.M. Ferrer, P. S. Lemos, F. A. L. Porta, A. C. Hernandes and E. Longo, Sci. Rep. 5, 5391 (2014).
[3] W. da Silva Pereira, J. Andrés, L. Gracia, M. A. San-Miguel, E. Z. da Silva, E. Longo and V. M. Longo, Phys. Chem. Chem .Phys. 17, 5352 (2015).
[4] Longo, E. et al. In situ Transmission Electron Microscopy observation of Ag nanocrystal evolution by surfactant free electron-driven synthesis. Sci. Rep. 6, 21498 (2016).
[5] Giovani M Faccin, Miguel A San-Miguel, Juan Andrés, Elson Longo e Edison Zacarias da Silva. J. Phys. Chem. C, 121 (12), pp 7030–7036 (2017)

Fábio Ribeiro - Cordoba

Understanding hydrodesulfurization at the atomic level: a computational science approach applied to catalysis

Environmental science is nowadays in the spotlight of many researchers due to the necessity to understand and find solutions to the anthropogenic impact on Earth. One of the major air pollutants today is sulfur dioxide (SO_2), that has a direct effect on the atmosphere and human health. SO_2 emissions result from burning fuels with high sulfur content, which is the case of most petroleum products. In order to reduce these emissions, there has been in the last decades an increasing international effort to regulate and limit the amount of sulfur present in fossil fuels and natural gases. The chemical process of removing sulfur from these materials is called hydrodesulfurization, that requires catalysts to speed up the reaction. In particular, a relevant catalyst used by the petroleum industry is MoS_2. For the distilleries, its use is almost irreplaceable due to its low cost and efficiency. MoS_2 has been the topic of many studies, specially in the last 5 years, and its structure has been already characterized by many different methods. Its role as a catalyst for hydrodesulfurization, however, is not well understood yet, and a lot of research has been performed in this matter.

This work focus on the study of the hydrodesulfurization reaction by the MoS_2 catalyst. Several simulation techniques are used to determine the relevant reaction steps and energies, providing an atomic-level description of the whole process, determining why MoS_2 is such a good catalyst for this reaction.

Maurice de Koning - UNICAMP

Glassy Dynamics at Pre-melted Grain Boundaries in Ice Ih

Using first-principles and classical molecular dynamics simulations, we study pre-melting phenomena in pristine grain boundaries (GBs) in proton-disordered hexagonal ice Ih at temperatures just below the melting point Tm. The results are consistent with experimental estimates for the pre-melt layer thickness of low-disorder impurity-free GBs and provide key insight into the mobility of water molecules in the pre-melted layers. In particular, the translational motion of the water molecules is found to be sub-diffusive for time scales longer than 10 ns. Furthermore, it is well-described by a continuous-time random walk model characterized by a waiting-time distribution with a power-law decay, suggesting that the dynamics in the pre-melt layers at GBs in ice I is glassy in nature, even at temperatures close to Tm.

Helena M. Petrilli - USP

Computer simulations of materials through ab-initio electronic structure calculations performed at IF-USP

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Some examples of the research actually performed in our group at IFUSP using ab initio electronic structure calculations in the framework of the Density Functional Theory in the Kohn-Sham scheme will be shown. Currently under study are electronic, magnetic, hyperfine and spectroscopic properties of materials with focus on nanomagnetism, multiferroic, hybrid and systems with nanobiotechnological applications.

Jose Hoyos - USP

Cluster-glass phase in pyrochlore XY antiferromagnets with quenched disorder

We study the impact of quenched disorder (random exchange couplings or site dilution) on easy-plane pyrochlore antiferromagnets. In the clean system, order-by-disorder selects a magnetically ordered state from a classically degenerate manifold. In the presence of randomness, however, different orders can be chosen locally depending on details of the disorder configuration. Using a combination of analytical considerations and classical Monte-Carlo simulations, we argue that any long-range-ordered magnetic state is destroyed beyond a critical level of randomness where the system breaks into magnetic domains due to random exchange anisotropies, becoming, therefore, a glass of spin clusters, in accordance with the available experimental data. These random anisotropies originate from off-diagonal exchange couplings in the microscopic Hamiltonian, establishing their relevance to other magnets with strong spin-orbit coupling.

J. Carlos Egues - USP

Topological and non-topological edge states in quantum dots and Chern Insulators

Common wisdom has it that edge states appear only in topological systems, e.g., topological insulators and topological superconductors. In this talk I will discuss edge states in topological and non-topological InAsBi quantum dots described by a confined Bernevig-Hughes-Zhang model. Interestingly we find that these quantum dots exhibit protected helical edges states both in the topological and non-topological regimes [1]. We also investigate edge states in Chern insulators and find that they display trivial edge states not arising from band topology (Chern number) [2]. We identify the approximate chiral symmetry of the Chern insulator (exact only in the nodal semimetal) as the relevant ingredient behind the appearance of these trivial edge states. This work was supported by CNPq, CAPES, UFRN/MEC, FAPESP, PRP-USP/Q-NANO, German Science Foundation (DFG) via Grant No. SFB 1170 "ToCoTronics" and the ENB Graduate School on Topological Insulators and the Center for Emergent Materials, and NSF MRSEC under Award No. DMR-1420451.

[1] D. R. Candido, M. E. Flatté and J. C. Egues, accepted in Phys. Rev. Lett. (arXiv:1803.02936)
[2] D. R. Candido, M. Kharitonov, J. C. Egues, and E. Hankiewicz, Phys. Rev. B, Rapid Commun. (to appear).

Belita Koiller - UFRJ

Atomically placed P in Si as quantum simulators and transport-based devices*

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Atomically precise placement of dopants in Si permits creating P nanowires by design. High-resolution images show that these wires are few atoms wide with some positioning disorder with respect to the Si structure sites, which is expected to lead to electronic localization. Experiments, however, report good transport properties in quasi-1D P nanoribbons. We investigate their electronic properties using an effective single-particle approach based on a linear combination of donor orbitals (LCDO), keeping the ground state donor orbitals' oscillatory behavior due to interference among the six states at the Si conduction band minima. Our model for the P positioning errors accounts for the presently achievable placement precision [1].

For monatomic chains, we show that electronic properties of donor nanowires in Si can be controlled by design to emulate Hubbard systems. We find that correlation properties remain robust up to 4K, even allowing for some disorder effects [2]. We infer transport properties from the calculated decay length ξ at the half-filling. For 1 to 3 atoms thick wires, ξ shows a rich non-monotonic behavior with respect to target placement parameters. We consider different positioning scenarios to explore how transverse and longitudinal aimed interdonor distances can be chosen to optimize and control the ξ for specific device applications.

Presenting author

[1] Dusko et al Phys Rev B 94, 115425 (2016)

[2] Dusko et al npj Quantum Information 4:1 (2018)

Marcio Varella - USP

Positronic Molecules

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The development of experimental techniques has allowed for the production and manipulation of antiparticles at extremely low energies. A wealth of new science arose from the interactions of such low-energy antiparticles, most notably antiprotons [1], muons [2] and positrons [3], with electrons, atoms and molecules.

One of the most interesting aspects of the research on positrons would be the formation of positronic compounds, i.e., bound states formed in scattering experiments in which a positron attaches to a vibrationally excited molecular core. The formation of about 60 positronic molecules has been reported [4], and theoretical models [5, 6] have also been proposed to describe the attachment and vibrational dynamics underlying the formation of such compounds. New possibilities for low-energy positron Physics and Chemistry also arise from positronium (Ps) manipulation advances. Ps2 molecules [7], Ps−anions [8], as well as laser spectroscopy of Ps and Ps2 [9] are now experimental facts, and even control over annihilation in excited Ps atoms has been achieved [10], among other breakthroughs.

We report on a fundamentally new kind of positronic compounds, which are not formed by positron attachment to stable molecules. Two otherwise repelling atomic anions are bound together by a positron, and the formation of positronic covalent bonds is discussed [11]. The calculations were performed with the Any-Particle Molecular Orbital (APMO) approach [12] implemented in the Lowdin [13] computer code, which has been previously employed to obtain positron binding energies to ordinary molecules [14, 15]. Our results were obtained at different levels of theory and always indicate the existence of stable positron-bonded diatomic molecules. Finally, we will also briefly discuss ongoing studies of solvated Ps atoms.

References

[1] G. B. Andresen et al., Nature 468, 673 (2011).

[2] D. G. Fleming et al., Science 331, 448 (2011).

[3] J. R. Danielson et al. Rev. Mod. Phys. 87, 247 (2015).

[4] G. F. Gribakin et al., Rev. Mod. Phys. 82, 2557 (2010).

[5] G. F. Gribakin C. M. Lee, Phys. Rev. Lett. 97, 193201 (2006).

[6] S. d'A. Sanchez et al., Phys. Rev. Lett. 107, 103201 (2011).

[7] D. B. Cassidy, A. Mills Jr, Nature 449, 195 (2007).

[8] K. Michishio et al., Nat. Commun. 7, 11060 (2016).

[9] D. Cassidy et al., Phys. Rev. Lett. 108, 133402 (2012).

[10] A. M. Alonso et al., Phys. Rev. Lett. 115, 183401 (2015).

[11] J. Charry et al. Angew. Chem. Int. Ed. Engl. 57, 8859 (2018).

[12] S. A. Gonz alez et al. 2008, Int. J. Quatum Chem. 108 1742.

[13] R. Flores-Moreno et al., Int. J. Quatum Chem. 114, 50 (2013).

[14] J. Charry et al., Phys. Rev. A 89, 052709 (2014).

[15] J. Romero et al., J. Chem. Phys. 141, 114103 (2014).

Kaline Coutinho - USP

Caio Lewenkopf - UFF

Quantum thermodynamics: Entropy evolution in strongly coupled mesoscopic systems

We develop a theory of the entropy evolution in time-dependent, strongly coupled electron systems [1]. The formalism naturally avoids the problem of the system-bath distinction by defining the entropy current in the attached leads. This current can then be used to infer changes of the entropy of the system which we refer to as the inside-outside duality. We carry out this program in an adiabatic expansion up to first order beyond the quasistatic limit. When combined with particle and energy currents, as well as the work required to change an external potential, our formalism provides a full thermodynamic description, applicable to arbitrary noninteracting electron systems in contact with reservoirs. This provides a clear understanding of the relation between heat and entropy currents generated by time-dependent potentials and their connection to the occurring dissipation.

[1] A. Bruch, C. Lewenkopf, and F. von Oppen, Phys. Rev. Lett. 120, 107701 (2018).

Eric Andrade - USP

Uncovering novel phases in j=3/2 Mott insulators

Mott insulators with strong spin-orbit coupling are promising candidates for realizing novel phases of matter, for instance, quantum spin liquids. One of the best examples is the effective model for materials with local j=1/2 moments on the honeycomb lattice, the Kitaev-Heisenberg model, whose phase diagram contains a quantum spin liquid with a Dirac spectrum of Majorana fermion excitations. In this talk, I will present phase diagrams of effective models describing j=3/2 local moments, which are relevant, for instance, to Mott insulators with heavy magnetic ions in 4d^1 or 5d^1 configuration. The additional pseudo-orbital degree of freedom contained in this model can potentially enhance quantum fluctuations, via frustrating compass-type interactions or even unexpected SU(4)-symmetric interactions. As an example, I will discuss a possible quantum spin-orbital liquid on the hyperhoneycomb lattice and in the recently synthesized twisted bylayer graphene.

Posters

Willian Natori - USP

The search for exotic states of matter induced by the combined effects of strong correlation and spin-orbit coupling has stimulated the study of transition metal oxides with 4d and 5d elements. We have developed theoretical tools to describe the magnetism of these compounds when the heavy ion is in the d1 configuration in previous works (PRL 117, 017204; PRB 96, 125109). In the present work, we study the effective spin-orbital model that describes the magnetism of 4d1 or 5d1 Mott insulators in ideal tricoordinated lattices (arXiv:1802.00044). The model is displays anisotropic and bond-dependent interactions between multipoles of j=3/2 angular moment operators. However, in the limit of vanishing Hund's coupling, the model has an emergent SU(4) symmetry. We demonstrate that this large symmetry can be made explicit by means of a Klein transformation on pseudospin degrees of freedom. A geometrical criterion for the emergence of this SU(4)-invariance was proposed. Taking the hyperhoneycomb lattice as an example, we employ parton constructions with fermionic representations of the pseudospin operators to investigate possible quantum spin-orbital liquid states. The energies of the projected wave functions were computed using variational Monte Carlo methods. Our numerical results show that the lowest-energy quantum liquid corresponds to a zero-flux state with a Fermi surface of four-color fermionic partons. We also show that this quantum spin-orbital liquid is stable against tetramerization and has a much lower energy than the simplest ordered states even when Hund`s coupling induced perturbations are included.

Pedro M. Cônsoli - USP

Stability of ordered phases of the Heisenberg-Kitaev model in a magnetic field

In 2006, A. Kitaev presented the exact solution of an anisotropic spin-1/2 model with bond dependent interactions on the honeycomb lattice. His work and the following realization that such a system consists of a quantum spin liquid spurred an intense search for materials properly described by this hamiltonian. Once its generating mechanism was understood, it became clear that the Kitaev interaction complements the Heisenberg term in Mott insulators with strong spin-orbit coupling. While the properties of the resulting Heisenberg-Kitaev model have been extensively studied, several questions related to the effects introduced by an external magnetic field remain unanswered. Thus, we apply here spin-wave analyses in order to study the canted zigzag and canted stripy phases subject to a [100]-oriented magnetic field. Besides showing dispersions for both cases, we present a modified phase diagram which includes magnetically disordered phases originated by quantum fluctuations. Finally, we suggest that the same framework be applied to investigate more complex phases which arise in a [111]-oriented field. In particular, interesting candidates for future studies are two vortex phases whose chiral classical configurations might indicate the existence of edge modes, a typical topological signature.

Rui Aquino dos Santos da Silva - UERJ

Dynamical phase transitions in two-dimensional Fermi liquids with quadrupolar interactions

Quantum nematic phases of Fermi liquids have been observed in several highly correlated systems, such as high Tc superconductors, heavy fermions and quantum Hall systems. The isotropic-nematic quantum phase transition can be understood as a Fermi surface instability, driven by attractive quadrupolar interactions. Using bosonization, the non-Fermi liquid character of this transition has been explicitly shown. In this work, we focus on the dynamics of the isotropic phase when the isotropic-nematic transition is approached. For this purpose, we study collective excitations of a two-dimensional Fermi surface considering density-density, as well as quadrupolar interactions.Using a semiclassical approximation in the bosonized theory, we write an evolution equation for Fermi surface fluctuations, analog to the Landau Fermi liquid formalism. By expanding the Fermi surface deformations in an angular momentum basis, the system is reduced to a set of infinitely coupled harmonic oscillators. Each oscillator describes a Fermi surface deformation mode with a specific symmetry. Focussing on the isotropic and the quadrupolar modes, we integrate out all other higher angular momentum components to compute the exact Green's functions. To do this, we use a "decimation" technique. Truncating the system to n modes, we are able to compute a recurrence relation in which the order Green's function is written in terms of the order one. Then, by carefully taking the limit , we compute the exact Green's function. The normal frequencies are computed from .The dispersion relation of the normal modes depends on two Landau parameters, and , that codify the density and the quadrupolar interactions respectively. We compute the dynamical fase diagram, where we display the normal modes in the plane. We show that, in specific regions of the plane, the dynamics of the Fermi surface fluctuations changes abruptly, signalling a dynamical phase transition.

L. Cabral - USP

Azobenzene Adsorption on the MoS2(0001) Surface: A Density Functional Investigation within van der Waals Corrections

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Light sensitive organic molecules, such as azobenzene, has attracted the attention due to their ability to functionalize two-dimensional layered systems and to engineer their electronic structure. Azobenzene is an organic molecule formed by the functional group azo, {N{{ N{ , and two aromatic benzene rings. Here, we study the adsorption properties of the cis- and trans-azobenzene conformations on the molybdenum disulde MoS2(0001) layer [1]. Our investigations are based on density functional theory within the van der Waals corrections to improve the description of the weak molecule-surface interactions. By performing total energy calculations, the stability of the azobenzene in gas-phase and placed on the surface is discussed. We found that the lowest energy configurations are the trans-isomer in gas-phase and the conformations located horizontally on the MoS2(0001) substrate. We observed an increase in the relative total energy among the azobenzene isomers (trans and cis) in the gas-phase and the azobenzene supported on the MoS2(0001) surface, which can be explained by the contact of the two rings of the trans-isomer with the surface. We also analyzed the adsorption energy and work function for each configuration. Thus, our results establish how the azobenzene changes the local environment on the MoS2(0001) monolayer.

[1] L. Cabral, Fernando P. Sabino, Matheus P. Lima, Gilmar E. Marques, Victor Lopez-Richard and Juarez L. F. Da Silva: \Azobenzene Adsorption on the MoS2 (0001) Surface: A Density Functional Theory Investigation within van der Waals Corrections", J. Phys. Chem. C 122, 18895 (2018).

Michel Miranda - USP

Phase Transitions in Frustrated Magnets

Classical Monte Carlo simulations indicate that the Palmer-Chalker--Paramagnet phase transition in easy-plane pyrochlores is of fluctuation-driven first order. This is in striking contrast with experiments which indicates a continuous phase transition. Since the experiments are performed near the quantum phase transition between the Palmer-Chalker and the order-by-disorder ψ_2 phase, we intend to investigate the role played by the quantum fluctuations. Our strategy is to study the effective action for the transition incorporating quantum fluctuations via a $1/S$ (spin-wave) approximation. In this way, we hope to better understand the interplay between quantum and thermal fluctuations in frustrated magnets.

Joao Carlos Gatelina - USP

Scaling of correlation functions of the random XX spin-1/2 chain

We study the spin-spin correlation functions of the random XX spin-$1/2$ chain via an exact numerical diagonalization of the Hamiltonian. Using higher numerical precision, we verified a universal power-law decay of the average correlation function, as predicted by the strong-disorder renormalization-group method. Therefore, recent claims of logarithmic corrections to the scaling are not consistent with our data. We have verified that the typical correlation function decays as a stretched exponential with the distance when measured with respect to the associated localization length. In addition, the associated exponent prefactor of the respective scaling function does not vary significantly with disorder. Finally, we also show that the universal correlation function distribution weakly violates the single-parameter scaling theory.

Denis R. Candido - USP

Edge states across the topological phase transition due to approximate chiral symmetry in quantum anomalous and spin Hall systems

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In this work [1] we demonstrate that a quantum anomalous Hall system [2] (Chern insulator) always exhibits edge states right at the phase transition (except when the system becomes charge-conjugation symmetric), where the Hamiltonian is gapless, and in the vicinity of the topologically trivial and non-trivial gapped phases. We show that the origin of these edge states can be attributed to the approximate chiral symmetry of the Hamiltonian. Additionally, we demonstrate that while the non-trivial quantum Hall topology is responsible only for the existence of these edge states within the energy gap region, the approximate chiral symmetry is the ingredient responsible for the edge state existence in the remaining energy range in both topological and trivial phases. This behavior is described by the realistic one block of the BHZ model [3] of a quantum spin Hall system, which was already noticed [4] but remained unexplained. This work was supported by German Science Foundation (DFG) via Grant No. SFB 1170 "ToCoTronics", the ENB Graduate School on Topological Insulators, CNPq, Capes, FAPESP and PRP-USP/Q-NANO.

[1] Denis R. Candido, M. Kharitonov, J. C. Egues, and E. M. Hankiewciz, Phys. Rev. B 98, 161111(R) (2018)

[2] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).

[3] B. A. Bernevig, T. L. Hughes, and S. C. Zhang, Science 314, 1757 (2006).

[4] J. Li, R.-L. Chu, J. K. Jain, and S.-Q. Shen, Phys. Rev. Lett. 102, 136806 (2009)

Denis R. Candido - USP

Blurring the boundaries between topological and non-topological phenomena in dots

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In this work [1] we first predict using the k.p method and the valence band anti-crossing theory that the common III-V InAs0.85Bi0.15/AlSb quantum well becomes a room temperature 2D topological insulator for well thickness dc>6.9nm. Second, we analytically solve the correspondent BHZ model [2] for our TI by introducing a cylindrical confinement defining cylindrical quantum dots (QDs). Surprisingly, we find for the non-topological QDs "geometrically protected" discrete helical edge states, i.e., Kramers pairs with spin-angular- momentum locking, similar to the topological protected helical edge states within the gap in the topological QDs. We calculate the circulating currents associated to both trivial and topological edge states and find no substantial difference between them. The two terminal conductance calculation for two pairs of edge states as a function of the QD radius and the gate controlling its levels with respect to the Fermi energy of the leads shows a double peak at 2e2/h for both topological and trivial QDs. In conclusion, our results blur the boundaries between topological and non-topological QDs as for the protection of the helical edge states, their calculated circulating currents and their two terminal conductance measurements. This work was supported by CNPq, CAPES, UFRN/MEC, FAPESP, PRP-USP/Q-NANO and the Center for Emergent Materials, an NSF MRSEC under Award No. DMR-1420451.

[1] Denis R. Candido, Michael E. Flatté and J. Carlos Egues, Accepted to Phys. Rev. Lett. (2018)

[2] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Science, 314, 1757 (2006).

Bruno Focassio*, Cedric Rocha Leão - UFABC

Organic cation effect on electronic and optical properties of hybrid organic-inorganic perovskites

We studied the effect of different organic cations on several hybrid perovskites, a promising material for making the absorption layers in solar cells. Perovskite-based solar cells already have comparable efficiency to silicon-based devices and other commercial semiconductors despite being searched for this purpose for a much shorter time. The application of this class of materials, however, is hampered by its degradation upon exposure to high temperature, UV radiation. The degradation of the material can be decreased by engineering the effect of the organic cation placed in the inorganic framework within the perovskite. Hybrid materials combining the inorganic perovskite structures with organic molecules is a way to tune the properties of the material, optimizing then for application in solar cells. It is also a way to slow degradation. We used atomistic parameter free simulations, based on the density functional theory (DFT) to obtain the optimized perovskite structure for different compositions. We based the studies in the inorganic perovskite with formula $CsPbI_3$. This material presents a structure where the cesium (Cs) atoms are surrounded by lead triiodide (PbI_6) octahedrons organized to form a cubic or tetragonal or orthorhombic lattice as a function of temperature. In our study the Cs+ cation was replaced by organic cations: methylammonium (MA), ethylammonium (EA) and formamidinium (FA) and by the inorganic cation Rb +. In each combination, the band gap and absorption coefficient was obtained. Maintaining the composition of the material, the gap decreases with increasing order of crystalline structure, i.e., orthorhombic > tetragonal > cubic, the difference between gaps was lower between MA and EA than for FA and larger for Cs. The cubic structures presented an absorption coefficient more suited to absorb solar radiation.

Krys E. A. Batista - USP

A Theoretical Investigation of 55-Atom Metal Nanoclusters (42 Systems) and the Atomic Radius Role in the Structural Formation of the Pt_nTM_{55-n} TM = Y, Zr, Nb, Mo, and Tc) Nanoclusters

Nanoclusters (NCs) with a diameter size from 1 nm to 2 nm are important in the development of several technological applications and, therefore, the understanding of structural, energetic and electronic properties is fundamental. In this context, Platinum-based NCs have been widely studied due to the possibility to tune the physical and chemical properties as a function of shape, size, chemical composition, etc. However, due to several challenges, such as the identification of ground state structures through experimental and theoretical techniques, the problem becomes complex, making it difficult to understand and requiring more studies. Thus, we performed an *ab initio* investigation of the structural, energetic, and electronic properties of the 55-atoms metal NCs which includes 4 alkali, 4 alkaline-earth, 30 transition, and 4 post- transition metals [1,2]. For 16 systems, we found a strong preference for the compact Mackay icosahedron structure, while 6 systems adopt alternative compact structures such as poly- tetrahedron, and 10 structures, are derived from crystalline face-centered cubic and hexagonal close-packed fragments. However, the 10 remaining systems adopt less compact structures based on the distorted reduced-core structure, tetrahedral-like, and one hexagonal close-packed wheel-type structure [1,2]. The binding energy shows a quasi-parabolic behavior as a function of the atomic number, and hence, the occupation of the bonding and anti-bonding states defines the main trends (binding energy, equilibrium bond lengths, etc). In addiction the binding energy for NCs is, on average, 79% of the cohesive energy of the respective bulk metals. From the results, we combine Pt with TMs from the beginning of the 4d serie (TM = Y, Zr, Nb, Mo, and Tc), searching for the mechanisms that control the Pt localization in the nanocluster [3]. From excess energy analysis we have obtained that the maximum stability is reached at Pt-rich compositions (n = 35−42). The number of hetero- bonds maximizes the charge transfer among the Pt−TM species, and its magnitude depends on the electronegativity difference, coordination, and location (core or surface) of both species. For PtTM in which Pt is slightly larger or has a similar size as the TM atoms (Tc, Mo, and Nb), Pt atoms prefer the surface sites, which helps to release the strain energy. For PtTM in which TM (Zr and Y) is larger than Pt, contrary to what would be expected, there are some Pt atoms in both regions, resulting in a cationic surface. Thus, the release of the strain energy is obtained by symmetry breaking [3].

[1] K. E. A. Batista, et. al. J. Chem. Phys. 144, 054310 (2016).

[2] M. J. Piotrowski, et. al. J. Phys. Chem. C 120, 50, 28844 (2016). [3] K. E. A. Batista, et. al. J. Phys. Chem. C 122, 13, 7444 (2018).

Augusto C. H. Da Silva - USP

Ab Initio Investigation of the Ligand Effects on Core-Shell Nanoclusters: The Example of [(CuAl)55(CP*)1,12]

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Introduction: The compositional and structural variety of the Hume-Rothery phases and their increasing significance in catalytic applications, are the main theme in this project, presenting an ab initio investigation, whose object is to study transition metals nano clusters, combining with group 13 monovalent metal [1]. These systems formed by CuAl have been studied in the context of intermetallic glasses [2], due to their excellent combination of mechanical and magnetic properties, corrosion resistance, and processability [3]. There are open lacks on the understanding of the fundamental physical-chemical characteristics in these systems, the present work is part of a joint effort to elucidate some characteristics of this type of nano clusters [4].**Computational Methodology/Experimental Details:** Our spin polarized density functional theory calculations were performed using the FHI-aims package [4] and the semi-local functional PBE [5]. The Kohn-Shan orbitals were expanded using numerically tabulated atom- centered orbitals (NAOs), with *light-tier2* basis set.

Results and Discussion: The 55-atom CuAl bimetallic nanoclusters were previously studied in our group [7] employing the revised basin-hopping Monte Carlo (RBHMC) algorithm combined with the embedded atom method (EAM). We observed that, once formed the bimetallic nanoclusters, the cluster's shape assumes a nearly icosahedron (ICO) structure. Once the free 55 atoms ICO nano cluster were studied, we carried out the cyclopentadienyl (CP*) coordination studies. For the single CP*/ICO nano cluster, were observed the sigma and pi-oriented binding, with the pi interaction energetically favorable by at least 2.90 eV in relation to the sigma. The magnetic moment for these systems has different values for the free ICO cluster in comparisonwith the coordinated system. The π-coordination changes the magnetic moment values from 3 and 5, to 3 in

both cases, Cu43Al12 and Cu42Al13 systems, respectively. In the σ-coordinated cases, the electron pairing occurs only at the Cu42Al13 system, changing its value from 5 to 3. The CP*-ICO binding energy combined with the electron pairing was observed as the stabilization factor for these systems, once the pi-oriented systems are strongly bonded by at least 1.98 eV, and the systems where was observed the major electron pairing, however, the stability order for the coordinated 55 atoms ICO nano clusters remains the same as the free system, after the CP* unit coordination. The saturated system, with12 CP* units coordination, were consider for the calculations only the systems with Al atoms allocated at the outermost shell on 55 atoms ICO cluster. Was observed that the π-oriented coordination still favorable, inrelation to the σ-oriented, by at least 3.38 eV. The Cu43Al12 system shows slightly short bonding lengths in comparison to the Cu42Al13, average 0.12 Å smaller bonding. The shorter bond lengths go towards the higher CP* bonding energies, observed for the Cu43Al12 system, the values average 0.20 eV per CP* unit higher than the Cu42Al13 system values.

References

[1]. Ganesamoorthy, Chelladurai, Weßing, Jana, Kroll, Clarissa, Seidel, Rüdiger W., Gemel Christian, and Fischer, Roland A., Angew. Chim. Int., **2014,** *53*, 7943-7947.

[2]. Laws, K. J, Laws, Miracle, D. B. and Ferry, M., Nat. Commun. **2015**, *6,* 8123.

[3]. Wang, W. H., Dong, C. and Shek, C. H., Mater. Sci. Eng. R., **2004,** *44*, 45

[4]. Weßing, J., Ganesamoorthy, C., Kahlal, S., Marchal, R., Gemel, C., Cador, O., Da Silva, A. C. H., Da Silva, J. L. F., Saillard, J., Fischer, R. A., Angew. Chim. Int., **2018**, 57, 1.

[5]. Blum, V.; Gehrke, R.; Hanke, F.; Havu, P.; Havu, V.; Ren, X; Reuter, K.; Scheffler, M. *Comput. Phys. Commun.,* **2009**, *180*, 2175-2196.

[6]. Perdew, J. P.; Burke, K.; Ernzerhof, M. Phys. Rev. Lett. 1996, 77, 3865–3868.

[7]. De Souza, Douglas G., Cezar, Henrique M., Rondina, Gustavo G., de Oliveira, Marcelo F. and Da Silva, Juarez L. F., J. Phys.: Condens. Matter, **2016,** *28,* 175302 (12pp)

Priscilla Felício-Sousa - USP

Ab initio Investigation of the Oxide and Mixed Oxide Clusters of Ce and Zr: Energetic, Structural and Electronic Properties

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Transition-metal oxides such as CeO2 and ZrO2 have attracted considerable attention due to the possibility to modulate their physical and chemical properties, which allows an extensive number of applications in nanocatalysts, etc.[1] Thus, it is crucial to obtain an atomistic understanding of the mechanisms that drive the structural formation of those clusters and mixed oxides, which defines the physical and chemical properties. For that, we employed *ab initio* density functional calculations as implemented in FHI-aims combined with the tree-growth scheme and Euclidean similarity distance algorithm, to investigate the (MO2) n clusters with M = Zr, Ce and n = 1-15,[3] as well the mixed $Ce_mZr(15-m)O$
30 clusters for m=0-15.[5] We identified the putative global minimum configurations (pGMC) for all clusters studies upon the total energy screening of several thousand configurations, which provided a deep understanding of the evolution of the structural, energetics, and electronic properties in function of the (MO2) n clusters, and the identification of the magic size clusters by the analysis of the stability function. In general, as expected, the physical and chemical properties approach the bulk values for large values of n. Using atomic configurations obtained for n = 15, the mixed oxides were designed from the pGMC and the bulk fragment. We found negative values for the enthalpy of formation (T = 0 K), which indicates an energetic preference for mixing of those oxides, and the highest stability is obtained for m = 4, which correspond to about 26.6% of ceria, i.e., in close agreement with experimental observations.[6] We found an energetic preference for the Zr atoms have a strong preference for the core region of the particles, which can be explained by the smaller atomic size of the Zr atoms compared with Ce, i.e., it helps to release the strain energy. This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - Finance Code 001, and also supported by FAPESP, project No. 2017/11631-2 and CNPq.

References

[1] Da Silva, J. L. F.; Ganduglia-Pirovano, M. V.; Sauer, J.; Bayer, V.; Kresse, G. Phys. Rev. B, 2007, 75, 045121.

[2] Tian, D.; Zeng, C.; Wang, H.; Luo, H.; Cheng, X.; Xiang, C.; Wei, Y.; Li, K.; Zhu, X. 2016, 671, 208–219 .

[3] Zibordi-Besse L.; Seminovski Y.; Rosalino I.; Guedes-Sobrinho D.; DA SILVA, J. L. F. In review process, almost accepted in *The Journal of Physical Chemistry C*.

[4] Grau-Crespo, R.; de Leeuw, N. H.; Hamad, S.; Waghmare, U. V. 2011, 467, 1925–1938.

[5] Felício-Sousa P.; Zibordi-Besse L.; Mucelini J.; Andriani K. F.; Seminovski Y.; Da Silva, J. L. F. Manuscript in process.

[6] Hosokawa, S.; Imamura, S.; Iwamoto, S.; Inoue, M. 2011, 31, 2463–2470.

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Ising antiferromagnetic quantum critical metal

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We study the non-Fermi liquid that arises at the antiferromagnetic quantum critical point with the Ising symmetry. In order to access the low- energy physics in a controlled way, we use the epsilon-expansion which tunes the co-dimension of Fermi surface [1]. To the leading order in epsilon, a non-Fermi liquid fixed point is found, which is characterized by a set of universal critical exponents. In contrast to the SU(2) symmetric case[2], the velocity of antiferromagnetic spin fluctuations flows to zero faster than the rate at which the Fermi surface becomes nested near the hot spots as the energy scale is lowered. The ratio between the velocities serve as a small parameter which suppresses a large number of higher order diagrams even when epsilon is not small. We comment on possible instabilities of the non-Fermi liquid promoted by the antiferromagnetic fluctuations.

Bibliography

[1] D. Dalidovich and S.-S. Lee, "Perturbative non-Fermi liquids from dimensional regularization," Phys. Rev. B 88, 245106 (2013).

[2] P. Lunts, A. Schlief, and S.-S. Lee, "Emergence of a control parameter for the antiferromagnetic quantum critical metal," Phys. Rev. B 95, 245109 (2017).

Bruno Mello - UFF

Conductance in the Anderson model according to EOM, NCA and OCA methods

In this work, we compare and study the range of validity of the numerical solutions of the single impurity Anderson model (SIAM) using the equation of motion method (EOM) [1], the non-crossing (NCA) and the one-crossing approximations (OCA) [2]. We calculate the conductance in the linear response limit and study its dependence on the chemical potential and on the several energy scales of the problem: interaction, temperature, coupling with the baths, paying special attention to the Kondo and Coulomb blockade regimes. We study the wideband limit. The interest in these methods is justified since they combine good accuracy (depending on the range of used parameters) and a relatively low computational cost. Such features are highly desirable for a full ab-initio (DFT+DMFT) [3] calculation of the transport properties of strongly correlated systems [4], our next goal.

[1] V. Kashcheyevs, A. Aharony, and O. Entin-Wohlman, Phys. Rev. B 73, 125338 (2006).

[2] C. N. Sposetti,L. O, Manuel, and P. Roura-Bas. Phys. Rev. B 94, 085139 (2016).

[3] G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti. Rev. Mod. Phys.7, 865 (2006).

[4] D, Jacob. J. Phys.: Condens. Matter 27, 245606 (2015).

Pamela C. Carvalho - USP

LOCAL MAGNETIC PROPERTIES AND DOMAIN WALL PROFILES OF METALLIC MULTILAYERED SYSTEMS

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In the last decade, the field of nanomagnetism has turned to the understanding of the formation, profiles, and physical properties of domain walls (DWs) due to its possible technological applications [1,2]. For example, the control of the DWs motions can be used on magnetic recording devices. In this case, the information can be interpreted via the DWs motion [1], which replaces the physical rotation of a hard disk. In materials with bidimensional symmetry, the presence of heavy non-magnetic transition metals provide an essential element for the appearance of a sense of rotation for the magnetization [3]: the high spin-orbit coupling, which gives rise to the anisotropic Dzyaloshinskii-Moriya (DM) interaction [4,5]. Then, the DW plane of rotation is determined by the competition between DM and other interactions with magnetic origin. Recently, in a theoretical study, a multilayered system composed by Co/Irn/Pt (n=0,1,2,...,6) has been addressed, and the fact that the presence of Ir can reverse the domain wall chirality from right-handed to left-handed [6] called attention to this system. Motivated by these results, we here use the Real Space - Linear Muffin-Tin Orbital - in the Atomic Sphere Approximation (RS-LMTO-ASA) method [7,8] to investigate the magnetic properties of the Co/Irn/Pt (n=0,1,2...,6) system and other multilayered systems based on the substitution of the Co layer by different transition metal elements, aiming to inspect the formation and profiles of DWs. The RS-LMTO-ASA method is an *ab initio* approach in the framework of the Density Functional Theory (DFT) that has been proven to correctly describe the local magnetic properties of metallic multilayered systems [9].

References

[1] S. S. P. Parkin et al., Science 320, 190 (**2008**).

[2] S. Emori et al., Nat. Mater. **12**, 611 (2013).

[3] M. Heide et al., Phys. Rev. B 78, 140403 (**2008**).

[4] I. E. Dzyaloshinskii, J. Phys. Chem. Solids 4, 241 (**1958**). [5] T. Moriya, Phys. Rev. 120, 91 (**1960**).

[6] G. J. Vida et al., Phys. Rev. B 94, 214422 (**2016**).

[7] S. Frota-Pessôa, Phys. Rev. B 46, 14570 (**1992**).

[8] A. Bergman et al., Phys. Rev. B 73, 174434 (**2006**).

[9] D.C.M. Rodrigues et al., Phys.Rev. B 94, 014413 (**2016**).

Eduardo Diaz Suarez - USP

Insights on the UV-Vis spectra of porphyrins: TMPyP as a study case

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Porphyrins are macrocycle organic compounds with many applications such as photosensitizers for light harvesting and chemical reactions, molecular electronics and enzymatic catalysis. Its optical spectra characterized by the presence of a dominant so called Soret band plus a Q-band structure, whose positions and shapes offer a method to characterize porphyrins in various environments. Here, the electronic and spectroscopic properties of tetracationic 5,10,15,20-tetrakis(1-methyl4-pyridyl)-21H,23H-porphyrin (TMPyP) are investigated in the framework of the DFT and compared to experimental results. For the purpose, a family of GGA and Meta-GGA exchange correlation functionals (E_{xc}) were employed, the modeling of implicit solvent and charge effects. The TMPyP environment tests show that among few conditions studied, the best description of the species was achieved employing water implicit solvent and a +4 total charge state. Afterwards, a systematic investigation on different E_{xc} were carried out, whereas the CAM-B3LYP shown the best fitting for the electronic UV spectrum in comparison to experimental results. Moreover, it was investigated the UV-Vis absorption properties on the geometry of the first excited state. These results allowed us to quantitatively reproduce the Soret and Q-band of the TMPyP. In conclusion, it is possible to infer the TMPyP main electronic transitions and the ring distortion influence the overall structure stability, addressing a new open question to literature regarding its optical mechanism on different environments.

Keywords

DFT, Porphyrin, Excited State, UV-Vis, Torsion Barrier, CAM-B3YLP

Dimitros Voliotios - USP

Multifractal Dimensions in aperiodic quantum spin chains.

Recently has been investigated that the ground-state wave function of the one-dimensional quantum spin-1/2 chain models is multifractal in general with non-trivial fractal dimension. We are studying these phenomena for the quantum Ising chain in the presence of aperiodic perturbation. By performing an analytical block real-space renormalization scheme, we extract the multifractal dimension and spectrum for chains with different wandering exponent. Negative wandering exponent leads the results similar to the uniform chain, while for vanishing exponent, the results vary with the coupling ratio. Finally for positive wandering exponent, we observe a different non-analytical behavior.