

Invited Talks

1 – Heat pumping mechanisms in electronic and phononic systems

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We analyze mechanisms for heat transfer from a cold to a hot reservoir in two kinds of systems: (i) Electronic systems under time-dependent driving by local AC voltages and (ii) Nanomechanical systems under periodic modulation of the sound velocity.

2 – Spontaneous Quantum Hall Effect in Frustrated Magnets

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I will present results on the Kondo Lattice models on a triangular lattice for band filling factors $n=3/4$ and $n=1/4$. We will see that a simple non-coplanar chiral spin ordering with uniform scalar chirality is naturally realized for different coupling regimes of each of the two filling factors under consideration. The $n=3/4$ case corresponds to a weak-coupling instability driven by perfect nesting of the Fermi surface. The $n=1/4$ instability takes place in the intermediate coupling regime. The resulting triple-Q magnetic ordering is a natural counterpart of the collinear Neel ordering of the half-filled square lattice Hubbard model. We will also see that the obtained chiral phase exhibits a spontaneous quantum Hall-effect with $\sigma_{xy} = e^2/h$.

*Work done in collaboration with Ivar Martin and Yasuyuki Kato.

3 – Electronic structure calculations for correlated materials

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Materials with strong Coulomb correlations are challenges for electronic structure calculations. During the last years new methods for their description have been developed. The combination of dynamical mean field techniques with density functional theory allows for the calculation of electronic properties of materials from first principles, taking into account the effect of arbitrarily strong Coulomb interactions.

We will give an introduction to dynamical mean field theory and its use within electronic structure calculations. For illustration, results on transition metal compounds and iron oxypnictides will be described. Finally, we will close by discussing the current limitations and perspectives of how to go beyond current LDA+DMFT techniques.

4 – Density of topological defects across phase transitions

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The state of a system taken through a phase transition is plagued with topological defects, be them domain walls, vortices, monopoles or other depending on the particular case at hand. As the system evolves after the quench their spatial distribution changes and, typically, their density decreases. The mechanisms whereby this occurs depend on the microscopic dynamics. Realizations of such "phase ordering kinetics" in condensed-matter are manifold including the relaxation of vortices in planar magnets or monopoles in magnetic spin-ice, both thermally quenched. The characterization of the density of topological defects has also been of interest in cosmology and the standard description in this context is given by the so-called Kibble-Zurek mechanism. We have critically revisited this theory in two characteristic cases: a second order phase transition with discrete spontaneous broken symmetry [1] and the Berezinsky-Kosterlitz-Thouless infinite order phase transition [2]. In this talk I shall explain our vision of this problem and make some concrete predictions on the time and cooling rate dependence of the density of defects after crossing the phase transition.

[1] Kibble-Zurekmechanism and infinitely slow annealing through critical points, G. Biroli, L.F. Cugliandolo, and A. Sicilia, *Phys. Rev.* **E 81**, 050101 (2010).

[2] Annealing through a Kosterlitz-Thouless phase transition, A. Jelic and L.F. Cugliandolo, in preparation

5 – Electric transport in nanowires and nanotubes

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The transport properties of nanostructures have become the subject of increasing interest. In such systems, quantization effects play an important role, leading novel behaviors. Based on the Boltzmann formalism and within the relaxation time approximation, we have investigated the electronic transport in cylindrically shaped nanowires and nanotubes as a function of their geometry. We have analytically shown that, due to the quantization of the carrier angular momentum L , the axial conductivity can be written as a sum of contributions associated with each of the allowed values of L . The number of terms in the sum, and consequently the number of allowed angular momentum, is determined by the geometry of the wire or tube, in particular by its external radius. The analogy between the observed behavior and the Shubnikov-de Haas effect is pointed out. We have extended the theory so as to include the effects of an externally applied magnetic field parallel to the tube axis.

6 – Switchable magnetization and polarization using multiferroics

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Multiferroic-based materials and heterostructures hold promises of potentially relevant functionalities. Most of them are based on the fact that these materials could show the ability of switchable ferroelectric polarization by a magnetic field or the magnetic polarization by an electric field. However, due to the weak coupling of both magnetic orders distinct approaches are required for each purpose. Interface coupling between multiferroics and ferromagnets appear to be a very promising tool to achieve sizable electric control of the magnetization. Coupling may be mediated by the exchange interaction between a multiferroic antiferromagnet and a suitable ferromagnet and it can express itself as an exchange bias field. Enormous progress has been achieved using this approach to modulate magnetization of the ferromagnetic layer. However, important issues remain to be addressed. For instance, the relative role of antiferromagnetic domains or domain walls as microscopic mechanisms of exchange bias, or the contribution of the accompanying strain effects associated to ferroelasticity. In this presentation we shall overview some of recent progress. It will be shown that using judiciously chosen materials, ferroelastic contributions can be avoided thus leading to purely electric effects on exchange bias and, in turn, on the magnetization of a neighbouring ferromagnetic layer. Moreover, we will show that switching and resetting of the exchange bias and magnetization can be done isothermally using appropriately shaped electric pulses. A framework for understanding these streaking effects will be discussed. On the other hand, switching the ferroelectric polarization by an appropriate magnetic field could also lead to novel applications. Most probably this would require using of thin films. Here we will show that magnetically switchable polarization is observed in YMnO_3 thin films.

7 – Electron localization in cerium oxide-based materials

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In the many applications of ceria-based materials in heterogeneous catalysis, the reducibility of ceria is essential to the catalytic function. Moreover, the well-known strong influence of the support on the reactivity of ceria supported vanadium oxides (VO_x) in several important oxidation reactions is yet not understood. To this end, we apply density-functional theory (DFT) with the HSE hybrid functional as well as the DFT+U approach to study the $\text{CeO}_2(111)$ surface [1] and $\text{VO}_n/\text{CeO}_2(111)$ model catalysts ($n=0-4$)[2,3]. To compare their catalytic activity in oxidation reactions, we calculate the energy of oxygen vacancy formation (which relates to the reaction energy), and the energy of hydrogenation (which relates to the energy barrier of the rate determining step). We show that subsurface vacancies at the $\text{CeO}_2(111)$ surface are energetically more favourable than surface ones, and thus provide support for the most recent experimental result [4]. Additionally, we combine DFT with statistical thermodynamics and discuss the stability of VO_n species as function of the oxygen partial pressure and temperature. We argue that the high catalytic activity of vanadia supported on ceria has its origin in the ability of ceria to stabilize reduced states by accommodating electrons in localized f-states, which is promoted by the supported vanadia species. We further show that the preference for subsurface vacancies and the stabilization of the +5 oxidation state of vanadium upon reduction, are the result of defect-induced lattice relaxation. The relaxation effects are crucial to the localization of the electrons left behind upon oxygen removal driving the $\text{Ce}^{4+} \rightarrow \text{Ce}^{3+}$ reduction. Besides, we find that vacancies at the $\text{CeO}_2(111)$ surface are likely to be bound to Ce^{4+} ions rather than to Ce^{3+} as priorly suggested.

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[1] M.V. Ganduglia-Pirovano, J.L.F. Da Silva, J. Sauer, Phys. Rev. Lett. **102**, 026101 (2009).

[2] M. Baron et al., Angew. Chem. Int. Ed. **48**, 8006 (2009).

[3] M.V. Ganduglia-Pirovano et al., J. Am. Chem. Soc. **132**, 2345 (2010).

[4] S. Torbrügge et al., Phys. Rev. Lett. **99**, 056101 (2007).

8 – Structural and electronic pressure-temperature phase diagram of the new iron based superconductors

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The discovery of superconductivity in the iron based compounds had a great impact on the condensed matter community. The superconducting state evolves from a antiferromagnetically ordered state by doping or by application of an external pressure on the parent compounds. Up to now a lot of effort has been devoted to these materials but there are still a number of unsolved questions concerning the appearance of superconductivity. The study of the crystalline structure, transport properties and electronic structure under pressure is a powerful tool that helps to find clues to analyze the superconducting state. We have studied the effect of structural parameters under pressure on the superconducting properties on compounds belonging to the five representative Fe based families. In particular, we reported the evidence of different structural phase transitions under pressure, for example in the case of FeSe the high pressure phase induce an increase in the superconducting transition temperature (TC) with a maximum at 34K. We have also performed high pressure experiments in other compounds from the 111, 122 and 1111 families. The effect on TC of some characteristics parameters under pressure, like the inter(intra)layer distance, the angle Fe-As(Se)-Fe, interstitial ion ordering will be discussed in detail.

9 – Switching currents through molecules

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We investigate the zero-bias and zero-temperature conductance through π -conjugated annulene molecules weakly coupled to two leads for different source-drain configurations. We find an important reduction in the current for certain transmission channels and for particular geometries as a consequence of destructive quantum interference between states with definite momenta. An abrupt increase of the conductance occurs when translational symmetry is broken by an external perturbation, thus leading to the possibility of a large switching of the conductance through single molecules.

10 – Manipulation of Charge, Spin and Conformation in Single Atoms and Molecules

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We combine a variety of scanning tunneling microscope (STM) manipulation schemes with tunneling spectroscopy techniques to investigate and to manipulate properties of atoms and molecules on surfaces. This talk will include our recent results and achievements: In spintronic area, we will show that a magnetized STM tip can be used not only to manipulate individual atoms maintaining magnetic contrast but also imaging of their spin directions is possible [1]. In nanoscale superconductivity area, we will present the smallest molecular superconductor ever studied to date. Here, the finding of superconductivity in just four pairs of (BETS)2-GaCl₄ molecules opens the possibility of investigating superconducting phenomena locally[2]. In molecular machines area, entangled and synchronized rotations of artificial molecular rotors operated by using the electric field from an STM tip will be presented. These experiments are innovative, and are tailored to address several critical issues covering both for fundamental understanding, and for demonstration of novel atom/molecule based nanodevices.

[1]. D. Serrate, P. Ferriani, Y. Yoshida, S.-W. Hla, M. Menzel, K. von Bergmann, S. Heinze, A. Kubetzka, and R. Wiesendanger. Imaging and Manipulating the Spin Direction of Individual Atoms. *Nature Nanotechnology* **5** (2010) 350-354.

[2]. K. Clark, A. Hassanien, S. Khan, K.-F. Braun, H. Tanaka, and S.-W. Hla. Superconductivity in Just Four Pairs of (BETS)2-GaCl₄ Molecules. *Nature Nanotechnology* **5** (2010) 261-265.

11 – What is measured in the scanning gate microscopy of a quantum point contact?

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Peeping electrons going by is one of the most fascinating issues of Quantum Mechanics. Attempting such an experiment in a solid-state environment, like in a two-dimensional electron gas, involves subtle ingredients such as decoherence and many-body effects, as well as cross-talks and other technical limitations. The conductance changes measured under the influence of a local perturbation (e.g. Scanning Gate Microscopy, SGM) have often been interpreted in the last decade as a mapping of the electron current density along a nanostructured device. In agreement with the dictates of Quantum Mechanics, our perturbative analysis shows that the SGM measurements in a phase-coherent nanostructure are not given by a local quantity, but by two scattering states impinging from opposite electrodes [1]. In the case of a Quantum Point Contact (QPC) exhibiting conductance quantization, the first-order contribution for weak tip voltages is significant only on the conductance steps, while the second-order correction is the dominant one on the plateaus. The latter contribution is always negative, exhibits fringes, and has a spatial decay consistent with SGM experiments on QPC.

[1] "What Is Measured in the Scanning Gate Microscopy of a Quantum Point Contact?" R.A. Jalabert, W. Szewc, S. Tomsovic, and D. Weinmann, *Phys. Rev. Lett.*; in press.

12 – Electric pulse induced resistance switching in oxide - metal junctions

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We investigate the electric pulse induced resistance switching in oxide - metal contacts at room temperature. Using a multiterminal configuration, we find a "complementarity" effect where the contact resistance of pulsed electrodes at opposite ends -a non volatile memory device- show variations of opposite sign. These reversible variations are further studied using different electric protocols, to show properties of each electrode. We discuss the mechanism driving the effect both on LaPrCaMnO and TiO samples contacted with Ag electrodes, based on old [1,2] and recent [3] results.

[1] Quintero, Leyva & Levy, *APL* **86**, 242102 (2005)

[2] Quintero, Levy, Leyva & Rozenberg, *PRL* **98**, 116601 (2007).

[3] Rozenberg, MSánchez, Weht, Acha, GMarlasca & Levy, *PRB* **81**,115101 (2010); Ghenzi, MSánchez, GMarlasca, Levy & Rozenberg, *J. Appl. Phys.* **107**, 093719 (2010).

13 – Sub-wavelength photonics: controlling near-field interactions between nanosystems.

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Metallic and dielectric objects are surrounded by fluctuating electromagnetic fields due to thermal and quantum fluctuations of the charge and current density at the surface of the bodies. Immediately outside the objects, this electromagnetic field exists partly in the form of propagating electromagnetic waves and partly in the form of evanescent waves that decay exponentially with distance away from the body's surface. These fluctuating electromagnetic modes are responsible for a great variety of near-field phenomena such as the Van der Waals force, the Casimir force, near-field heat transfer, and non-contact friction forces. As devices evolve from micro- to nanoscale structures, these forces become relatively stronger, and their effect cannot be disregarded any further. To improve our understanding of these near-field interactions and to develop mechanism to control them, is extremely important for a diversity of seemingly different fields, such as nanomechanics, quantum computing with trapped ions, measurements of gravitational forces at the nanometer scale, and detection of single spins for magnetic resonance force microscopy. In this presentation I will describe the fundamentals of near-field forces, I will review recent scientific advances regarding manipulation of these interactions, and I will illustrate novel applications that could be enabled once we are capable of control these forces.

14 – What is wrong with DFT ?

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Electronic-structure modeling has become a very powerful tool to understand, predict, or design the properties of complex materials and devices. It is also an imperfect tool, with many open and urgent challenges in our quest towards qualitative and quantitative accuracy, and in our ability to perform quantum simulations under realistic conditions.

Several of these challenges stem from the remnants of self-interaction in our electronic-structure framework, leading to qualitative failures in describing e.g. mixed-valence complexes, electron-transfer excitations, and even single-particle energies. I'll discuss these effects in realistic case studies, and suggest possible solutions based on constrained DFT, on extended Hubbard functionals, or on imposing a generalized Koopmans' condition. I'll also highlight how the calculation of magnetic properties (NMR/EPR) or the use of wavefunction techniques can provide stringent validation criteria for novel developments.

15 – s_{\pm} Pairing Symmetry and Pairing Mechanism in Fe-based Superconductors

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I will briefly explain the basics of the spin-fluctuation induced superconductivity, and will discuss the Fe-based superconductors (FeBSC) in comparison with the cuprates and MgB₂. I will emphasize the interplay between the Fermi surface geometry and the structure of the spin fluctuation spectrum in the momentum space, and explain why it was so easy to come up with the basic prediction of the s_{\pm} superconductivity, and why physically very different models appear to lead to the same pairing symmetry.

16 – Frontiers in Spin Polarized Tunneling

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Electron tunneling phenomenon has richly contributed to our understanding of various branches of physics over the years. Spin polarized tunneling (SPT), sensing of the spin polarization of tunneling electrons using a spin split superconducting spin detector, discovered by Meservey and Tedrow forty years ago has led to many recent breakthroughs. SPT has set the field of spintronics into an extremely active field since many years. In this overview talk we will cover the field starting from its origin to tunnel magnetoresistance (TMR) effect, spin filtering, spin tunneling in organic semiconductors to tuning of superconducting state with spin current. Electrical spin injection/detection in a semiconductor including graphene, currently one of the most active areas, is strongly believed to succeed through the SPT approach. The successful observation of a large change in tunnel current in magnetic tunnel junctions (MTJ) in the mid nineties has brought extreme activity in this field - from the point of fundamental study to extensive application in mind (as sensors, nonvolatile memory devices, logic elements etc).

Work done in collaboration with Drs. Meservey and Tedrow, PhD students, postdoctorals, as well as high school students and undergraduates. NSF, ONR, DARPA and KIST-MIT project funds supported the research over the years.

[1] “*Spin Polarized Electron Tunneling*”, R. Meservey and P. M. Tedrow, *Phys. Rep.* **238**, 173 (1994)

[2] “*Frontiers in Spin Polarized Tunneling*”, J. S. Moodera, G-X. Miao and T. S. Santos, *Physics Today* p46 (April 2010)

17 – Competing Pairing Symmetries in a Generalized Two-Orbital Model for the Pnictides

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An extended “ t - U - J ” two-orbital model for the pnictides will be discussed. The Hamiltonian consists of the standard two-orbital Hubbard model plus additional Heisenberg terms, arising from the strong coupling expansion, that render the $(\pi, 0)$ spin order in the undoped limit very robust. This stabilizes electronic bound states even in the small clusters that are studied via the Lanczos algorithm. Focussing on the symmetry of these bound states and varying couplings, it will be shown that the A_{1g} pairing dominates at intermediate and large Hubbard U while B_{2g} is stable at small U . In addition, dynamical pairing susceptibility calculations also unveil low-lying B_{1g} states in the model, suggesting that small changes in parameters may render any of the three channels stable. These numerical results are in agreement with RPA studies, although addressing the problem from quite a different perspective, and they provide a rationalization for the puzzling material/technique dependent results in pnictides where both nodeless and nodal states have been reported.

18 – Structure of MgO nano-islands on metallic substrates: A semi-empirical, order N , Hartree-Fock simulation

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In the last decade, there have been intense efforts to synthesize ultra-thin oxide layers deposited on metal substrates. It has been recognized that, in most cases, their properties largely differ from their bulk analogues, and may be tuned as a function of orientation, thickness and support characteristics. In addition, lateral confinement gives additional degrees of freedom for engineering artificial objects. However, at small sizes, nano-objects are strongly influenced by the interaction with the substrate, both electronically and structurally. This raises questions related to epitaxial growth, formation of Moiré patterns, presence of interfacial dislocations, and elastic relaxation at the interfaces. In order to decipher the microscopic mechanisms involved, atomistic numerical simulations are of great help. They can complement other approaches based on linear elasticity or theoretical models such as the Frenkel-Kontorova model. However, atomistic simulations of nanooxides are presently subject to either severe size limitations if first principles methods are used, or suffer from a limited or absent account for the electronic degrees of freedom if classical methods are chosen (extended Born models, chemical potential equalization, etc). We have developed a semi-empirical Hartree-Fock simulation code, which scales quasi-linearly with the system size. It correctly treats the self consistent relationship between the charge distribution and the electrostatic potential acting on the electrons. The adjustable parameters are fitted as to reproduce experimental or first principles results on several periodic systems and on a variety of small clusters. In order to achieve order N scaling, a “divide and conquer” strategy is adopted. We will present the basis of the method, and discuss the epitaxial properties of metals-supported MgO square islands. We will discuss commensurability locking, interface dislocations, island magicity and local electronic properties. We will also show how these properties evolve as a function of the strength of interaction with the substrate and the lattice mismatch, thus producing a “phase diagram” in which size effects will be discussed. Finally, we will make a link with recent experimental results of MgO clusters or layers deposited on Ag(100) and Mo(100).

19 – Physical origins of the dependence of T_c on the As-Fe-As angle in iron superconductors : the 1111 and 21311 cases

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Early in the study of high temperature superconducting compounds it was established that the superconducting transition temperature T_c was strongly dependent with the As-Fe-As angle of the FeAs₄ tetrahedron: T_c was maximal for regular values ($109^\circ 47'$) of the angle. Several theories were put forward to explain this behavior, all based on particular details of the band structure, that were supposed to be universal, i.e. applicable to all systems, as the empirical T_c vs angle relationship was based on recollections of data from different samples or measurements of different groups. To verify this relationship, we have started a systematic study of the behavior of different compounds under pressure. We are able to follow under pressure both the superconducting T_c by electrical resistivity measurements, and the evolution of the structure through synchrotron radiation measurements. We can then calculate the electronic band structure on the measured atomic positions at each pressure to follow the electronic properties. This method allows us to determine in each particular case the physical cause behind the relationship, that does not seem to be universal. For superconducting Sm-1111 it turns out to be a charge transfer issue, that is optimized under pressure. While for superconducting Sr₂VO₃FeAs it is associated to the disappearance of multiple nesting features when the tetrahedron becomes irregular under pressure and the degeneracy of the bands is broken. Our results call for more general symmetry related reasons to explain the relationship, that would then appear through different ways in different compounds.

20 – Magnetic structure and superexchange pathways in CsV₂O₅

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The study of low dimensional spin-1/2 quantum systems has been a very prolific field of condensed matter physics during the last decades. The family of vanadates, in particular, has provided a rich variety of compounds with different behaviours and topologies.

Their magnetic structure and properties are primarily determined by the magnitude and the sign of the different exchange couplings arising between magnetic ions and therefore on the very details of their atomic and electronic structures. The sole consideration of the topology of a compound, based on idealized crystal structures, is often incomplete and even misleading.

In this work, the magnetic properties of the layered compound CsV₂O₅ have been investigated using density-functional calculations. The results show that this compound is built from strongly dimerized alternating chains oriented along the **c** axis. Moreover, we demonstrate that the largest interaction along the chains direction arises *between* the structural dimers, involving a superexchange pathway through the covalently bonded V⁽⁵⁺⁾O₄ bridging groups. These results should motivate further experimental investigations of the magnetic excitations in this compound.

21 – Scanning Tunneling Microscopy and First-Principles Theoretical Study of Manganese-induced Stripe Phase Superstructures on GaN(0001)

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The formation of magnetic nanostructures on semiconductor surfaces is a topic of considerable fundamental as well as technological interest. Gallium nitride is a next-generation semiconductor material with a bright future in optoelectronics; yet this material will also be of great interest for spintronics if it is possible to combine spin functionality with its amazing electronic properties. For this reason, we have explored the epitaxial growth of Mn on the pseudo-1x1 surface of gallium polar GaN(0001). At the appropriate deposition temperature near 250 °C, we find that Mn incorporates into the surface at sub-monolayer coverages first in narrow stripe phases having a Mn zig-zag $4 \times \sqrt{3}$ structure oriented along $[10\bar{1}0]$ surrounded by a sea of pseudo-1x1; while at higher coverage (but still less than 1 ML), the surface shows wider Mn stripe phases having $\sqrt{3} \times \sqrt{3}$ - R30° type structure. We explore both the narrow and wide stripe superstructures using a combination of scanning tunneling microscopy and first principles theory. Various models are considered for the wide stripe phases having $\sqrt{3} \times \sqrt{3}$ - R30° structure, including both adatom and substitutional models. Surprisingly, first principles theory using LDA/GGA + U finds that the lowest energy structural model is instead a rotated, in-plane structure. Such a novel structure has not previously been reported for Mn/GaN. The calculated spin-polarized local density of states is best fit to the experimental data using $U = 6$ eV, resulting in a dip and strong spin polarization near the Fermi level. Theory also finds a similar in-plane type model for the narrow $4 \times \sqrt{3}$ stripe structure; results are compared with the STM data, and in this case an antiferromagnetic ground state is calculated, consistent with STM images showing an asymmetry between the two Mn atoms of the Mn zig-zag chain.

22 – Spin orbit effects in quantum point contacts and quantum dots: from current polarization to Kondo effect

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The basic elemental unit in many electronic quantum devices, the *quantum point contact* (QPC), has been recently studied in systems where the spin-orbit interaction is relatively strong. In particular, we investigate how a *lateral* spin-orbit coupling, introduced by asymmetric lateral confinement potentials defining the QPC, affects the spin polarization of the current. We find that even in the absence of external magnetic fields, a variable nonzero spin polarization can be obtained by controlling the asymmetric shape of the confinement. These results suggest an approach to produce spin-polarized electron sources. Furthermore, this asymmetry-induced polarization provides a plausible explanation of recent observations of a “half” conductance plateau (in units of $2e^2/h$) in QPCs made on InAs quantum-well structures [1]. However, our estimates for the magnitude of such effect for realistic spin-orbit interaction strength in these systems do not support this explanation, and point to the important role that electron-electron interactions play in these systems [2].

This conclusion motivates our recent work incorporating the spin polarization of QPC tunneling in these structures. We discuss how even for slightly polarized injection, the Coulomb blockade and Kondo regimes of a quantum dot created with these QPCs are profoundly affected. We predict strong current polarization, intrinsically enhanced by the electronic interactions in the dot. The system behaves essentially as if the current were injected via ferromagnetic leads, despite the *total absence* of magnetization or magnetic fields. In particular, we show that while the Kondo effect is substantially affected, it remains strong and yet the resulting conductance exhibits spin polarization even for unpolarized current injection [3].

Supported by NSF MWN/CIAM and PIRE.

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23 – Atomic resolution views of complex oxide materials

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The success of aberration correction in the scanning transmission electron microscope (STEM) is revolutionizing the study of materials, especially those containing light atoms such as C based materials such as graphene or transition metal oxides. These are fascinating systems that exhibit the most disparate physical behaviors such as colossal magnetoresistance, orbital and/or charge ordering, magnetoelectronic phase separation or high T_c superconductivity to just name a few. Thanks to their relatively large lattice parameters and the fact that both O and transition metals exhibit absorption edges well within the reach of modern electron energy loss spectrometer (EELS) optics, they are ideal systems for such types of electron microscopy studies. Since many of the aforementioned phenomena exhibit characteristic length scales in the nanometer regime, they are affected by reduced dimensionality (e.g., thin films or heterostructures), proximity to other materials, or depend on nanometric active regions (e.g., defects, interfaces, etc.). Understanding such phenomena must therefore rely heavily on probes capable of studying simultaneously the structure, chemistry and electronic properties with atomic resolution in real space, such as STEM-EELS. In this talk the state-of-the art of the technique will be reviewed along with a number of applications to transition metal oxide interfaces based on perovskites. Examples such as the imaging of subtle O displacements across LaMnO₃/SrTiO₃ (LMO/STO) interfaces will be discussed. The LMO/STO relative layer thickness ratio changes the degree of epitaxial strain within the layers and dramatically affects the physical properties of the system, which can be tuned from insulating, mild ferromagnetic, to metallic ferromagnets. While STO is a cubic perovskite, LMO is characterized by a strong Jahn-Teller distortion and orbital ordering at low temperatures. We will show how the octahedral distortions of relaxed LMO layers can be tuned through different degrees of epitaxial strain and affect the O sublattice of ultrathin STO layers. These results will be discussed and combined with density functional theory, in connection with the magneto-transport properties.

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24 – Growth and magnetic properties of embedded Co nanowires with diameters in the 3-5 nm range.

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In this contribution, we report on the growth of embedded Co nanowires with diameters in the 3-5 nm range and length up to 400 nm. Such nanowires were observed to form spontaneously upon pulsed laser deposition of CoO and CeO₂ on SrTiO₃(001) in reducing conditions. The obtained samples consist in Co nanowires embedded in an epitaxial CeO₂/SrTiO₃(001) film exhibiting good crystalline quality. The structure of the Co nanowires was characterized by high resolution transmission electron microscopy and extended x-ray absorption fine structure. The nanowires orientation, diameter and internal structure depend sensitively on the growth conditions. The magnetic properties of these objects will be discussed in connection with their structure with a particular emphasis on the magnetization reversal.

This work has been supported by the Region Ile-de-France in the framework of C'Nano IdF. C'Nano IdF is the nanoscience competence center of Paris Region, supported by CNRS, CEA, MESR and Region Ile-de-France.

Talks

25 – Structural and magnetic properties of $\text{La}_2\text{CoMnO}_6$ produced by combustion synthesis

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Multiferroics (MF) are a class of materials which can exhibit both magnetic and electrical order. The coupling between these ordered states can be used in many technological applications such as magnetoelectrics random-access memory and magnetic field sensors. The main problem for the use these materials is the weak magnetoelectric coupling at room temperature, this can be attribute to the antiferromagnetic state present in many materials. The rare-earth manganites doped with Co and Ni are adequate materials to develop applications with these compounds. The preparation conditions are decisive key for the magnetic and electrical properties of these materials. In this context, we present the process of preparation of $\text{La}_2\text{CoMnO}_6$ synthesized by the combustion method, structurally characterized by X-ray diffraction complemented by Rietveld analysis and magnetically characterized by SQUID magnetometry. The powders obtained by combustion process were thermally treated between 800°C – 1300°C . The samples were submitted to three different heat treatment. The crystalline structure changes according to the heat treatment. The temperature dependence of the magnetization reveal that sample can presents a ferromagnetic order at 225 K or a ferromagnetic order at lower temperatures, bellow 170 K, according to the heat treatment. All samples are exhibits strong irreversibility in ZFC/FC sequences of measurements. And there are strong evidences of a new magnetic order at lower temperatures, which can either be a spin-glass or a weak antiferromagnetic phase.

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26 – Kondo effect vs RKKY in real lattices: A DMRG and ECA study

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Magnetic interactions between strongly correlated impurities coupled to a sea of conduction electrons is a subject of great interest from both, experimental and theoretical studies. When many magnetic impurities are attached to the same conduction band a rich phase diagram can arise. By one hand the magnetic impurities can be strongly coupled to the spin of the electrons of the conduction band forming a singlet. This is the well known Kondo effect. By the other, through electron of the conduction band, a spin-spin interaction between the impurities can appears as a consequence the Rutherford-Kittel-Kasuda-Yosida interaction. In this later case a singlet state between the impurities will appears. This new singlet will compete with the singlet formed by the Kondo effect. In this two effects is important the well description of the electrons with energy close to the Fermi level. Systems like the square lattice, with a van-Hove singularity at the middle of the band, or Graphene, with Dirac electrons, or Carbon nanotubes with multiple bands and multiples van Hove singularities need a proper description of the electrons in the lattice Hamiltonian.

In this work we present a numerical method to study problems with several magnetic impurities coupled to arbitrary lattices. First we separate the Hamiltonian in two parts. One part that contains the impurities and the coupling with the band and the other that have just the lattice Hamiltonian. Using the lattice sites that couples to the impurities as seed in a Lanczos-type procedure we manage to map the real-space lattice Hamiltonian into a ladder type Hamiltonian. This canonical transformation, known as block Lanczos tri-diagonalization, can be now solved using different numerical techniques as DMRG or ECA. This method is not restricted to analyze barvais lattice Hamiltonians but a wide variety of systems as a Bethe lattice or even systems with disorder can be also studied.

To introduce this method we will present a study of the competition between the Kondo effect and the RKKY interaction in a square and a rectangular lattices.

27 – Extraordinary Hall Effect on Fe-rich amorphous thin films and Fe-rich/Cu multilayers

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The extraordinary Hall effect (EHE), a spin-dependent scattering phenomenon observed in ferromagnetic materials occurs because the asymmetry of magnetic scattering is proportional to magnetization. Interest has been growing for thin films with potential applications as magnetic sensors or memory devices using the EHE. Ferromagnetic amorphous alloys are known to have a high degree of magnetic disorder and are good candidates for increasing spin-orbit scattering, a key ingredient for enhancing the EHE. In this study we investigated the magnetic and transport properties of thin Fe-rich amorphous films and Fe-rich/Cu multilayers. We compared the extraordinary Hall effect (EHE) in these two types of samples and discussed it in terms of thickness and sample structure. The thicker films exhibited stripe magnetic domains and a strong in-plane magnetic anisotropy. Decreasing film thickness reduced in-plane anisotropy while both saturated Hall resistivity and Hall sensitivity increase. A Hall resistivity value of 20 microOhm.cm is observed in 100 nm thick Fe-rich films at 12 K and a sensitivity of 1.3 Ohm/T is obtained at room temperature. Electrical conductance increases and Hall resistivity decreases when the films are sandwiched with Cu. EHE measurements at low temperatures provide hints on the magnetic response of the multilayers.

28 – Role of local correlation effects in bcc Fe, hcp Co, and Mn doped GaAs.

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The strength of local electronic correlation effects in the spin-dependent electronic structure of ferromagnetic bcc Fe and hcp Co has been investigated by means of the LDA+DMFT (local density approximation combined with the dynamical mean-field theory) scheme, and compared with spin and angle-resolved photoemission spectroscopy. Although strong improvements are seen with respect to standard one-particle theory, still a perfect quantitative agreement cannot be reached. In particular strong differences are found between the quasiparticle lifetimes and the corresponding linewidths of the experimental spectrum. These differences cannot be explained as non-electronic contributions, and are shown to be stronger for Fe and weaker for Co, suggesting that they become weaker with increasing of the atomic number. A possible explanation can come from the neglected non-local correlation effects, as pointed out by recent experimental studies.

Finally preliminary results on the application of the LDA+DMFT scheme to the dilute magnetic semiconductor Mn doped GaAs are presented. The spectral and magnetic properties of this material are calculated for several different dopings, and compared with standard *ab-initio* simulations by means of density-functional theory.

29 – Grazing Incidence Fast Atom Diffraction: a new in situ technique to study the Molecular Beam Epitaxy growth

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We have discovered and developed an alternative technique to investigate the growth morphology of thin films, in situ and in real time, based on grazing incidence scattering of high energy atoms. This technique, named GIFAD for grazing incidence fast atom diffraction, uses the same geometry as reflection high energy electron diffraction but is less invasive, more surface sensitive, and readily interpretable quantitatively. In order to test it we have specially customized a molecular beam epitaxy (MBE) growth machine. I will present the basis of this new technique and the first results obtained for a semiconductor prototypical II–VI compound, ZnSe(001). Besides providing lattice parameter with high accuracy, we show that GIFAD gives straightforward access to the surface valence electron density profile, allowing clear identification of an electron transfer from Zn to Se. Also, the last results of surface and growth studies of GaAs epilayer with the new MBE –GIFAD growth equipment will be presented.

30 – Electronic and structural distortions in graphene induced by carbon vacancies and boron doping

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We present an ab initio - DFT/GGA - study on the structural and electronic distortions of modified graphene by creation of vacancies, inclusion of boron atoms, and the coexistence of both, by means of total energy and band structure calculations. In the case of coexistence of boron atoms and vacancy, the modified graphene presents spin polarization only when B atoms locate far from vacancy. Thus, when a boron atom fills single- and di-vacancies, it suppresses the spin polarization of the charge density. In particular when B atoms fill a di-vacancy a new type of rearrangement occurs, where a stable BC₄ unit is formed inducing important out of plane distortions to graphene. All these findings suggest that new chemical modifications to graphene and new type of vacancies can be used to modify its electronic properties. [1] Faccio, R. et al. J. Phys. Chem. 2010 (in press)

31 – Local Quasiparticle Density of States of Superconducting $\text{SmFeAsO}_{1-x}\text{F}_x$ Single Crystals: Evidence for Spin-Mediated Pairing

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We probe the local quasiparticles density of states in micron-sized $\text{SmFeAsO}_{1-x}\text{F}_x$ single crystals by means of scanning tunnelling spectroscopy. Spectral features resemble those of cuprates, particularly a dip-hump-like structure developed at energies larger than the gap that can be ascribed to the coupling of quasiparticles to a collective mode, quite likely a resonant spin mode. The energy of the collective mode revealed in our study decreases when the pairing strength increases. Our findings support spin-fluctuation-mediated pairing in pnictides.

32 – Unconventional magnetization processes and thermal runaway in spin-ice $\text{Dy}_2\text{-Ti}_2\text{O}_7$

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Spin ice is a deceptively simple frustrated system. Composed of Ising spins on the vertices of a pyrochlore lattice with ferromagnetic interactions, it has a ground state formally equivalent to that of protons in the eponymous water ice.

In this talk I will briefly discuss some non-equilibrium effects in the magnetisation process of spin-ice. Magnetisation is increased through the propagation of monopolar excitations of opposite sign. Because these are gapped and have long-range attractive interaction, they act as a reservoir of Zeeman energy. As the magnetic field is increased, this energy builds up, and depending on additional conditions, such as the bath temperature, thermal conductivity and sweep rate, they can either relax through a normal combustion -analogous to gently charring a paper - or in a very sudden fashion -the magnetic analogue of deflagration of a combustible material.

33 – Spectral properties of a doped frustrated Mott insulator: a slave-fermion study

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We study the spectral properties of the $t - J$ model on the triangular lattice, at zero temperature and at low doping, in order to analyze the electron dynamics in the presence of strong correlation and magnetic frustration. We represent the projected electron operators by means of Schwinger-bosons and slave-fermions, and we solve the resulting Hamiltonian in an $SU(2)$ -invariant mean-field approximation. Within this scheme, there are significant antiferromagnetic correlations up to moderate doping, that strongly affect the electron dynamics. In general, the spectra exhibit two clearly distinguishable bands: a heavy one at the top, with a bandwidth of the order of the exchange integral J , and a light band below, with a tight-binding-like dispersion displaced by the magnetic wave vector \mathbf{Q} . The heavy band has its origin in the dressing of the holes by the spin fluctuations, and it has a relatively small spectral weight due to the presence of magnetic frustration, while the light band represents the almost free motion of the electrons at energies above J . As a consequence of these spectral features, we observe a transition between an incoherent metal at low doping and a conventional Fermi liquid for higher doping, driven by the spin fluctuations. In the strong coupling regime, $J/t = 0.4$, the critical doping is $\delta_c \simeq 0.12$.

34 – Transport in Carbon Nanotubes: 2LSU(2) regime reveals subtle competition between Kondo and Intermediate Valence states

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In this work, we use three different numerical techniques to study the charge transport properties of a system in the two-level $SU(2)$ (2LSU2) regime, obtained from an $SU(4)$ model Hamiltonian by introducing orbital mixing of the degenerate orbitals via coupling to the leads. $SU(4)$ Kondo physics has been experimentally observed, and studied in detail, in Carbon Nanotube Quantum Dots. Adopting a two molecular orbital basis, the Hamiltonian is recast into a form where one of the molecular orbitals decouples from the charge reservoir, although still interacting capacitively with the other molecular orbital. This basis transformation explains in a clear way how the charge transport in this system turns from double- to single-channel when it transitions from the $SU(4)$ to the 2LSU2 regime. The charge occupancy of these molecular orbitals displays gate-potential-dependent occupancy oscillations that arise from a competition between the Kondo and Intermediate Valence states. The determination of whether the Kondo or the Intermediate Valence state is more favorable, for a specific value of gate potential, is assessed by the definition of an energy scale T_0 , which is calculated through DMRG. We speculate that the calculation of T_0 may provide experimentalists with a useful tool to analyze correlated charge transport in many other systems. For that, a current work is underway to improve the numerical accuracy of its DRMG calculation and explore different definitions.

35 – Dewetting dynamics of crystalline thin films

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Thin solid films are the basic components in many devices. However since the deposition conditions generally are far from equilibrium, such 2D thin films, when annealed, may break up into 3D islands. Such a dewetting process is observed in many experimental systems. If a continuous film is required for applications, its dewetting clearly is a parasitic process but it could also be considered as a method to produce and control the formation of an assembly of nanocrystals. Here we report a quantitative characterization of the dewetting dynamics of silicon-on-oxyde (SOI) thin-films. From an experimental point of view we use low-energy electron microscopy to record real-time in-situ movies of the dynamics of the SOI dewetting process leading to the formation of 3D compact Si nanocrystals. The complex morphological evolution is reproduced by a simple Solid-on-Solid Kinetic Monte Carlo model in which enters only two physical ingredients: a wetting parameter and a reduced temperature. We also develop illustrative models that captures the essentials of the underlying physics that enable us to clearly identify the origin of the driving-force. Our results show (i) that the dewetting is a consequence of surface-free-energy-minimization mediated by surface diffusion and (ii) that the velocity of the dewetting front is limited by its thickening. We connect the rim growth mechanism to the growth dynamics of the dewetted area. The front edges instabilities that lead to the formation of local elongated structures (then to 3D islands by a pinch-off process) are closely connected to the local height instabilities of the rim. Finally the dewetting properties of SOI films are compared to those obtained for a few other systems.

36 – Issues in the ab-initio assessment of hcp transition metals self diffusion

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Since about a decade ago, first principles electronic structure techniques have started to impact traditional domains of Materials Science; among the reasons for this are the availability of reliable and efficient codes based on the Density Functional Theory, and the ever increasing power of computing hardware at affordable prices. Notably, under well controlled conditions, these calculations have demonstrated to be as reliable as experiment itself.

A couple of applications of those techniques relevant to the present context include, i) the formation energy of small cell (~ 10 atoms) perfect crystals, needed e.g. in the assessment of alloys phase diagrams, and ii) simulations of point defects, situation computationally more delicate and demanding (~ 100 atoms), some of which have shed light on fundamental aspects of radiation damage (in bcc metals and Fe in particular). With the exception of two pioneering works dealing with Si and Na, ab-initio studies on diffusion are of more recent date. Within the framework of Transition State Theory, these do not only involve energetic aspects of the defects but also their vibrational properties. In particular, the literature reports several studies dealing with Al, though only one of them can be considered to be fully self-consistent, that also has resulted in very good agreement with the experimental data.

Following the latter methodology, we use the SIESTA code to tackle the case of hcp transition metals, presently restricted to Zr and Ti. Several issues pertaining to this apparently hard case are commented and analyzed, elements of such a list including i) the suitability of available pseudopotentials, ii) the need to employ fine space grids for the numerical integrations, iii) the need of a rather large basis set, iv) the reliability of the simulation cell size and boundary conditions, etc. All of which impact the precision and convergence of the magnitudes to be evaluated, namely, assuming a standard diffusion mechanism, vacancy formation energy, vacancy formation entropy, and attempt frequency.

37 – When nothing really matters: finding the zeros of the fermionic many-body wave function.

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The emergence of parallel computing has altered the cost-benefit balance of the numerical methods used to study numerically the electronic structure of real materials. Sequential algorithms flourished during the 80's and 90's with single processors machines. However, they now suffer heavily from communication bottle necks in large parallel supercomputers. This is typically the case of methods based on density functional theory. Statistical methods, while dormant during many decades, are now taking over the front of electronic structure research since they can be easily distributed with a minimum of communication involved. Diffusion quantum Monte Carlo (DMC) is the many-body method of choice to study ab-initio systems with more than 12 electrons and has been used up to a few thousands. DMC is based on an analogy between the Schrödinger equation at imaginary time and the diffusion equation. DMC finds statistically the ground state energy of any many-body system without approximations. The ground state energy of most Hamiltonians is, however, the bosonic solution. For electronic problems one must first provide the exact surface where the many-body wave function changes sign (the node). Any error in the node increases the energy of the ground state found with DMC. Finding an approximation to the node belongs to the family of problems known as sign problems. In this talk we will outline a method that is able to find the node for electronic problems. The cost of the method is linear in the number degrees of freedom of the wave function. This method is not only able to find the node but also the many-body wave function itself. Applications to molecules and small clusters will be presented.

38 – The theory of optical properties of low-dimensional semiconductors in quantizing magnetic fields

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The base of the theory of light reflection and absorption by low-dimensional semiconductor objects (quantum wells, wire and dots) at both monochromatic and pulse irradiations and at any form of light pulses are developed. The semiconductor object may be placed in a stationary quantizing magnetic field. As an example the case of normal light incidence on a quantum well (QW) surface is considered. The width is arbitrary. For Fourier-components of electric fields the integral equation (similar to the Dyson-equation) and solutions of this equation for some individual cases are obtained.

39 – Spin-orbit and Kondo effect in graphene

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One of the greatest challenges for the development of spin-based devices is the understanding of mechanisms that give rise to spin-polarized currents. Advances in the field have been achieved by studying the effect of different types of spin-orbit interactions in semiconductor materials. Rashba spin-orbit interactions are of particular interest for systems with surfaces since they present a natural breaking of space-inversion symmetry, a condition for its existence. Graphene, a monolayer of graphite, is not expected to exhibit large Rashba couplings in isolation, but recently, several groups have successfully produced samples with band-splittings consistent with large values of the Rashba coupling. Two important effects result from large Rashba interactions: the linear dispersion at the Dirac points becomes quadratic (with the consequent change in the density of states) and new Dirac points are generated around the (K; K') points. The properties of zigzag graphene ribbons are equally affected, with edge states magnetization highly dependent on momentum[1].

Because Rashba changes the density of states in graphene, it is natural to wonder about its consequences on the Kondo effect. The role of spin-orbit interactions on the Kondo effect, an issue posed for the first time by D. Gainon and A. Heeger in 1969[2], has been the topic of much controversy in later years, with many partial (and sometimes contradictory) answers. We have obtained the exact solution for a two-dimensional Anderson impurity model in the presence of Rashba interactions and its effects in the Kondo regime, with and without particle-hole symmetry[3]. The main features are: a two-channel Kondo regime with antiferro- and ferromagnetic couplings and the presence of Dzyaloshiinski-Moriya interactions when particle-hole symmetry is broken. Interesting results are also obtained for graphene where an exponential enhanced Kondo temperature is predicted.

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40 – The Size-Dependent Ferroelectric Phase Transition in BaTiO₃ Nanocrystals Probed by Surface Plasmons

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Understanding the fundamental aspects of nanoscale ferroelectricity is important for various applications of ferroelectrics, such as non-volatile memories, pyroelectric and piezoelectric devices. At the nanoscale, in particular at nanocrystals (NCs) that are strongly confined, deviations from "bulk" properties are expected due to stronger depolarization fields. This leads to the idea of a critical correlation volume below which ferroelectricity cannot be sustained. Reports of the size dependent phase transition properties encompass a broad range of results and suggest a drop in Curie temperature with decreasing size. As NC size decreases and the surface layer takes a substantial part of the volume an average over surface and interior would be measured using techniques such as XRD and Raman scattering. Thus, in order to probe the phase transition at the nanoscale, a different method selectively sensitive to the surface of the ferroelectric NCs should be used. A technique for probing the temperature dependence of the dielectric constant of ferroelectric NCs using shifts in the localized surface plasmon resonance wavelength of gold nanoparticles attached to the surface of the ferroelectric NCs is demonstrated. We study the ferroelectric-to-paraelectric phase transition of Barium Titanate (BTO) nanocubes in three size regimes. Temperature-dependent Raman spectroscopy was applied to probe the whole volume of the NCs. It was revealed that ~ 16 nm BTO NCs were dominated by surface effects, and as the NC size increased bulk BTO behavior governed. This work strengthens the concept of having different surface and interior, bulk-like contributions to the ferroelectricity and to the phase transitions. It thus indicates on the absence of an intrinsic size-dependence of the transition temperature. In addition the surface ferroelectricity behaves differently from the bulk-like ferroelectricity and is characterized by long relaxation time scales.

41 – A test of the bosonic spinon hypothesis for the triangular antiferromagnet

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We show that the anomalous excitation spectrum of the spin-1/2 triangular Heisenberg model, recently found with series expansion by Zheng *et al.* [Phys. Rev. Lett. **96**, 057201 (2006)] , can be naturally interpreted in terms of spinon excitations using a Schwinger boson mean field theory. In particular, we find a qualitative and quantitative agreement of the strong renormalization of the high energy part of the spectrum with respect to spin wave results along with the appearance of roton like minima at the midpoints of faces of the hexagonal Brillouin zone. By looking at the dominant part of low energy peaks of the dynamical structure factor the roton like minima can be traced back to the crossing of the spinon branches shifted by $\pm \frac{\mathbf{Q}}{2}$, where $\mathbf{Q} = (4\pi/3, 0)$ is the magnetic wave vector of the 120° Néel order. We also find that near the location of the roton minima the contribution of the two spinon continuum to the static structure factor is about 40% of the total weight. The implications of our findings are contrasted with recent calculations within the context of $1/s$ spin wave expansions.

42 – Are Friedel oscillations in one-dimensional Hubbard chains noninteracting v-representable?

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The widely known Kohn-Sham (KS) formalism of density-functional theory leads to a restriction on the density: it needs to be noninteracting v-representable. This is a direct consequence of considering the non-interacting kinetic energy functional, which, on the other hand, can allow computational simplicity by means of the KS equations. Friedel oscillations in one-dimensional (1D) model systems are known to suffer a $2k_F - 4k_F$ crossover in the frequency as electronic interaction effects become more prominent. The current local density functionals which are applied to the 1D Hubbard model, however, are not seen to reproduce such a crossover, referring to a more fundamental question: Are the Friedel oscillations in such systems noninteracting v-representable? Or, is there an exchange-correlation potential which is able to correctly yield them? Finding an appropriate answer to both questions is our main task here, and by means of the exact many-body solution for small Hubbard chains, we show the answer to be positive.

Posters

Oxides and related topics

1 - 1 – Behavior of thermal expansion coefficient of $\alpha - MoO_3$ in function of the concentration of Nd^{3+}

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The molybdenum trioxide (MoO_3) and neodymium (Nd) has excellent physical and chemical properties that have made them useful in different applications. For example, the MoO_3 has been used as thermal sensor (thermochromic), in information display screen (photochromic), as cathode material in solid-state micro batteries and as gas sensor. On the other hand, the Nd^{3+} due to their photo emissive properties has been used mainly as active element in laser systems; it is important remember that the photoluminescence related with the neodymium is produced only by interaction with the crystal field of a suitable host material. In order to establish the physical mechanisms that determine the inclusion of neodymium in MoO_3 structure several samples were prepared, using the technique of liquid phase reaction, mixtures with different molar concentrations of Nd (0.1% to 20%). The mixtures were subjected to heat treatment, starting from room temperature to reach 823K, and analyzed in situ by X-ray diffraction (XRD). From the XRD analyses were calculated x_i (with $x=a, b, c$ lattice parameters) of molybdenum trioxide as a function of molar concentration Nd^{3+ion} , and allow us calculate thermal expansion coefficients ($\alpha_a = 7.7402 \times 10^{-4} \text{ } \dot{A}/^{\circ}C$, $\alpha_b = 5.7012 \times 10^{-5} \text{ } \dot{A}/^{\circ}C$, and $\alpha_c = -3.1031 \times 10^{-6} \text{ } \dot{A}/^{\circ}C$); the composition of these materials were determinate by X-ray dispersive spectroscopy (EDS). From the EDS analyses were found that the mixtures have concentrations of the 4.00to8.00%atomic the Nd.

1 - 2 – Behavior of the irreversibility line in the new superconductor $La_{1.5-x}Ba_{1.5+x-y}Ca_yCu_3O_z$

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The irreversibility properties of high-Tc superconductors are of major importance for technological applications. For example, a high irreversibility magnetic field is a more desirable quality for a superconductor [1]. The irreversibility line in the H-T

plane is constitutes by experimental points which divides the irreversible and reversible behavior of the magnetization. The irreversibility lines for series of $La_{1.5-x}Ba_{1.5+x-y}Ca_yCu_3O_z$ polycrystalline samples with different doping were investigated. The samples were synthesized using the usual solid state reaction method. Rietveld-type refinement of x-ray diffraction patterns permitted to determine the crystallization of material in a tetragonal structure. Curves of magnetization ZFC-FC for the system $La_{1.5-x}Ba_{1.5+x-y}Ca_yCu_3O_z$, were measured in magnetic fields of the 10 Oe to 20000 Oe, allowed to obtain the values for the irreversibility and critical temperatures. The data of irreversibility temperature allowed demarcating the irreversibility line, $T_{irr}(H)$. Two main lines are used for the interpretation of the irreversibility line: one of those which supposes that the vortexes are activated thermally and the other proposes that associated to T_{irr} , it happens a phase transition. The irreversibility line is described by a power law. The obtained results allow concluding that in the system $La_{1.5-x}Ba_{1.5+x-y}Ca_yCu_3O_z$ a characteristic bend of the Almeida-Thouless (AT) tendency is dominant for low fields and a bend Gabay-Toulouse (GT) behavior for high magnetic fields. This feature of the irreversibility line has been reported as a characteristic of granular superconductors and it corroborates the topological effects of vortexes mentioned by several authors [1,2].

[1] Dawood Ahmad, Tae Kwon Song, Insuk Park, G. C. Kim, Y. C. Kim. Current Applied Physics 10 (2010) 1345-1348. [2] P. Rodrigues Jr, J. Schaf, P. Pureur, Phys. Ver. B 49, 15292 (1994).

1 - 3 – Synthesis, structure and magnetic properties of the double perovskite Sr_2SbMnO_6

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We report the structural and magnetic properties of the perovskite Sr_2SbMnO_6 , which has been synthesized by the standard solid state reaction recipe. Crystalline structure was studied by means of Rietveld refinement of X-ray diffraction data. This study indicates that the structure is tetragonal, space group 128.

The magnetic behavior was studied for several temperatures between 5 and 300 K, through measurements of magnetization in function of field, AC and DC susceptibility in function of temperature and ZFC–FC magnetization curves. The ZFC and FC curves show a magnetic transition/glassy freezing at ~ 13 K and was observed that the behavior is not pure Curie Weiss; also, at 300 K $\text{Sr}_2\text{SbMnO}_6$ show a pure paramagnetic behavior. Was studied field dependence of magnetization data at 8 K, which show that there are ferromagnetically coupled clusters in the ordered/glassy state. However, there are significant details that distinguish the observed behavior from a standard spin glass. The measurements of AC susceptibility at 125 Hz and 1000 Hz show two peaks, one of these indicating the magnetic transition glassy at 13 K, and the second about 40 K show up the beginning of glassy dynamics. These results are in agreement with reports of other authors.

This work was partially supported by the Dirección de Investigaciones (DIN) of the Universidad Pedagógica y Tecnológica de Colombia (UPTC).

1 - 4 – Evolution of the structural ordering of the $\text{Sr}_2\text{SbMnO}_6$ perovskite in function of temperature

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Polycrystalline samples of $\text{Sr}_2\text{SbMnO}_6$ material has been synthesized by means of the conventional solid state reaction method, using powder oxides SrO , MnO_2 and Sb_2O_3 . Our route of synthesis differs of others reported in the literature by the use of SrO instead of SrCO_3 as the precursor of the Sr. X-ray diffraction (XRD) pattern obtained was studied by means of the Rietveld refinement method. This study reveals that the $\text{Sr}_2\text{SbMnO}_6$ material has tetragonal structure, space group 128. Furthermore, XRD patterns were registered for temperatures between 25°C and 1400°C . The Rietveld refinements of these patterns show that the structure correspond to the space group 128 until 200°C , change to space group 87 for temperatures between 300 and 1000°C and, finally is cubic, space group 225 for temperatures above 1000°C . Additionally, is discussed the evolution of the lattice parameters in function of the temperature. The study of this material is important because it has been attracted the attention due to its ferroelectric and magnetic properties.

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1 - 5 – Critical temperature above 92 K in a new superconducting material $\text{Yb}_{1.8}\text{Sm}_{1.2}\text{Ba}_5\text{Cu}_8\text{O}_{18}$

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We report the synthesis, structural ordering and superconducting measurements of a new material $\text{Yb}_{1.8}\text{Sm}_{1.2}\text{Ba}_5\text{Cu}_8\text{O}_{18}$, which was made by means of the conventional solid state reaction method, based on commercial oxide powder precursors. To determine the crystal structure of the $\text{Yb}_{1.8}\text{Sm}_{1.2}\text{Ba}_5\text{Cu}_8\text{O}_{18}$, the X-ray diffraction pattern was refined by Rietveld method. This study reveals that the material has a single phase with complex orthorhombic perovskite structure, space group 25.

Results of magnetization measurements in function of temperature show that the $\text{Yb}_{1.8}\text{Sm}_{1.2}\text{Ba}_5\text{Cu}_8\text{O}_{18}$ material undergoes a superconducting transition at $T_c \sim 98$ K. This results are in agreement with the observation of a high transition temperature in $\text{Y}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ system, reported by Aliabadi et. al[1].

This work was partially supported by the Dirección de Investigaciones (DIN) of the Universidad Pedagógica y Tecnológica de Colombia (UPTC).

[1] A. Aliabadi, Y. Akhavan Farshchi and M. Akhavan, *Physica C*, **469** 2012–2014, (2009).

1 - 6 – Production and characterization of the type Superconducting Perovskites $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$, (RE= Y, Sm, Dy, Ho)

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In this work we report the synthesis and characterization of the system $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ (RE=Y, Sm, Dy, Ho), in order to reproduce the results reported by A. Aliabadi et. al.[1] about the $T_c \sim 100$ K for the superconducting system $\text{Y}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ and, to evaluate the superconductor behavior of $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ samples (RE=Sm, Dy, Ho). The system $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ (RE=Y, Sm, Dy, Ho), was produced by the method of solid state reaction following a thermal process similar to that used for the superconductor RE:123 and different to that used by Aliabadi. The experimental results obtained by the technique of X-Ray Diffraction and Rietveld analysis show that these samples have the expected

crystal structure. On the other hand, the resistivity measurements of samples produced ensure the superconductor transition in the system $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ (RE=Y, Sm, Dy, Ho), with critical temperatures near $T_c = 96\text{K}$ for the system $\text{Y}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ and a T_c above 92K for the system $\text{RE}_3\text{Ba}_5\text{Cu}_8\text{O}_{18}$ (RE=Sm, Dy, Ho). This work opens a new avenue of research in the area of superconductivity for systems RE:358.

This work was partially supported by the Dirección de Investigaciones (DIN) of the Universidad Pedagógica y Tecnológica de Colombia (UPTC).

[1] A. Aliabadi, Y. Akhavan Farshchi and M. Akhavan, *Physica C*, **469** 2012–2014, (2009).

1 - 7 – Shot noise in HTc superconductor quantum point contact system.

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We study the electrical transport properties of a quantum point contact between a lead and a High Tc superconductor. For this, We use the Hamiltonian approach and non-equilibrium Green functions of the system. The electrical current and the shot noise are calculated with this formalism. We consider $d_{x^2-y^2}$, d_{xy} , $d_{x^2-y^2} + is$ and $d_{xy} + is$ symmetries for the pair potential. We find that for d_{xy} symmetry there is no a zero bias conductance peak; for $d + is$ symmetries there is a displacement of the transport properties. From shot noise and the current, the Fano factor is calculated and we find that it takes values of effective charge between e and $2e$ depending on the pair potential symmetry, it is explained by the diffraction of the quasiparticles in the contact. These results are compared with the obtained for a plain junction.

1 - 8 – Magnetic properties and structural characterization of $\text{Sr}_2\text{RuHoO}_6$ complex perovskite

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We report an experimental study of the crystallographic lattice, morphologic characteristics and magnetic feature of $\text{Sr}_2\text{RuHoO}_6$ complex perovskite, which is used as a precursor in the fabrication process of the superconducting ruthenocuprate $\text{RuSr}_2\text{HoCu}_2\text{O}_8$. The samples were produced through the standard solid state reaction. A careful Rietveld

refinement of the experimental X-ray diffraction patterns shows that the material crystallizes in a monoclinic structure, which belongs to the $P21/n(\#14)$ space group, with lattice parameters $a = 5.7719(6)\text{Å}$, $b = 5.8784(5)\text{Å}$, $c = 8.1651(9)\text{Å}$, and tilt angle $\beta = 90.200^\circ$. The calculated tolerance factor of material was 0.9170, which is in agreement with a monoclinic crystallographic cell. The inter-atomic distance and occupancy calculated through the Rietveld refinement of experimental data is reported too. Micrograph of Scanning Electron Microscopy for $\text{Sr}_2\text{RuHoO}_6$ double perovskite, obtained from ETD detector, show the granular characteristic of material with mean size between 2.0 and $7.5\mu\text{m}$. Through semiquantitative Energy Dispersive X-ray analysis, we determined that the composition of the material is 98% in agreement with theoretical values calculated from stoichiometry of $\text{Sr}_2\text{RuHoO}_6$ material. From the structural, morphologic and compositional characteristics we deduced that no other crystallographic phases or impurities are present in the sample. Magnetic susceptibility measurements reveal the occurrence of an antiferromagnetic behavior for a Néel temperature $T_N = 10.1\text{K}$. From the Curie-Weiss fitting of the paramagnetic regime we obtain an effective magnetic moment of $11.31\mu_B$. The antiferromagnetic ordering is attributed to Ru-O-O-Ru superexchange interaction and a ferromagnetic transition for a Curie temperature of 17K , which are related with the Ru-O-Gd interactions.

1 - 9 – Formation of a magnetic composite by reduction of Co-Nd doped strontium hexaferrite in a hydrogen gas flow

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Co-Nd strontium hexaferrite nanoparticles synthesized by the self-combustion method were treated in a hydrogen flow at different temperatures and times. The samples were characterized structurally by scanning electron microscopy and x ray diffraction and magnetically with a vibrating sample magnetometer. Phase identification showed decomposition of the hexaferrite structure into Fe_3O_4 , Fe_2O_3 and different strontium mixed oxides. The sample treated at 500° for 30 minutes shows good magnetic properties due to the formation of a magnetite/hexaferrite composite. In this case saturation magnetization is very close to the original sample while the coercivity slightly diminishes. The hexagonal phase is almost completely transformed into non-magnetic oxides at a reducing temperature of 500° for 120 minutes. The obtained results are analyzed in terms of the phase composition and of the magnetic susceptibility of the studied samples.

1 - 10 – Impedance spectroscopy and structural properties of the perovskite-like $\text{Sn}(\text{Ba},\text{Sr})\text{O}_3$ stagnate

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In the last decades, the study of perovskite materials has attracted great interest of researchers in the ceramics area due their physical and chemical properties at several temperatures, which are required for technological applications. In this work we perform an exhaustive study of structural, electrical and transport properties in bulk samples of the perovskite stagnate $\text{Sn}(\text{Ba},\text{Sr})\text{O}_3$. The synthesis of the $\text{SnBa}_{1-x}\text{Sr}_x\text{O}_3$ compounds was performed by the solid state reaction recipe. Seven tablets were obtained with different concentrations of $\text{SnBa}_{1-x}\text{Sr}_x\text{O}_3$ with $0 \leq x \leq 1$. The crystallographic structure was studied by the X-ray diffraction technique and the analysis of the experimental data was performed from the Rietveld refinement by using the GSAS code. Results reveal that the material synthesized in a Pnma structure (space group #62). The approximate grain size was found from experiments from Scanning Electron Microscopy images to be $2\mu\text{m}$. The semi-quantitative composition was established from Energy Dispersive X-ray experiments, which permitted to establish that the chemical compositions of our samples are 97% in agreement with the expected stoichiometry. The response of the impedance as a function of frequency at room and low temperatures were obtained by the Impedance Spectroscopy technique from 10.0mHz up to 0,1MHz, also obtaining the respective equivalent circuit, using the fitting the Cole-Cole diagrams. Electric polarization measurements for SnSrO_3 and SnBaO_3 were determined through polarization experiments, using a polarization equipment produced by Radiant Technologies. Curves of polarization as a function of applied electric fields reveal the hysteretic behavior which is characteristic of the ferroelectric materials. From the saturation polarization it was determined that SnSrO_3 and SnBaO_3 have dielectric constants of 64.7 and 95.2 respectively. The ferroelectric parameters for these materials are presented and discussed.

1 - 11 – Size Dependent Ferroelectric Polarization in BaTiO_3 Nanocrystals Probed by Electron Holography

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In bulk ferroelectric crystals and thin films, the paraelectric to ferroelectric phase transition is accompanied by the formation of polarization domains to minimize the system energy with respect to the depolarization field and mechanical strain. While experimental data is available for thin perovskite films only few studies address the electric polarization properties of ferroelectric nanocrystals. Hence, it is yet to be established what is the minimal nanocrystal (NC) size and geometry that could support the ferroelectric crystal phase in the absence of external support such as a substrate, metal electrodes or adjacent high dielectric constant material. It is not established experimentally whether a small isolated NC exists as a single ferroelectric domain, or that its high depolarizing field causes other forms of ferroelectric order. Here, we present images of ferroelectric polarization in isolated BaTiO_3 (BTO) NCs obtained with nanometer resolution using off-axis electron holography, above and below the Curie temperature (T_C). It is found that the polarization magnitude within 20-55 nm NCs is size dependent, forming complex configurations in the larger nanocrystals with polarization values surpassing the bulk values quoted in the literature. In addition, the polarization appears to decay or re-orient near free NC surfaces to minimize the depolarization energy.

1 - 12 – Magnetotransport Properties in Manganite $\text{La}_{1/3}\text{Ca}_{2/3}\text{MnO}_3$ (FM) and $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$ (AF): A Monte Carlo Approach

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Manganese perovskites have recently been the focus of renewed interest, due to the "colossal" magnetoresistance (CMR) effect and the coupled metal-insulator and magnetic transitions displayed at the

spin-ordering temperature TC by some of these compounds. In this work, a magnetotransport properties simulation of ferromagnetic (FM) $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$ and antiferromagnetic (AF) $\text{La}_{1/3}\text{Ca}_{2/3}\text{MnO}_3$ is presented and discussed. Our study is addressed by using the Monte Carlo method. Moreover, magnetic Kronig-Penney model based on the thermodynamics of a Heisenberg can be used for describing the colossal magnetoresistance (CMR) phenomenon for the FM phase and insulating behavior for the AF phase. The model consists on tunnelinglike transmission process of hopping electrons in a magnetically dynamic lattice containing magnetic clusters. In this model, electrical transport features are mainly governed by the magnetic states, neglecting the lattice strain effects. By means of the theoretical fundamentals described here, intrinsic temperature and field dependences of the resistivity and magnetoresistance, typically observed in these manganites were obtained and analyzed.

1 - 13 – Effect of the heat treatment conditions on the synthesis of Sr-hexaferrite

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The effect of the heat treatment conditions under oxygen atmosphere on the $\text{SrFe}_{12}\text{O}_{19}$ (Sr-M ferrite) synthesis is analyzed. We study the effect of the partial evacuation of the gases of decomposition of the organometallic precursor on the phase composition of different samples. An accurate structural analysis of samples obtained between 250 °C (with Sr-M crystallite size, \varnothing , around 20 nm) and 500 °C (\varnothing 40 nm) is reported. From the structural analysis two secondary phases, hematite and maghemite, are identified. The amount of secondary phases (between 10% and 30%) can be manipulated through the control of the heat treatment conditions, and therefore, this constitutes a methodology to manipulate the phase composition of the nanopowders. The influence of secondary phases on the magnetic properties of the samples is also studied. The quantitative determination of phases is performed by structural refinement of X-ray powder patterns, by using Rietveld analysis. Magnetic study is done by Magnetization vs Temperature and Magnetization vs Applied Magnetic Field.

1 - 14 – Copper adsorption on magnetite chitosan composites: a kinetic and equilibrium study

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The accumulation of heavy metals in water is an important environmental problem, caused by industrial effluents. One possibility for removing these contaminants is the use of adsorption on biopolymers, such as chitosan. It is of interest to prepare an adsorbent material with magnetic properties, allowing the separation of the material with a magnet.

A composite of magnetite and the biopolymer chitosan was prepared as microspheres and used to adsorb copper ions which were chosen as model of contaminant metal in water. Fe_3O_4 particles of nanometric size were obtained by the oxidative hydrolysis of a FeSO_4 solution. The ferrofluid made of magnetite nanoparticles and chitosan was transferred dropwise on the surface of an alkali solution to form microspheres, which were then crosslinked with glutaraldehyde. The resulting material contained 35% w/w of chitosan, determined gravimetrically.

The adsorption of copper on the surface of the magnetic microspheres was studied in a batch process, with different aqueous solution of Cu (II) concentrations ranging from 40 to 1100 ppm. The residual metal concentration in solution was determined by a spectrophotometric method.

Kinetic and equilibrium aspects of the adsorption process were studied. The time-dependent Cu (II) adsorption data were well described by a pseudo-second-order kinetic model. Moreover, it was found that the equilibrium data fitted well to the Langmuir isotherm, with a maximum adsorption capacity of 500 mg Cu per g chitosan.

The microspheres were removed after use with a magnet and following a chemical treatment with a complexing agent the material could be reused as an adsorbent.

In conclusion, the prepared microspheres have proved useful in the removal of copper ions through an adsorption process whose kinetic and equilibrium characteristics have been analyzed.

1 - 15 – High Temperature-induced phase transitions in $\text{Sr}_2\text{GdRuO}_6$ complex perovskite

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We report experimental and theoretical study of crystallographic lattice and electronic structure of $\text{Sr}_2\text{GdRuO}_6$ complex perovskite, which is used as precursor in the fabrication process of superconducting ruthenocuprate $\text{RuSr}_2\text{GdCu}_2\text{O}_8$. Samples were produced by the standard solid state reaction. Rietveld refinement of experimental X-ray diffraction patterns shows that material crystallizes in a monoclinic structure, which belongs to the $P2(1)/n$ (14) space group, with lattice parameters $a=5.8019(6)$ Å, $b=5.8296(5)$

\AA , $c=8.2223(7)$ \AA , and tilt angle $\beta=90.2580^\circ$. Measurements of X-ray diffraction in the range between 298 K and 1273 K show that lattice parameters a , b and c of complex perovskite Sr_2GdRuO_6 suffers volume expansion in the three coordinate axes. The results show that as temperature increases the value of cell parameter c increases approximately linearly, while the values of cell parameters a and b tend to be equal and the tilt angle β decreases to 90° . The value of cell parameter a increases approximately linearly and takes the value of cell parameter b at temperature of 753 K. From this temperature the values of two parameters are similar, and arguably presents a phase transition in complex perovskite Sr_2GdRuO_6 , when the tilt angle β tends to $90.073(3)^\circ$. In Agreement with these results have a tetragonal structure, in which $a=b$, c is arbitrary and $\alpha=\beta=\gamma=90^\circ$. Then the complex perovskite Sr_2GdRuO_6 adopts an tetragonal perovskite structure with space group $Ibmm$, which is characterized by rotation of GdO_6 octahedra about the pseudocubic two-fold axis.

1 - 16 – Resistive switching in ceramic multiferroic $\text{Bi}_{0.9}\text{Ca}_{0.1}\text{FeO}_3$ oxide

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Resistive switching (or RS) [1] is defined as the reversible change of the resistance of a material under the application of electrical pulses. RS in transition metal oxides has been observed in many binary and complex compounds, being the basis for the development of novel non-volatile resistance random access memories (RRAM). While in the case of binary oxides the RS effect is believed to arise from the creation/destruction of conducting filaments, in complex oxides the effect is interface-related, that is, it takes place at the interface between a metal electrode and the oxide, playing a key role the presence of oxygen vacancies that modulate the interface resistance. Here we study the RS effect in ceramic samples of the multiferroic oxide $\text{Bi}_{0.9}\text{Ca}_{0.1}\text{FeO}_3$ with different metallic electrodes. Samples were prepared by means of standard solid state reactions. We show by means of Mössbauer spectroscopy that the Fe valence remains unchanged (3+) upon Ca doping, suggesting a charge compensation mechanism via formation of oxygen vacancies. We studied the dependence of the RS effect with the type of electrode and with the intensity and number of pulses. RS values of up to 100 per cent were obtained, a figure that is lower than that found in thin films samples [2]. We argue that this is due to the low electrical fields achievable in ceramic samples with metallic electrodes separated by distances of the order of millimetres. In addition, the RS effect is found to relax with time, with typical relaxation times that depend on the number and intensity of the

previously applied electrical pulses. We rationalize our results by considering the Nernst-Planck equation and the migration of oxygen vacancies to and from the metal-oxide interface.

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1 - 17 – Magnetic behavior of Mg - Al - Zn - Fe mixed oxides from precursors layered double hydroxide

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Mixed oxides of Mg-Al-Zn-Fe were obtained by calcination of layered double hydroxides (LDH) prepared by coprecipitation reaction with hydrothermal treatment. The structural characterization of precursors and the mixed oxides was carried out by X rays diffraction, showing a increases of ZnO phase with the increase of the zinc content. Magnetic behavior was studied by vibrating sample magnetometer (VSM) and by a superconducting quantum interference device (SQUID) showing both ferromagnetic and superparamagnetic behavior depending on both particles size and composition.

1 - 18 – Structural, Magnetic and Electric behavior of new $\text{Ba}_2\text{TiMoO}_6$ material

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The $\text{A}_2\text{BB}'\text{O}_6$ double perovskites tend to order in a NaCl-type superlattice structure. Compounds where A is an alkaline earth cation and B= Cr, Fe, Mg; B'= Mo, Re, are ferromagnetic [1]. Interest in this type of compounds was revived because they exhibit

properties like intrinsic tunneling-type magnetoresistance (TMR) at room temperature [2], show evidence of electronic conductivity attractive for applications as anodes or cathodes in solid-oxide fuel cells [3] and half-metallicity [4]. These characteristics suggest the possible technological applications of perovskites in magnetoelectronic devices and make them promising candidates for future spin electronics. We report synthesis and characterization of the new $\text{Ba}_2\text{TiMoO}_6$ material. X-ray diffraction experiments reveal characteristic reflections for complex perovskite systems. A Rietveld refinement of the diffraction pattern shows that $\text{Ba}_2\text{TiMoO}_6$ crystallizes in a tetragonal structure, which corresponds to the space group $P_{4/mmm}$ (#123), with lattice parameters $a = b = 3.906 \text{ \AA}$; and $c = 11.732 \text{ \AA}$. Images of scanning electron microscopy (SEM) reveal small, sphere-shaped grains from $3.0 \mu\text{m}$ up to $5.0 \mu\text{m}$ size.

Measurements of the magnetization as a function of temperature after Zero field cooling and field cooling were carried out by using a MPMS Quantum Design SQUID magnetometer. We find paramagnetic behavior down to 5 K. Electric polarization curves were measured by means of a radiant ferroelectric tester, which include a 10 kV source for experiments in bulk samples. Hysteresis curves of the polarization as a function of the applied voltage exhibit a ferroelectric response for $\text{Ba}_2\text{TiMoO}_6$.

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1 - 19 – Growth of Ba-titanate and Ba-hexaferrite bilayers: effect of BTO layer in magnetic properties of BaM phase

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Bilayers of barium titanate, BaTiO_3 (BTO) and barium ferrite, $\text{BaFe}_{12}\text{O}_{19}$ (BaM) were grown by Pulsed Laser Deposition, using (100) LaAlO_3 substrate in the BaM/BTO configuration and (0001) Al_3O_4 substrate in BTO/BaM configuration, maintaining identical conditions of growth in both

samples. Stoichiometric control of the plasma emission during the deposition of BTO and BaM films was made by optic emission spectroscopy (OES). The structural characterization was achieved by X-ray diffraction and preferential growth it was found for the BTO phase in the BaM/BTO bilayer, and for BaM phase in the BTO/BaM bilayer. The magnetic properties of BaM phase was studied by SQUID magnetometer over a temperature range of the 5-300K and for different magnetic field applied. The dependence with temperature of the coercive field and squareness ($Sq = M_R/M_S$) present strong influence with structural characteristic of BaM, besides, significant differences were found between $Sq(T)$ of BaM single phase and the squareness of BTO/BaM bilayer, both deposited on Al_3O_4 , indicating the influence of BTO layer.

1 - 20 – Displacive Disorder, Anti-site Disorder and Magnetic Properties of Cubic Pyrochlores $\text{Bi}_2\text{MM}'\text{O}_7$ with $\text{M} = \text{Sc, Cr, Mn}$ and Fe and $\text{M}' = \text{Nb, Ta}$ and Sb

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Pyrochlore oxides are being the subject of renewed interest because of their many interesting applications. Specifically those with formula $\text{A}_2\text{MM}'\text{O}_7$ were recently informed to be alternative cathodes for IT-SOFCs [1]. Proton conductivity has also been observed in doped $\text{Sm}_2\text{Sn}_2\text{O}_7$ [2] and dielectric properties were informed for doped $\text{Bi}_{1.5}\text{Zn}_{0.92}\text{Nb}_{1.5}\text{O}_{6.92}$ [3]. Many other important applications make the synthesis of new pyrochlore oxides and their fundamental studies a very interesting area of research. The typical pyrochlore compound has the general formula $\text{A}_2\text{B}_2\text{O}_7$, with a cubic crystal structure Fd-3m (SG 227), and it is well described as $\text{A}_2\text{B}_2\text{O}_6\text{O}'$ comprising two interpenetrating sublattices with the formulae $\text{A}_2\text{O}'$ and BO_6 . Non spherical ions (like Bi^{3+}) inside the classic cubic structure can be accommodated through displacive disorder. This disorder results in the appearance of hkl reflections where $h = 4n$, $k = 4n$, and $l = 2n$. Its appearance is rationalized by a static displacement of the A ions toward the surrounding ring of O atoms. The synthesis of new $\text{Bi}_2\text{MM}'\text{O}_7$ pyrochlores with a combination of both, a magnetic ion and a spectator ion on the M sites (where $\text{M} = \text{Sc, Cr, Mn}$ and Fe and $\text{M}' = \text{Nb, Ta}$ and Sb) have been selected as an interesting family to study their fundamental properties. They were successfully synthesized

by solid state method, from stoichiometric quantities of the corresponding binary oxides and appropriated thermal treatments. XRD patterns, combined with Mössbauer spectroscopy for Fe containing compounds, allowed establish the displacive disorder and site disorder presence for all compounds. Their structures were refined by Rietveld analysis of PXRD patterns, and the comparison between the ideal cubic and displaced cubic pyrochlores was carried too. Resulting cell parameters are consistent with the M^{3+} cation in high spin configuration in octahedral coordination. Magnetic measurements were made in a commercial SQUID in the 10-300 K temperature range, and they allowed observe a wide range of magnetic characteristics, starting by expected diamagnetism for Sc pyrochlores, and indications of magnetic frustration for Fe pyrochlores.

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1 - 21 – Zero-valent iron nanoparticles and magnetite as solid catalysts for benzene degradation

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Fenton's reagent, a solution of hydrogen peroxide and ferrous iron catalyst, is used for an in-situ chemicals oxidation of organic contaminants. Recent studies of Fenton's reaction are concentrated on improving the remediation technique by minimizing the addition of extrinsic materials into subsurface systems and by using environmentally benign chemicals. Natural iron catalyst as a means of minimizing the extrinsic chemical addition was examined by many researchers. Although still in the emerging phase, zero-valent iron nanoparticles represent a highly promising agent of environmental remediation technologies. Nanoparticles containing magnetic materials such as Fe_3O_4 , Fe_2O_3 are particularly useful for imaging and separation techniques. They are considered to be biologically and chemically inert. The high ratio area/volume increase the catalysts properties. In this work we report the preparation and characterization of a magnetite ferrofluid and zero-valent iron nanoparticles by the method of ferric iron reduction by sodium borohydride. A comparative kinetic analysis between magnetite and zero-valent iron nanoparticles for the degradation of an aqueous solution of benzene is presented. The results are related to previous experiences developed in our laboratory with ferrous sulphate with the traditional Fenton's method. The experiences were performed at 20°, at a fixed molarity of benzene, hydrogen peroxide and catalyst. Prelimi-

nary results indicate that zero-valent iron nanoparticles show promising results compare to magnetite at one hour.

1 - 22 – Characterization of magnetite nanoparticles used for adsorption of As

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Magnetite may be used for remediation purposes, because of its physical properties that allow a magnetic separation of the oxide from polluted natural and industrial sources. In this work we characterize several samples of pure and doped nanomagnetites used for the adsorption of As(V), a ion that originates in some natural processes of mineral dissolution, mining operations and through the use of fertilizers and pesticides [1-3]. We have obtained nanosized pure magnetite (MP), doped Mn-magnetite (MMn) and doped Co-magnetite (MCo) by a chemical co-precipitation method using $FeCl_2 \cdot 4H_2O$ and $FeCl_3 \cdot 6H_2O$ in the molar ratio $\frac{1}{2}$. The ionic force was increased to assure the formation of nanoparticles [4]. The doped samples were obtained by replacing 10% of the Fe(II) ions by Co(II) and Mn(II) using $CoCl_2 \cdot 6H_2O$ and $MnCl_2 \cdot 4H_2O$. To analyze the influence of the preparation media on the morphology and hyperfine properties of the obtained particles, similar series were prepared in urea 0.4 M (samples named MPUREA, MCoUREA, and MMnUREA).

The effect of the dopants and the preparation media on the magnetite nanoparticles was evaluated by 77K Mössbauer spectrometry, FTIR, SEM and EDS measurements. The adsorption studies were performed at 25 °C, using 0.1 KNO₃, As(V) (40 ppm) and 80 mg of the iron oxide. The pH was kept at 4.00 using KOH 0.1N and HNO₃ 0.1N.

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1 - 23 – Structural stability and electronic properties study of the Sr_2MnSbO_6 perovskite

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The Sr_2MnSbO_6 perovskite has been reported as a ferroelectric and ferromagnetic compound in the tetragonal I4m phase and exhibits very interesting dielectric properties in the cubic Fm-3m phase, that make it a technological alternative for use in microelectronics devices. In addition, it is also very interesting the co-existence of both ferromagnetic and ferroelectric phenomenon, which is very important in spintronic applications such as the spin valves, reading devices in magnetic disks and recording devices.

In this work, first-principles calculations have been performed to study the structural and electronic properties of the Sr_2MnSbO_6 perovskite in cubic (Fm-3m), tetragonal (I4m) and P4/mnc phases. The calculations are performed in the framework of the spin density functional theory (DFT). We have employed the full potential linearized augmented plane waves (FP-LAPW) method as implemented in the WIEN2k code. The exchange and correlation effects were treated using the generalized gradient approximation (GGA), and the local density approximation (LDA). (GGA)+U approaches has been used in order to describe the strong on-site Coulomb repulsion among the localized d-Mn electrons; the results are compared with experimental results. Also we present a structural stability analysis based on fitting of the total energy values to the Murnaghan equation of state and a thermodynamic study of the phase transitions was carried out by means of the calculations of the Enthalpy. On the other hand, the study of the electronic properties was carried out by means of the representation of the bands structure and the densities of states for the two spin polarizations, which this show the half-metallic behavior in the cubic phase while that in the tetragonal phases is comported as semiconductor material.

1 - 24 – Electronic Structure of α - Al_2O_3 Slabs: a local environment study.

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In this work we performed an *ab initio*/DFT study of structural and electronic properties of the (001) α - Al_2O_3 surface. For this study we used two methods

with different basis set: the Augmented Plane Wave plus local orbital (APW+lo) and a linear combination of numerical localized atomic orbital basis sets, employing the Wien2K code and SIESTA code, respectively. In order to calculate the structural and electronic properties of the reconstructed surface, we calculated the final equilibrium atomic positions with the SIESTA code and then we calculated the Electric-Field Gradient (EFG) tensor with the APW+lo code at the optimized positions. Using this procedure we found equilibrium structures with less energy than those obtained by using only the APW+lo method. The EFG tensor and the local structure for Al were study as a function of the depth from the surface, for relaxed structures. We found that distances down to 6 Å from the surface are sufficient to converge the EFG and the Al-O distances to bulk values. The predicted bulk EFG is in good agreement with the experimental results. These results can be used for local probe purposes, for example in the case of doping, with important sensitivity for probes located close to the top of the surface, in particular for distances lower than 6 Å

1 - 25 – Study of the formation of $Co_3(BO_3)O_2$ by oxidation of Co_3B nanoparticles

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Until recently, the physical properties of the homometallic cobalt ludwigite, $Co_3(BO_3)O_2$, were unknown. The interest in this compound is due to the low-dimensionality of its structure, that is composed of low-dimensional subunits in the form of three-leg ladders, and the unexpected strong ferromagnetic ordering observed below 42 K that do not occurs in the compound $Fe_3(BO_3)O_2$ that have similar structure. The goal of our work is study the formation of the $Co_3(BO_3)O_2$ during the oxidation of Co_3B nanoparticles and the effect of antiferromagnetic spurious phases in its magnetic properties. The nanoparticles were prepared by reduction of Co^{2+} ions by sodium borohydride in 2-propanol and its specific surface area obtained by application of BET method in the N_2 adsorption isotherm is 52 m²/g. Thermogravimetric analysis of oxidation process of these nanoparticles, combined with X ray diffratograms (XRD) of samples calcined in different temperatures, showed the formation process of the phases Co_3O_4 , $Co_3(BO_3)_2$ e $Co_3(BO_3)O_2$. The Rietveld analysis of XRD patterns revealed that the sample calcined at 800 °C is composed by 55.3% of $Co_3(BO_3)_2$ and 44.7% of Co_3O_4 , while the sample calcined at 900 °C is formed by 71.7% of $Co_3(BO_3)O_2$, 13.8% of $Co_3(BO_3)_2$ and 14.5% of Co_3O_4 . The magnetization curves of the sample calcined at 800 °C show features similar to the Co_3O_4 nanostructures, possibly due to the entanglement of the phases. An increase of coercivity of

the phase $\text{Co}_3(\text{BO}_3)_2\text{O}_2$ due to the presence of antiferromagnetic phases was observed. The results of this work contribute to understanding of the formation of $\text{Co}_3(\text{BO}_3)_2\text{O}_2$ that will allow in a future work the control of the preparation process and the study of the particle size effects in its magnetic properties.

1 - 26 – Dynamic hyperfine interactions in $^{111}\text{In}/^{111}\text{Cd}$ -doped ZnO semiconductor: PAC results supported by *ab initio* calculations

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During the last 25 years, dynamic hyperfine interactions have been observed in several Time-Differential γ - γ Perturbed-Angular-Correlation (PAC) experiments when the probe isotope ^{111}Cd , obtained after the electron-capture (EC) decay of its parent ^{111}In , was used in certain semiconducting and insulator oxides. These dynamic interactions are originated in the electronic relaxation of the probe atom, usually called "after-effects" (AE), which follows the EC decay of the ^{111}In isotope. This relaxation must occur during the life time of the intermediate-sensitive-nuclear state of the γ - γ cascade, time-window in which we measure the hyperfine interaction at the probe nucleus with external fields by means of the PAC technique. Up to now it was believed that the ECAE can only be detected if the probe atom was a non-isovalent impurity in the system under study.

Following these ideas, we present here results of PAC experiments performed in an oxide, ZnO, where the ^{111}Cd probe atom is an isovalent impurity. But this time the observed behavior will be analyzed enlighten by recent *ab initio* calculations of the electric-field gradients (EFG) as a function of the charge state of the Cd atom.

PAC experiments carried out on ^{111}In -diffused polycrystalline ZnO have been performed in order to measure the EFG at (^{111}In (EC) \rightarrow) ^{111}Cd nuclei located at the cation site of the ZnO crystal structure. The PAC experiments were performed in the temperature range 77 K-1075 K. The presence of dynamic hyperfine interactions with low intensity was observed, fitting the spectra with a perturbation factor based in the Båverstam and Othaz model [U. Båverstam et al., Nucl. Phys. A 186, 500 (1972)]. The experimental results were compared with *ab initio* calculations performed with the Full-Potential Augmented Plane Wave plus local orbital (FP-APW+lo) method, in the framework of the Density Functional Theory

(DFT), using the Wien2K code. The dependence of the EFG at the Cd sites as a function of the charge state of the supercell was determined. From this *ab initio*-experimental comparison we can correlate the strength dynamic hyperfine interaction with the dependence of the EFG on the charge state of the impurity Cd atom.

1 - 27 – Synthesis and characterization of thin films of Zn-Mn - Al - O system obtained by PLD

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Among semiconductor II-IV compounds, oxide zinc (ZnO) is one of the most promising for technological applications for its optical, electrical, piezoelectric and magnetic properties. In particular ZnO films exhibit unique properties that are appropriate for devices and magnet-optics applications. Incorporating aluminum and manganese allows obtaining a material known as diluted magnetic semiconductor (DMS) that continues showing a high bandwidth prohibited, retains its transparency in the visible range and is able to generate a magnetic order at room temperature. Starting from precursors ZnO, MnO_2 and Al_2O_3 , by conventional ceramic method were obtained powders, ZnO + 3% wt. of Al, + 2% ZnO at. Mn, + 2% ZnO at. Mn + 3% wt. of Al, and ZnO + 5% at. Mn + 3% wt of Al. These materials cold pressed to make the targets employees in pulsed laser deposition (LDP). (Deposits were made using a Nd-YAG (532 nm) laser in atmosphere oxygen on a substrate (SI 100) / SiO_2 /nitride) at 450 °C. The structural properties-obtained by DRX - and magnetic properties of powders and films were compared. Also the films were characterized surface and morphologically; determining presence of oxide of zinc and other oxides of Mn in powders samples. Also Zn oxide is detected in all films. Contrary to expectations, ferromagnetic ordering has not been detected, in films at room temperature.

1 - 28 – Structural and magnetic properties of pyrochlore $Gd_{2-x}M_xRu_2O_7$ (M = Ho, Y)

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Compounds with the pyrochlore structure, face centered cubic $A_2B_2O_7$, have been intensively studied in recent years due to its variety of properties arising from the different elements that can occupy the sites A and B. In this work, we present a systematic study of structural and magnetic properties the ruthenium pyrochlores $Gd_2Ru_2O_7$ as well as the effect of doping Gd site in the structure $Gd_{2-x}M_xRu_2O_7$ (M= Ho and Y). The X-ray diffraction patterns were analyzed by Rietveld refinement, allowing the identification of single-phased compounds and verification of the lattice parameter contraction with increasing doping concentration according to Vegard's law, independent of the dopant. The study of magnetic properties show that doping with Ho and Y, in site of Gd ions causes an increase and a dilution in magnetic moment of the compounds, respectively. The Curie constant and Weiss temperature calculated from experimental data show an indication of antiferromagnetic ordering below 35 K, in both compounds studied. It was verified that the addition of Ho increases the magnetic response of the material and decreases sharply the magnetic irreversibility present in the pristine sample, observed in the temperature range 9 - 16K. We conclude that by adding Ho one can tune the magnetic ordering of the sample by changing it from antiferromagnetic, in the absence of Ho, to ferromagnetic in the absence of Gd. It is observed that the Y doped samples preserves the magnetic order of the compound. It presents an antiferromagnetic order for all the dopant concentration studied. Nevertheless, it was also found that by increasing Y one can get a spin glass behavior. Work financed by CAPES, CNPq and FACEPE.

1 - 29 – Magneto-optic study of the behavior of magnetic domains walls in ferrimagnetic garnet films placed over samples with in-plane magnetization.

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Magneto-optic (MO)imaging is based on Faraday rotation of a linearly polarized incident light beam illuminating a sensitive MO layer placed in close contact to the sample. For in-plane magnetized layers of $Lu_{3-x}Bi_xFe_{5-y}Ga_yO_{12}$ ferrimagnetic garnet films, zig-zag domain formation occurs whenever the sample stray parallel field component changes sign. In this work we study the behavior of zig-zag domain walls that appear when the garnet is placed over samples with in-plane magnetization like audio tapes recorded with different signals. We describe the zig-zag walls considering the anisotropy, exchange and magneto-static energies in the Neel tails and the contribution of an applied magnetic field. Using different recorded signals we have been able to control the gradient of stray parallel field component on the garnet, changing the distance between domains and the size of zig-zag walls. We could even avoid the appearance of these zig-zag domain walls and obtain closed domains structures. We also study the behavior of the domain walls when an external magnetic field is applied parallel to the sample.

1 - 30 – Magnetic properties of Co doped $CeO_{2-\delta}$ nanopowders.

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The development of spintronics has promoted the study of materials with strong coupling between their electric and magnetic properties. For that kind of applications, the materials should have a high spin polarization and also present structural compatibility with existing semiconductors. Among materials that meet these requirements are the diluted magnetic oxides such as Co doped CeO_2 . The pure compound is a diamagnetic insulator, but on doping with magnetic ions like Co, Mn or Fe, the system can become paramagnetic or ferromagnetic. The great capability to accommodate oxygen vacancies in its structure seems to be the responsible for this particular behavior. In this work we study the magnetic properties of Co doped CeO_2 nanopowders, as a function of doping and the relative concentration of oxygen vacancies, by performing thermal treatments of the samples in a vacuum chamber. Our results indicate that magnetism is enhanced in samples with higher concentration of oxygen vacancies.

1 - 31 – *Ab initio* study of F-centers in alkali halides

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The structural and electronic properties of an electron trapped at vacant anion sites in alkali halides (F-center) have been investigated using *ab initio* band-structure calculations with the super-cell method. Despite of the underestimated transition energies we could obtain a qualitative agreement with the known experimental UV/Vis absorption energies.

We used the Full-Potential Linearized Augmented Plane Waves plus local orbital (FP-APW+lo) method in the framework of the Density Functional Theory (DFT), with a vacancy dilution of 1:64 in order to determine the spatial electronic charge density and the vertical transition energies.

1 - 32 – Electric-Field Gradients at ¹⁸¹Ta impurities in Sc₂O₃ semiconductor

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In this work we present a combined *ab initio* and experimental study of ¹⁸¹Ta-doped Sc₂O₃ semiconductor. An extrapolation to 0 K of the experimental electric-field gradient (EFG) results obtained by Perturbed Angular Correlations (PAC) as a function of temperature suggested a reinterpretation of the charge state of the impurity in this semiconductor.

The experimental temperature dependence of the EFGs at ¹⁸¹Ta probes located at defect-free cation sites C and D of the Sc₂O₃ structure was determined in the range 373 K - 1173 K.

The theoretical calculations were performed at diluted Ta impurities located at both cationic sites, using the Full-Potential Augmented Plane Wave plus Local Orbital (FP-APW+lo) method in the framework of the Density Functional Theory (DFT), with a impurity dilution of 1:32. The structural atomic relaxations and the EFGs were studied for different charge states of the cell in order to simulate different ionization states of the double donor Ta impurity (with a

neutral cell, and removing 1 or 2 electrons from the cell). These APW+lo results were found to be in excellent agreement with the experimental values.

1 - 33 – Dielectric and impedance spectroscopy studies on YBa₂Cu₃O_{7-δ}-Sr₂YSbO₆ composites

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We have studied the dielectric behaviour of YBa₂Cu₃O_{7-δ}-Sr₂YSbO₆ composites as a function of YBa₂Cu₃O_{7-δ} and Sr₂YSbO₆ volume fractions. Frequency dependence of complex impedance spectroscopy studies have been investigated in the frequency range from 1 Hz to 100 kHz. The experimental results showed that the composite undergoes a change in the electric behaviour, from resistive to dielectric for ~ 0.24 YBa₂Cu₃O_{7-δ} volume fraction. Fitting of permittivity in function of YBa₂Cu₃O_{7-δ} volume fraction shows a percolative behaviour, with a sudden change of permittivity value at percolation threshold of 0.24. The critical exponent for the permittivity is $u = 0.78$, which is in agreement of percolation theory. The complete study of the dielectric characteristics in function of volume fraction of components and of the frequency is discussed.

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1 - 34 – Structural and Magnetical properties of La(Fe, Cr, Mn)O₃ nanostructured systems

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The nomenclature *multiferroics* has been used to name materials in which two or more ferroic ordering simultaneously, i. e., ferroelectrics, ferromagnetics, and ferroelastics coexist in the same phase [1,2]. These materials have attracted innumerous researchers because of its perspectives of both fundamental physics and practical applications have to offer [3]. Although there exist many works in literatura devoted to the materials in bulk form, few works in these nanostructured materials have been reported in literature.

Besides, these materials are not easy to produce as single phase. In this sense, we have studied the synthesis process of $LaMTO_3$ (MT = Mn, Cr and Fe) in both bulk and nanostructured form using co-precipitation method. X-ray diffraction results added to the Rietveld refinement analysis confirm the formation of the crystalline phase of $LaFeO_3$, $LaCrO_3$ and $LaMnO_3$ identified as system orthorhombic, rhombohedral and orthorhombic, respectively with particles average size among 25 and 70 nm, calculated using Scherrer equation. DC-magnetization measurements carried out on a magnetometer SQUID point out an increasing in the magnetization with decreasing particles size. Beside, the magnetization measurements as a function of temperature show a change in T_N for samples obtained at different temperature, in which we have associate to the particle size. These results show to be promise with respect to the possibility of making small multiferroic nanostructures for future technological applications. (CNPq)

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[2] G.A. Smolenskii and I.E. Chupis, *Sov. Phys. Usp* **25**, 475 (1982).

[3] Y. Wang, *Appl. Phys. Letters*, **88**, 142503 (2006).

1 - 35 – Non equilibrium Thermodynamics and entropy production spectra: a tool for ferrimagnetic materials characterization under electromagnetic field applied

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The entropy production and its evolution in the frequency domain upon application of electromagnetic fields to ferrite materials has been investigated. The spectral entropy of $NiZn$ ferrites doped with different amount of SiO_2 has been studied by numerical simulation. The system under the application of oscillating electromagnetic field is out of equilibrium, since there are entropy production due to dielectric and magnetic polarization. A system subjected to applied electromagnetic fields $E(\omega)$ and $H(\omega)$ at constant temperature T has been considered. For the numerical simulation of the behavior of the entropy production due to the magnetic relaxation a recent published causality model has been used. For the dielectric relaxation the well known Cole-Cole model has been used. The behavior of the entropy as a function of the frequency with the correlation of the amount of SiO_2 has been analyzed in terms of entropy production due to increasing the electric resistance between the boundary grains and the response of the magnetic

and dielectric properties. Entropy production related to magnetic response could be associated with domain wall resonance and spin rotation relaxation. Entropy production related to dielectric processes could be associated with the delay of the different components of the polarizability as a function of the frequency of the applied field and the correlation with the transport charge mechanism in the material. Then the entropy spectra will be transformed in a tool for ferrimagnetic material analysis

1 - 36 – Hyperfine interactions and site localization of Sc impurities in Sapphire

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Single electric-field gradient (EFG) obtained from γ - γ Perturbed Angular Correlation (PAC) experiments at $^{111}\text{In}/^{111}\text{Cd}$ impurity sites in $\alpha\text{-Al}_2\text{O}_3$ have been already reported in the literature [1,2]. In these works the hyperfine interaction observed were assigned to ^{111}Cd probes localized at substitutional cation sites in the corundum structure. Nevertheless, other authors [3,4] claimed that the ^{111}Cd isotope could be localized at interstitial sites after the electron-capture decay of ^{111}In .

In this work we present a theoretical study of Sc impurities in $\alpha\text{-Al}_2\text{O}_3$ performing electronic-structure *ab initio* calculations for different impurity charge states and site localizations (substitutional and interstitial) and compare the EFG predictions (in magnitude, orientation and symmetry) with preliminary experimental results obtained in singlecrystals doped with the $^{44}\text{Ti}/^{44}\text{Sc}$ probe. The structural relaxations and the electronic properties induced by the presence of the Sc impurity at both sites (substitutional and interstitial) in the $\alpha\text{-Al}_2\text{O}_3$ lattice are also discussed. The *ab initio* calculations were performed with the FP-APW+lo (Full-Potential Augmented Plane Wave plus Local Orbitals) in the framework of the Density Functional Theory, using the Wien2K code. From the comparison between theory and experiment both substitutional and interstitial scenarios are possible, in order to explain the two hyperfine interactions present in this impurity-host system.

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[2] J. Penner and R. Vianden, *Hyp. Int.* **158**, 389 (2005).

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[4] G. C. Farlow, P. S. Sklad, C. W. White and C. J. McHargue, *J. Mater Res.* **5**, 1502 (1990).

1 - 37 – Magnetic properties of lamellar aluminosilicate structure rich in Fe

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Layers of Si-Al-O can be formed when the ratio $O/(Si + Al) = 2.5$ is obeyed, giving rise to lamellar structures aluminosilicates type, which have interesting physical properties, eg, transport and controlled release of drugs in anti-cancer therapies. In natural samples, there is a very high possibility of ionic exchange, allowing the formation of a lamellar structure consisting of transition metals, particularly iron. Natural samples from the coast of Sergipe, Brazil were collected, washed and separated from sand by a permanent magnet. Analysis by SEM,EDS, XRF and XRD showed a Biotite-like mineral as the major component of the sample. SEM show clearly a lamellar structure presented by typical true micas and in the association with the high level of Iron showed by EDS and XRF analysis and, with help XRD phase identification, this material has a ferriphlogopite-like structure. Another phase founded was a clinocllore-like mineral, namely chamosite and goethite. When in raw mode, the original sample showed the presence of quartz, rutile and possibly crossite. Magnetic measurements (saturation magnetization, remanence magnetization and coercive force) and the anisotropy constant $K(T)$ have been determined at room temperature and at low temperatures using magnetic fields up to 7 T. Influenced by the lamellar structure, the average value of K for an applied field parallel to the lamellae, was 2082 and 3.3 *emu.Oe/g* at 2 and 300 K, respectively. For an applied magnetic field perpendicular to the lamellae, was 1338 and 3.8 *emu.Oe/g* at 2 and 300 K, respectively. The H_c versus T curve showed a minimum of 34 Oe about 15 K due to the presence of pseudo-single-domains probably formed by the buildup of $\alpha FeOOH$, revealed by analysis of SEM.

1 - 38 – Synthesis and structural and electrical characterization of new materials $Bi_3R_2FeTiO_{15}$

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In this work we report the synthesis of polycrystalline samples of Bi_5FeTiO_{15} (BFT) and $Bi_3R_2FeTiO_{15}$ compounds with

$R = Nd, Sm, Gd, Dy, Ho, Yb$. The materials were synthesized by the standard solid state reaction recipe from high purity (99.99%) powders. The structural characteristics of materials were analyzed by x-ray diffraction experiments. Results reveal that materials crystallized in orthorhombic single-phase structures and space group to be $Fmm2$, Rietveld refinement by the GSAS code was performed, taking the input data from the ICSD 74037 database. Measurements of polarization as a function of applied electric field were carried out by using a Radiant Technology polarimeter. We obtain a hysteretic behavior, which is characteristic of ferroelectric materials that can be used as nonvolatile memories. Rapid growth is appreciated on the $2E_c$ and $2P_r$ with increasing external electric field applied to polarize the compound.

1 - 39 – Magnetic properties of the disordered barium titanium manganite $BaTi_{1/2}Mn_{1/2}O_3$.

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Oxides materials with perovskite structure are outstanding examples of materials used in technological applications as well as in fundamental studies in condensed matter physics because of the observed ground states which include multiferroicity, high-temperature superconductivity, colossal magnetoresistive effects, ionic conductivity, etc. The ideal formula unit is ABO_3 , where A is a large cation, e.g. K, Sr, Ba, La, and B is a smaller cation like Ti, Mn, Co, Ni. When a second (B') transition metal atom is added to the above structure, an ordered double perovskite type structure $A_2B'B''O_6$ (where $B', B'' = 3d, 4d, 5d$ metals) as well as a disordered $AB'_{1/2}B''_{1/2}O_3$ perovskite-type structure might be formed, which have attracted great attention due to their potentiality as magneto-electronic devices.

In this work we present the results of the low temperature specific heat and magnetization measurements as well as the high temperature magnetization data of the barium titanium manganite $BaTi_{1/2}Mn_{1/2}O_3$. This 12R-type hexagonal perovskite is a modest dielectric insulator at room temperature with high permittivity at both radio and microwave frequencies and its magnetic behavior as a function of temperature remains unclear. We have performed detailed specific heat and magnetization measurements as a function of the applied field and temperature in order to understand the detailed magnetic behavior of the Mn^{+IV} ions. Our results show

the presence of a ferromagnetic phase at high temperature ($T > 300$ K) coexisting with a previously reported low temperature antiferromagnetic phase. We evaluate and discuss the mechanisms that drive the coexistence of the magnetic interactions.

1 - 40 – Magnetic measurements in double perovskite $\text{Ca}_2\text{FeMoO}_6$ single crystal

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In the 1990's decade materials exhibiting colossal magnetoresistance (CMR) were widely studied due to technological interest. A range of compounds were found to exhibit intrinsic CMR, most of them are manganese perovskites based on LaMnO_3 . A few years later, some members of the family of double perovskites of composition A_2MTO_6 (A = alkali earths, M , T = transition metals) have been proposed as halfmetallic ferromagnets, as an alternative to perovskite manganites. We focused our attention on the Ca analogue of the A_2FeMoO_6 family. $\text{Ca}_2\text{FeMoO}_6$ perovskite has been prepared in single crystalline form by a floating zone technique as described elsewhere.[1] This high quality material has been studied by X-ray powder diffraction (DRX), thermal analysis, and magnetic measurements. The crystal structure is monoclinic, space group $\text{P}2_1/\text{n}$, with $a = 5.41(1)$ Å, $b = 5.52(1)$ Å, $c = 7.71(2)$ Å, and $\beta = 89.9(8)^\circ$ at room temperature (RT). The crystal contains alternating FeO_6 and MoO_6 octahedra, considerably tilted due to the relatively small size of the Ca^{2+} cations. Magnetization as a function of temperature indicates a Curie temperature of 380 K, in agreement with the obtained by others authors in polycrystalline sample.[2] The dependence of magnetization with magnetic field at 5 K, 100 K and 300 K are typical of a ferromagnet with a saturation magnetic moment of approximately $2.1 \mu_B$, $2.0 \mu_B$ and $1.4 \mu_B$ per formula unit, respectively. Magnetism indicate a large component of itinerancy for down-spin Fe t_{2g} electrons. M

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1 - 41 – Electromagnetic properties of lithium zinc ferrites doped with aluminium

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Ferrites form a very good class of electrical materials because of their high resistivity and low loss behaviour, and hence have vast technological applications over a wide range of frequencies. Ferrites assume special significance in the field of electronics and telecommunication industry because of their novel electrical properties which makes them useful in radiofrequency circuits, high quality filters as electromagnetic interference (EMI), rod antennas, transformer cores, read/write heads for high digital tapes and other devices. The dielectric properties of ferrites are dependent on several factors, such as method of preparation, heat treatment, sintering conditions, chemical composition, cation distribution and crystallite size. We present the results of the effect of Al substitution on the magnetic and electrical properties of $\text{Li}_{0.2}\text{Zn}_{0.6}\text{Fe}_{2.2-x}\text{Al}_x\text{O}_4$ ferrites (where $0 \leq x \leq 0.5$) prepared by the standard ceramic technique. The characterization has been performed using XRD, SEM, magnetic and dielectric response in frequency. XRD analysis confirms that the system exhibits polycrystalline single phase cubic spinel structure only to low dopant content. Dielectric loss tangent are lower by replacing in the whole frequency range analyzed. Doping decreases the conductivity of the ferrite in more than two orders of magnitude. Reflection losses has a maximum near 50MHz for $x=0$ and they decrease significantly to high levels of aluminium. these ferrites can be used as EMI devices.

1 - 42 – Determination of critical exponents of inhomogeneous Gd films

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An understanding of thermal phase transition behavior of inhomogeneous ferromagnets has been an outstanding problem in the science of magnetism. On the other hand, homogeneous magnetic films have been an important case study due to the fact that their universality class is relatively well understood and adequate fabrication methods have been devised. In this work, we explore the role of inhomogeneity on the critical behavior of Gd films. The films were prepared as $\text{Cr}(50\text{nm})/\text{Gd}(100\text{nm})/\text{Cr}(50\text{nm})$ multilayers grown onto $\text{Si}(110)$ single crystal substrates by

means of ultra high vacuum sputter deposition. The sample inhomogeneity was controlled by annealing at different temperatures, $T = 500, 400,$ and 200 C). VSM magnetometry was used for the magnetization M vs. T measurements at different external fields H . To extract the critical exponents and the distribution of intrinsic Curie temperatures T_c we applied a linear superposition theory [1] which views the $M(T)$ dependence as a distribution of power laws centered at specific T_c s. We found that this method allows us to extract reliable values of the critical exponents for all annealing temperatures, which enabled us to study the effects of disorder onto the universality class of Gd-films.

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1 - 43 – Synthesis and characterization of cobalt-doped manganese oxides

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In this work, cobalt doped and undoped manganese oxides materials were synthesized by soft chemical reactions, specifically by oxido-reduction method, which allows us to generate metal mixed oxide. The synthesized materials were characterized using chemical analysis which shows the presence of cobalt, XRD reveals a spinel type structure and SEM analysis shows morphology with fine aggregate of particles. Vibrating sample magnetometry was used to determinate the hysteresis loops at different temperatures. We observed different magnetic behavior, when the manganese oxide material is cobalt doped.

1 - 44 – Structural and electronic properties influenced by high pressure in $\text{La}_{0.325}\text{Pr}_{0.300}\text{Ca}_{0.375}\text{MnO}_3$

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Because of the strong coupling between their different degrees of freedom (i. e. magnetic, electronic and structural), manganites are nowadays one of the most studied in the family of strongly correlated electrons systems. The enormous capacity of tuning its properties by the application of moderated

external excitations (magnetic and electric field, hydrostatic pressure, etc.) converts manganites in one of the most investigated systems for potential technological applications. The effect of high pressure in the structure of manganites is one of the less studied topics, mainly due to the complexity of the experimental procedure. In this work we have studied the temperature-magnetic field-pressure phase diagram of $\text{La}_{0.325}\text{Pr}_{0.300}\text{Ca}_{0.375}\text{MnO}_3$ using magnetization (M), X ray diffraction (XRD) and resistivity (R) measurements. At room pressure, we observed a paramagnetic state above 220K, followed by a region of coexistence of ferromagnetism and charge ordered phase between 200K and 75K, and a purely ferromagnetic state below 75K. The existence of all these phases has been shown by different techniques like M , XRD and R . In this presentation we will show the effect of external applied pressure on the transport and the structure up to 300kbar. We will correlate the crystallographic and the electronic phases in order to clarify the phase diagram.

1 - 45 – Magnetic Hydrophobic Nanocomposites: Silica Aerogel/Maghemite

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In this work we present a new material: Magnetic hydrophobic aerogels (MHA). It consists of iron-oxide nanoparticles hosted in hydrophobic silica aerogels. In this work, we discuss about the fabrication and characterization of this nanocomposite. We also investigate the relation between the MHA's porosity and magnetic nanostructure.

Silica aerogel/iron oxide nanocomposites were fabricated by means of the sol-gel process followed by supercritical drying. The gel obtained in this process was synthesized from tetraethylorthosilicate (TEOS) and methyltrimethoxysilane (MTMS), with a molar ratio $\text{MTMS}/\text{TEOS} = 0.5$. MTMS was added to achieve the aerogels' hydrophobic property. As Fe oxide precursor, we incorporated iron nitrate. We fabricated samples with different $m_{\text{Fe}}/m_{\text{Si}}$ ratios: 0.083, 0.207, and 0.330. The molar ratios $\text{alcohol}/\text{TEOS} = 2.3$ and $\text{H}_2\text{O}/\text{TEOS} = 1.8$ were kept fixed in all of them.

The structural and magnetic properties of $\text{Fe}_2\text{O}_3 - \text{SiO}_2$ nanocomposite porous aerogels were systematically investigated by XRD, Mössbauer Spectroscopy, TEM, SQUID magnetometry and with SAXS and XAF by using synchrotron radiation at LNLs.

These materials exhibit an accessible internal porous structure, both in the meso and in the micro

scale. Porosity structure was studied by SAXS and displays the typical fractal power law behaviors with primary particle radius of 20 nm.

Field cooled and zero field cooled magnetization curves indicate that the composites behave as an assembly of non-interacting superparamagnetic nanoparticles for the three compositions studied. The samples become blocked at a temperature TB between 27 and 40K.

Direct magnetic particle size determination is not an easy task because these materials exhibit low crystallinity and low contrast for TEM. Here we attempt this determination using SAXS: hydrophobicity allows the aerogel to be loaded with an organic liquid to lower the silica/porous contrast and highlight the nanoparticle/silica contrast. Contrast studies and the feasibility of a direct determination of magnetic structure from the scattering data are discussed.

The results provide new insights into innovative materials and on the relation between the compositional and microstructural features, and the properties of magnetic nanocomposite.

1 - 46 – Specific Loss Power of ferrofluids under Radiofrequency fields

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Ferrofluids (FF) are liquid suspensions of magnetic nanoparticles. When FF are submitted to a radiofrequency (RF) magnetic field, the nanoparticles dissipate energy. In the case of single domain particles two relaxation mechanisms exist, known as Néel and Brown mechanisms. Néel relaxation depends on particle magnetic anisotropy, whereas Brown relaxation depends on fluid viscosity. Both types of relaxation depend on temperature and particle size, but through different functional expressions. Except for the infrequent situation in which the two relaxation times are equal, relaxation occurs almost entirely by one of the two mechanisms.

In this work we study aqueous FFs of $Zn_xFe_{3-x}O_4$ ($0 \leq x \leq 0.5$). We have determined the FF Specific Loss Power (SLP), defined as the power dissipated per mass unit of nanoparticles, as a function of RF field parameters (amplitude H_0 and frequency f) and FF concentrations. H_0 was varied up to 700Oe and discrete f values between 160 kHz and 260 kHz were used. The nanoparticles mass/water volume ratio, $R = m_{NP}/V_{FF}$, was varied from about 1 g/l to 10 g/l.

We observed that measured SLPs did not depend on R . On the other hand, SLP f and H_0 dependences deviate slightly but clearly from the behaviors found

in the literature. It was reported that SLP depends linearly and quadratically with f and H_0 , respectively [1]. The experimental results indicate that for field amplitude larger than about 500 Oe, SLP increases at a slower rate than predicted by the power H_0^2 law, suggesting saturation effects. Simulations based on the Stoner-Wholfahrt model modified for finite temperature conditions, give a consistent account of the observations. The simulations illustrate how the M-H minor loops shape determines the previously mentioned dependences.

[1] Kallumadil, M., Tada, M., Nakagawa, T., Abe, M., Southern, P., Pankhurst, Q.A., *Journal of Magnetism and Magnetic Materials* 321 (2009) 1509-1513.

1 - 47 – Electrical transport properties of manganite powders under pressure.

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We have measured the electrical resistance of micrometric to nanometric powders of the $La_{5/8-y}Pr_yCa_{3/8}MnO_3$ (LPCMO with $y=0.3$) manganite for hydrostatic pressures up to 4 kbar. By applying different final thermal treatments to samples synthesized by a microwave assisted denitration process, we obtained two particular grain characteristic dimensions (40 nm and 1000 nm) which allowed us analyze the grain size sensitivity of the electrical conduction properties of both the metal electrode interface with manganite (Pt / LPCMO) as well as the intrinsic intergranular interfaces formed by the LPCMO powder, conglomerate under the only effect of external pressure. We also analyzed the effects of pressure on the phase diagram of these powders. Our results indicate that different magnetic phases coexist at low temperatures and that the electrical transport properties are related to the intrinsic interfaces, as we observe evidences of a granular behavior and an electronic transport dominated by the Space Charge limited Current mechanism.

1 - 48 – Resistive switching topology in metal-complex oxide interfaces

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In order to determine the key parameters that control the resistive switching mechanism in metal-complex oxides interfaces, we have studied the electrical properties of metal / YBa₂Cu₃O₇ (YBCO) interfaces using metals with different oxidation energy and work function (Au, Ag, Pt) deposited by sputtering on the surface of a YBCO ceramic sample. By analyzing the IV characteristics of the contact interfaces and the temperature dependence of their resistance, we inferred that ion migration may generate or cancel conducting filaments, which modify the resistance near the interface, in accordance with the predictions of a recent model.

1 - 49 – Electric transport through nanometric CoFe₂O₄ thin films investigated by conducting atomic force microscopy

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The ferrimagnetic insulating spinel CoFe₂O₄ (CFO) is considered a promising candidate material for spintronic devices, e.g as spin filtering tunnel barrier capable to work at room temperature. However, although spin filtering through CFO thin films has been successfully demonstrated, up to now reported efficiencies are clearly below expectations.

In the search of optimized CFO thin films, we have used conducting atomic force microscopy (CAFM) to perform a systematic study of electric transport through thin (1-8nm) CFO films deposited on SrRuO₃ thin film bottom electrodes. Samples were grown on (111) and (001) oriented SrTiO₃ substrates using either rf sputtering or pulsed laser deposition (PLD).

Experimental procedures to investigate tunnel transport through thin insulating films by CAFM are revised. The potential of differently prepared CFO films for the use as spin filtering barrier is assessed. Samples prepared by PLD on SrRuO₃/SrTiO₃ (001) are found to offer improved properties compared to rf sputtered CFO thin films.

1 - 50 – Light induced negative magnetoresistance in ZnO Films.

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Transient photoconductivity and magnetotransport measurements were used to investigate the spin interaction in pure ZnO thin films grown under N₂ pressure. Light induced temperature dependent negative magnetoresistance was measured at 300K in ZnO films growth on c-plane Al₂O₃. There is a correlation between the magnetoresistances and the existence of defect-induced magnetic order already reported in these films. The oxygen and/or nitrogen 2p orbitals are responsible of the magnetic exchanges interaction. The experimental results support theoretical predictions of photoinduced ferromagnetism interaction in diluted magnetic semiconductors.

1 - 51 – Effects of Dopant Cation Order in 3D and Layered Perovskite Manganites

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The 3-dimensional and layered La,Sr-doped manganites, (La_{1-x}Sr_xMnO₃)_n·SrO, exhibit a delicate interplay between charge, spin and orbital degrees of freedom which gives rise to a number of intriguing collective states. Depending on cation doping (x) and dimensionality (n), these materials can exhibit ferromagnetic, antiferromagnetic, charge and orbital ordering. Recently, our group has shown that ordering the A-site cations through the atomic-monolayer control of molecular beam epitaxy can uncover additional physics in the 3-dimensional (3D) systems, including a metal-insulator transition, higher anti-ferromagnetic ordering temperatures, and modulated in-plane ferromagnetic and antiferromagnetic ordering as a function of depth. Here, we investigate the effects of A-site cation order on the magnetism, transport and magnetotransport of two related systems: (1) the 3D, ferromagnetic and colossal magnetoresistant La_{1-x}Sr_xMnO₃ (x=1/3) and (2) its 2-dimensional analog, single layered La_{1-x}Sr_{1+x}MnO₄ (x=1/3), which in bulk only exhibits a spin-glass phase below 20K. We find that in both systems, while the in-plane magnetism appears largely unaffected

by the dopant cation order, the out-of-plane magnetism perpendicular to the cation-ordered sheets is enhanced. Additionally, in the single layer manganite, large differences in magnetic anisotropy and low temperature transport mechanisms between the cation ordered and disordered films suggest that ordering the dopant cations in this layered compound results in a new preferred orbital ground state.

1 - 52 – Electric Pulse Induced Resistive Switching Contacts for Non Volatile Memory Devices

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Non volatile memory concepts for electronic applications are presently based on resistance change rather than in charge storage. Electric pulse induced resistance switching (RS) was shown to produce useful retention time capability for massive applications. Several basic and applied research teams are presently devoted to the study of transition metal oxides contacted through metal electrodes driven by appealing fast switching and scalability.

We study manganite (LaPrCaMnO) and titanium dioxide (TiO) samples contacted with metallic electrodes, under different experimental conditions. Evidence for an oxygen diffusion mechanism by means of electric transport measurements was obtained using the Hysteresis Switching Loop procedure in which pulses of varying amplitude determine the state of the interface, and a small bias is used to test the remnant state, in a loop mode. Obtained results can be explained by oxygen vacancy detrapping at the oxide-metal interface. Besides, we study the characteristics of RS applying a closed-loop control protocol of the amplitude pulse to attain a certain resistance level.

Low dimensional systems, nanostructured materials, and nanomagnetism

2 - 1 – B3LYP/cc-pVTZ study on the growing pattern of small Al/P clusters

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Semiconductors formed by group 13/15 elements have growing importance due to the potential application in the preparation of thin films for electronic devices [1]. The interest in the study of AlN atomic clusters is based on the fact that the application in thin films requires a profound understanding of properties at atomic level as well as the growing pattern followed by the aggregates.

Results obtained for clusters up to five atoms are reported, with emphasis on the growing pattern followed for the aggregates. Al/P aggregates were studied with tools from density functional theory (DFT); using the B3LYP hybrid exchange and correlation functional [2], with cc-pVTZ triple- ζ basis functions [3], as implemented in the Gaussian 03 program [4]. Equilibrium geometries were obtained starting from the AlP dimer and adding up aluminium and phosphorus atoms to grow the aggregates. The increase in the binding energy per atom was used to evaluate the growing. The preferred growing pattern was found to be AlP (³A) - AlPP (²A) - PAIPP (³A) - PPAIPP (²A). Molecular electrostatic potentials (MEP), spin densities and charges derived from electrostatic potentials were calculated to get a quantitative picture of the whole process. It is found that Al-P clusters tend to grow following a non planar pattern, preferring zones in which MEP's are negative and where unpaired electrons are located.

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[2] A. D. Becke and J. Chem. Phys. 98 (1993) 5648; C. Lee, W. Yang and R. G. Parr, Phys. Rev. B 37 (1988) 785.

[3] T. H. Dunning, Jr. J. Chem. Phys. 90 (1989) 1007; T. H. Dunning, Jr. J. Mol. Struct. 388 (1996) 339.

[4] M. J. Frisch, et al., Gaussian, Inc., Wallingford CT, 2004, Gaussian 03, Revision D.01.

2 - 2 – Theoretical study of the structural, electronic and magnetic properties of small Molybdenum clusters and their reactivity towards H₂ adsorption and dissociation

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Small neutral and ionic Mo_N clusters, with N = 2-6, are studied within the framework of the density functional theory (DFT) [1]. After an extensive test of several exchange and correlation functionals, it is found that the BLYP one [2] provides the best results for some selected properties of atomic Mo and Mo₂. In all cases, the basis functions used are of triple-zeta quality with polarization functions. The calculations are carried out with the ADF program [3-5]. Geometries of isolated clusters are optimized without symmetry constraints. The electron spin multiplicity is also considered as a variable during optimizations. Eigenvalues of the hessian matrix are determined to confirm that the optimized structures are indeed minima on the potential energy surface of the aggregates and not saddle points. For the most stable clusters of every size, the interaction of the hydrogen molecule with different possible sites are investigated. Special emphasis is laid on those sites being able to dissociate the molecule.

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2 - 3 – Thermoelectric effects in the (111)-FCC Al surface coupled to an interacting quantum dot

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We study the thermoelectric transport properties through the (111)-FCC Al surface coupled to a gate-defined quantum dot (QD). The local density of states (DOS) for the surface have been calculated using the Quantum-EXPRESSO package, which calculates the electronic-structure properties within Density-Functional Theory, using a Plane-Wave basis

set and pseudopotentials. The calculations were carried out with a (1×1) slab of five atomic layers. We obtain the surface Green's function (GF), linked to the (111) -FCC Al plane, using that surface DOS. The interaction between the QD and the surface is described employing the Anderson impurity model (AIM), in the frame-work of the Atomic Approach [1]. The localized state in the AIM is linked with the QD, considering finite U electronic repulsion inside it, the surface is associated with the continuous states in the model. The thermoelectric transport coefficients were obtained by the Keldysh non-equilibrium GFs technique with the Onsager relation in the linear regime automatically satisfied [2]. We compute the thermopower S , linear thermal conductance K , linear electric conductance G and the thermoelectric figure of merit Z , for all the regimes of the system, as function of the QD energy and the temperature T . Our results are similar to the obtained for a quantum wire with a side coupled QD [3,4] and for metallic surfaces with Kondo absorbed impurities (G results) [5]. We discuss the possibility of practical applications of the system in mesoscopic cooling process, based in the results of the ZT product.

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2 - 4 – Magnetic and structural properties of $Co_{1-x}TM_x$ (Fe, Cr and Mn) nanoparticles

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In the last years metal nanoparticles have drawn much attention because of their potential for development in building ultrahigh density hard drives, devices for biomedical applications and chemical sensing [1,2]. Therefore, for that materials can to have applications is necessary a good control of well-defined size, geometry and surface chemistry effects for minimize coalescence between the particles. In this sense several synthesis process (chemistry and physics) have

been extensively investigated. In this work we have studied the structural and magnetic properties of $Co_{1-x}TM_x$ (Fe, Mn and Cr) nanocrystalline alloys using X-ray diffraction and magnetic measurements. The nanocrystalline alloys were obtained chemical route via co-thermolysis of metallic acetylacetonate precursor in oleylamine surfactant/phenylether at low temperature ($TS \approx 250^\circ C$). X-ray diffraction results and Rietveld refinement analysis show for samples with concentrations lower than 20% of TM, the crystalline structure is similar to the cubic structure of the Co with average size of 5 nm. Magnetizations measurements as function of field show that the particles present to be soft magnetically. Zero-Field-Cooling and Field-Cooling magnetization curves suggest that the surface anisotropy prevail at low temperature and the systems are strongly interacting and same for samples disperse on the polymeric matrix. Transmission Electronic images would be shown to verify the morphology and size distribution of the nanoparticles. (CNPq)

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[2] S. Sun *et al.*, *Science* **287**, 1989 (2000).

2 - 5 – Fe-based bulk metallic glass plates with Y and Gd addition

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Fe-based bulk metallic glasses (BMG) have been developed since 1995 and achieve an interesting combination of physical and mechanical properties. While conventional metallic glasses require rapid solidification with a cooling rate of about 10^6 K/s, BMGs can be formed at cooling rates between 1 and 100 K/s, leading to the possibility of casting much thicker objects. At first, Fe-based BMGs were developed with the purpose of obtaining very good soft ferromagnetic properties owing to the structural isotropy of the material (high Fe content alloys in Fe-B-Si system). However, during the last decade, researchers were able to prepare these materials with less Fe content, so that they become paramagnetic at room temperature. These materials were named structural amorphous steels (SAS) [1]. There were then obtained SASs with a maximum thickness of 16 mm, very high strength, high hardness and excellent corrosion resistance, but highly brittle. The aim of this work is to present our recent studies on amorphous alloys with composition (at%) $Fe_{48}Cr_{15}Mo_{14}C_{15}B_6Gd_2$ (A) and $Fe_{48}Cr_{15}Mo_{14}C_{15}B_6Y_2$ (B1). Copper-mold injection

casting in air atmosphere was used to obtain plate samples with a fix thickness of 2 mm and variable lengths between 10 and 20 mm. In order to evaluate the possibility of commercial application of the material, 56% (wt) of B1 alloy was replaced with commercial AISI430 steel and was cast into rods of 2 mm diameter (B2). The structure and microstructure of the obtained samples was studied by means of optical microscopy, X-ray diffraction and scanning electron microscopy. DSC measurements showed a glass transition temperature of 856 K for alloy A and 841 K for alloy B1, and an onset crystallization temperature of 887 K for alloy A and 885 K for alloy B1. Furthermore, the hardness of the alloy was measured by means of nanoindentation tests and was found to be around 13 GPa for both alloys. The role of Y and Gd on the formation of the glassy phase under adverse casting conditions including air atmosphere and the partial replacement of pure elements with commercial steel will be discussed.

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2 - 6 – Synthesis and characterization of Co_3O_4 Nanoparticles with addition of organic precursor

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In the last years several methods to synthesize nanostructured materials have been extensively explored to control the size, size distribution and morphology. Considerable interest in these properties is related to the good control in the physical properties that these materials can present. Besides of these properties, in particular, the magnetic nanoparticles (NP's) need to be in monodisperse suspensions. The head of this high demand is related to the new physical and chemical properties that arise in these materials with a decrease in their size compared to in bulk form. Thus, it is essential to search for methods of synthesis that produce nanoparticles with controlled size and morphology. In this paper we have use co-precipitation to synthesize Co_3O_4 NP's at low temperature, controlling the growth with the addition of an organic precursor (OP) to study the structural and magnetic properties. The nanoparticles were synthesized at temperatures of 80°C for 72h and 200°C for 3h with and without addition of OP. Results of X-ray diffraction together Rietveld refinement confirmed the formation of single crystalline phase for all samples. The results show that the crystallite average size of the resulting products ranges between 47

and 54nm for samples without addition of OP and a mean of 19nm for samples with OP, respectively. Results of Scanning Electron Microscope show particles with spherical morphology and sizes consistent with those obtained with the Scherrer formula trough values extracted by Rietveld refinement. Preliminary measures of magnetization as a function of applied field at room temperature, show a superparamagnetic behavior. Measurements of magnetization in SQUID magnetometer will be held to a more wide characterization of the magnetic behavior of the samples.

2 - 7 – Monte Carlo simulation of Geometrical Influence on Magnetic Properties of Ferromagnetic Nanotubes

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A computational model was developed for describing magnetic properties of ferromagnetic nanotubes. They were based on the Monte Carlo method with nearest neighbors interaction employing Metropolis dynamics. Magnetization per magnetic site, magnetic susceptibility, ferromagnetic energy and specific heat were computed for nanotubes with square and hexagonal unit cells. These properties were simulated varying parameters as the system size, temperature, and anisotropy; also an external magnetic field was taken into account. The dependence on the exchange parameter of the nanotubes geometrical appearance was also discussed. A strong influence on the magnetic properties, especially the Curie temperature because of the difference in the interactions density of the nanotubes was observed.

2 - 8 – Superparamagnetic nano magnetites forming oriented structures in elastomer composites

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Structured magnetoelastic composites are promising materials for its applications in field sensitive devices, such as field-modulated inductances and sensors of magnetic field and pressure. The central aspect is that smart materials can be obtained by combining the magnetic properties of fillers nanoparticles with the elastic characteristic of a hosting elastomeric polymer matrix, particularly when anisotropy is induced in the composite. In the present work the preparation and characterization of structured composites is presented, using nanoparticles of magnetite as fillers and polydimethylsiloxane (PDMS) as the elastomer matrix. The strategy for obtaining structured magnetoelastomers was preparing the magnetite-PDMS mixture before casting and then curing the mixture in the presence of a uniform, and relatively intense, magnetic field.

Magnetite nanoparticles were prepared by the coprecipitation method, dissolving stoichiometric amounts of the precursors (Fe(II) and Fe(III) chlorides), in acid media, which was added to a basic solution at controlled pH and temperature. The precipitation of dark brown nanoparticles occurred immediately. The obtained material was magnetic, with superparamagnetic behavior at room temperature (determined by Vibrating Sampling Magnetometer, VSM). XRD pattern was compatible with magnetite structure, while SEM images shown particles of 15 nm average size.

Mixtures of magnetite-PDMS at defined proportions were placed for curing inside a cylindrical mould, which is part of a designed device that allows curing the samples at a given temperature in the presence of an applied magnetic field, while rotating the sample at constant speed. Formation of chains (needles) of magnetite aggregates, oriented in the direction of the applied field, appears after polymerization. Chains as long as 1.5 mm length and 40 microns diameters were observed, which are composed by aggregation of particles with individual sizes about 20 nm. Anisotropic effects are under quantification at present, both for the magnetic and elastic properties, by VSM, SQUID and texture analysis(1).

It is remarkable that the anisotropic composite is obtained using superparamagnetic particles, while for the case of cobalt-iron oxides, structured composites were obtained when using ferromagnetic nanoparticles only.

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2 - 9 – Nickel ferromagnetic nanoparticles of different sizes in anisotropic magnetoelastomer materials

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Magnetoelastomers are dispersions of magnetic particles into an elastomer polymer matrix [1,2]. These materials combine magnetic and elastic properties in the same material. In this work, nickel ferromagnetic nanoparticles were synthesized, following Sidhaye et al [3]. The syntheses were performed at different concentrations and temperatures (up to 60° C) in order to explore their influence in the properties of nanoparticles. The X-ray powder diffraction patterns indicate that the formation of Ni nanoparticles is favored at low concentration of reactants and at room temperature. As the concentration of reactants and the temperature of synthesis are increased, formation of hydroxides and oxides nanoparticles of Ni(II) and Ni(III) is observed. SEM images show a significant decrease in the particle size when both the concentration of reactants and temperature of synthesis are increased. VSM (Vibrating Sample Magnetometer) measurements are in good agreement with the results of XRD and SEM. First, in the case of nanoparticles synthesized at room temperature and low concentrations of reactants, a ferromagnetic behavior is observed. Moreover, a saturation magnetization of about 40 emu/g is obtained. Second, with other synthesis conditions, a marked decrease of the saturation magnetization is observed, due to the presence of hydroxides/oxides of Ni(II) and Ni(III). Composites of PDMS (poly-dimethylsiloxane) and nanoparticles synthesized at room temperature were prepared. In the absence of an external magnetic field during curing, composites of uniform distribution of nanoparticles are observed in SEM images. On the other hand, when curing is performed in the presence of an external magnetic field, formation of macroscopic needles oriented along the direction of the magnetic field is observed. Those needles were also observed by SEM, being wider when preparing

composites with nanoparticles with higher saturation magnetization. Finally, the composites were characterized by VSM and texture measurements. From those results it is concluded that the material have both magnetic and elastic anisotropy.

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2 - 10 – Nanostructured ZnO layer fabrication by pulsed electrodeposition for morphology control

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ZnO electrodeposited layers have properties strongly dependent on their morphology. Their applications are directly linked to the obtained properties. On this paper a fabrication method based on pulsed electrodeposition is presented with good results on final morphology control. The samples are fabricated over ITO sputtered glass substrates. Process optimization is guided through AFM analysis of the nucleation stage according to different pulse train designs. SEM characterization and electrochemical techniques allow the evaluation of the morphology and the properties obtained. Optical properties characterization allows a bandgap measurement correlated to the obtained morphology through the Tauc plot.

2 - 11 – Study of Al-doped Zinc Oxide nanocrystalline powders subjected mechanical milling

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The interest in new materials of nano-sized scale for applications in industry, medicine and other fields has led to research in the many ways of producing them with good efficiency and trying to improve the quality of the final products. Of the many techniques of obtaining nanomaterials, mechanical ball-milling has the virtues of being efficient in producing large

amount of material, obtaining incorporation of doping material into the main structure and/or creating blends, alloys, non-equilibrium phases and oxide-reduction reactions, etc. This is of particular importance in the study of semiconductors, like ZnO, whose electrical/optic/other properties can be ameliorated with doping of metals or metal-oxide substances. The aim of this article is to study the final products of milling ZnO powders doped in different proportions (5, 10 and 30 at%) with Al powder. We have used X-ray diffraction (XRD) for following the structural ZnO changes. We have observed that under certain circumstances ZnO can be reduced in milling with Al without obtaining alumina. XRD patterns corroborate the incorporation of aluminum into the wurtzite ZnO structure. Ternary oxides of the form $Zn_{1-x}Al_xO$ are obtained in all samples subjected to 16 hours of milling time. Avoiding the reduction of ZnO in mechanical milling with Al is a question of low doping fraction and large milling duration.

2 - 12 – Ab initio study for ultrathin Fe films onto MnAs

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Recent magnetic anisotropy measurements of Fe thin films epitaxially grown on MnAs/GaAs(001) [Phys.Rev. B 82,094423 (2010)] show that Fe films are magnetically decoupled from the MnAs substrate at low temperatures. This unexpected behaviour motivated us to tackle this system by means of first principles calculations.

We compute the magnetic interaction of Fe ultrathin films onto a MnAs slab taking into account different possible interfaces between them. Our calculations suggest that the Fe magnetic properties are independent of the magnetic configuration of the MnAs substrate and that interfacial effects seem to play an important role in the decoupling mechanism.

2 - 13 – Gas Sensing Properties of Nanostructured MoO₃ Thin Films Prepared by Spray Pyrolysis

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Molybdenum oxides are extremely interesting from a chemical point of view because of their wide exploitation in both, catalytic and industrial processes of

industrial relevance. In recent years, a strong research effort has been made for developing gas sensors based on these materials. In this work, thin films of molybdenum trioxide (MoO_3) were deposited on common glass using the chemical spray pyrolysis technique. A $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24}\text{H}_2\text{O}$ solution 0.1M was used as precursor one. The influence of substrate temperature on the crystallographic structure, surface morphology and electrical behavior of MoO_3 thin films was studied. MoO_3 can exist in two crystalline forms, the thermodynamically stable orthorhombic α - MoO_3 and the metastable monoclinic β - MoO_3 phase. XRD-spectra showed a growth of α - MoO_3 phase percentage as substrate temperature increases from 450K up to 700K. Films deposited in the 500-600K range have a clearly porous surface structure of nanometer order as can be seen in SEM images. Changes up to six magnitude orders were observed in MoO_3 thin films electrical resistance when films temperature varied from 100K up to 500K. The sensing property of these MoO_3 films was also studied. The sensitivity was investigated in the temperature range 160K and 360K for H_2O and CO gases. Both of them are of reducing nature. In all studied cases sensitivity decrease slowly as film temperature is raised. At room temperature the sensitivity changes from 15 up to 70 depending on substrate temperature. The sensitivity for CO gas was found to be lower than that of H_2O .

2 - 14 – Dynamic coercivity of Mo-doped FINEMETs

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Over the past decades, there has been an important interest in nanocrystalline soft magnetic materials due to their attractive magnetic properties compared with conventional crystalline alloys. These materials are suitable for a wide range of applications at ac field such as transformer cores, inductive devices, sensors, etc. and, therefore, it is important to know their frequency dependence of their magnetic properties.

In previous works, the structure and some magnetic properties of a series of FINEMET-type alloys with a partial replacement of Nb by Mo has been studied including: i) the magnetostrictive behaviour of the series, ii) a thorough analysis of the phase transformations occurring during the crystallization process of the alloys and finally, iii) the estimation of amorphous and crystalline phases' fractions, chemical compositions and contributions in the magnetization of the sample.

It is the aim of the given contribution to present a study of the frequency dependence of the coer-

civity in as-quenched (amorphous) and isothermally annealed (nanocrystalline) samples of composition $\text{Fe}_{73.5}\text{Si}_{13.5}\text{B}_9\text{Nb}_{3-x}\text{Mo}_x\text{Cu}_1$ ($x = 0, 1.5$ and 3 ; Mo0, Mo1.5 and Mo3, respectively). Although the general form of the curves coercivity vs frequency is the same for all ribbons, a clear distinction in the values was observed between the amorphous and the nanocrystalline samples. Moreover, a molybdenum-content dependence of the dynamic coercivity was seen.

2 - 15 – Magnetic coupling and exchange-bias on multilayers with CoFe_2O_4 as pinner layer

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Multilayered films composed by two decoupled ferromagnetic thin layers separated by a non-magnetic (NM) spacer layer are the basic architecture of spin valve devices and magnetic random access memories (MRAM). The decoupling can usually be obtained by different methods, one of them is the use of a synthetic antiferromagnet (such as $\text{Ir}_{20}\text{Mn}_{80}/\text{Co}/\text{NM}/\text{Ni}_{81}\text{Fe}_{19}$) [1]. The natural CoFe_2O_4 ferrimagnet is a suitable candidate for its use as pinner layer for these systems grown by pulsed laser deposition technique [2]. We prepared $\text{CoFe}_2\text{O}_4(340\text{nm})/\text{FM}(50\text{nm})/\text{NM}(5\text{nm})/\text{FM}(50\text{nm})$ multilayered films (NM = AlO_x and TiO_2 , FM = Fe and $\text{Ni}_{80}\text{Fe}_{20}$) by pulsed laser deposition (Nd-YAG, $\lambda = 355$ nm). The films were grown on a $\langle 100 \rangle$ Si substrate. The structural properties of the samples were analyzed by X-ray diffraction and scanning electron microscopy. At low temperature (50K), a good coupling between free and pinned FM layers was observed only for $\text{CoFe}_2\text{O}_4/\text{Fe}/\text{TiO}_2/\text{Fe}$. For both multilayers with FM = $\text{Ni}_{80}\text{Fe}_{20}$, it was observed a vertically biased cycle that is originated in uncompensated magnetic moments at the interface between CoFe_2O_4 and pinned $\text{Ni}_{80}\text{Fe}_{20}$ layers. Moreover in these samples, ZFC and FC measurements show a monotonically decrease with T, fact that also reinforces this hypothesis.

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[2] Fix, T., et al., Nanotechnology, 18 (2007), 495708. doi: 10.1088/0957-4484/18/49/495708.

2 - 16 – Synthesis and Magnetic Properties in Fe₂O₃ Nanorod obtained using chelating agent

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Much attention has been gained on the magnetic nanomaterials by researchers from various fields such as physics, medicine, biology, and materials science due to their multifunctional properties such as small size, superparamagnetism and low toxicity [1]. In this work Fe₂O₃ nanopowders were synthesized in nanoscale dimensions by co-precipitation method on the addition of a chelating agent. X-ray diffraction and Rietveld refinement analysis results added to the magnetism results show that the addition of organic precursor in the synthesis influence significantly on the control particles sizes distribution. Transmission and scanning electron microscopy images show that the particles change your shape from 5 nm for faceted particles and 8x30 nm² for nanorods to depend of the agent chelating concentration. These results also show a preferential growth in 110 crystalline plane for nanorod. Therefore for samples prepared without organic precursor present average size of 75nm and temperature-dependent field cooling magnetization showed that there was Morin transition, in which indicate a large particle size distribution. ZFC-FC magnetizations curves show that samples obtained at low temperature present a superparamagnetic behavior with blocking and irreversibility temperatures around 95 and 135K, respectively, which increase with increasing of synthesis temperature. Moreover, we have found that the presence of chelating agent in the synthesis inhibited the coalescence effect (CNPq, FAPITEC-SE).

[1] Y.S. Kang et al., Chem. Materials 8 (2006) 2209.

2 - 17 – Raman characterization of bulk ferromagnetic nanostructured graphite

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Despite the fact that in the last 20 years have regularly appeared reports with experimental verification of the presence of ferromagnetism in pure carbon materials, still exists skepticism about this phenomenon being intrinsic. Previously, we presented a method for modifying pristine graphite in order to obtain ferromagnetic graphite at room temperature. This method is relatively easy to implement and economically affordable, which makes it particularly interesting for technological applications. Such materials could be used in magnetic imaging in medicine, communications, electronics, sensors and/or catalysis. In this work Raman spectroscopy was used to characterize bulk ferromagnetic graphite samples. The G:D band intensity ratio, the position of the 2D band and the presence of a band around 2950 cm⁻¹ showed a high degree of disorder in the modified graphite sample, with a significant presence of exposed edges of graphene as well as a high degree of attached hydrogen atoms.

2 - 18 – Electronic properties of NbS₂ and TiS₂ low dimensional structures.

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Transition metal dichalcogenides are well known because of their laminar structure, weakly bound through van der Waals interactions. Due to their technological applications in catalytic processes the bulk structure of many of them has been widely studied in the last 30 years. Some of them, such as NbTe₂ and TiSe₂, show superconductivity and, due to this, have been the subject of intense study. In 2004 Novoselov *et al* achieved to isolate not only graphene but also other bidimensional crystals, among them monolayers of some dichalcogenides [1]. These bidimensional crystals preserve their monocrystallinity under normal ambient conditions, keeping the crystal structure of the bulk. In this contribution we study the magnetic and electronic properties of 2D monolayers of NbS₂ (metallic in 3D) and TiS₂ (semimetallic in 3D) and the presence and characteristics of edge states of quasi 1D stripes of different widths cut out of these layers.

[1] K.S. Novoselov, D. Jiang, F. Schedin, T.J. Booth, V.V. Khotkevich, S.V. Morozov and A.K. Geim, PNAS 102, 10451 (2005)

2 - 19 – FESEM and GIXRD characterization of nanostructured NiCr thin films

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The application of NiCr thin films is widely well established in several microelectronic applications due to its relative large resistivity, more resistant to oxidation and a low temperature coefficient of resistance (TCR). These interesting properties of NiCr thin films show a strong dependence on their preparation conditions, i.e. the deposition environment and subsequent annealing treatments.

In this case, NiCr thin films were deposited by RF magnetron sputtering on a Si/Si₃N₄ substrate using a 3-inch Ni/Cr (80/20 %wt) alloy target. The thickness for each sample was 50 nm. Annealing treatments were subsequently performed at three different temperatures during 6 hours at 400, 600 and 800 °C in air and N₂ ambient, respectively. These temperatures were chosen in order to appreciate the change of the crystal size and the surface composition of the thin films according with the recrystallization temperature. In this work, the appreciation of the three stages in the annealing process of a NiCr metallic alloy in a nanostructured scale is aimed. The annealing process is split in three stages: recovery, recrystallization and grain growth, respectively. To observe this effect, surface composition of each sample is determined. It is also studied, how the crystal growth in N₂ ambient was formed and stabilized due to the suppression of oxidized substance on the film surface. Crystallographic structure as well as interatomic spacing of this nanocrystalline material is also characterized.

The characteristics of these films such as crystal structure and changes of microstructure are analyzed as function of annealing temperature and atmosphere conditions. In this work, surface composition and crystallography of the samples are determined by means of field emission scanning electron microscopy (FESEM/EDAX) and X-ray diffraction in the grazing incidence mode (GIXRD) methods, respectively.

Comparisons of structural and crystallographic properties of the nanostructured RF sputtered NiCr thin films under the variation of annealing conditions will be presented on final paper.

2 - 20 – Electron Spin Resonance studies of Magnetic Ions (Er³⁺, Yb³⁺ and Mn²⁺) Diluted in Ag Nanoparticles

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Ag nanoparticles doped with Er are of particular interest in industry of photonics, due to the remarkable enhancement of the Er³⁺ photoluminescence intensity. In this paper we describe the synthesis of nanoparticles doped with Re = Er³⁺, Yb³⁺ and Mn²⁺, by reducing the AgNO₃ and oxides of transition ions. We have performed the structural characterization and the study of the magnetic properties of these ions (concentration = 5%) diluted in colloid Ag nanoparticles. Electron Spin Resonance experiments indicate that magnetic ions are located in the matrix cubic in the AgRe. The exchange interaction, $J_{fs}\mathbf{S}_f\cdot\mathbf{s}$, between the Re localized magnetic moment and the host's conduction-electrons has no effect on the ESR data, in contrast to bulk system.

2 - 21 – Electronic Structure of TiO₂ and related nanostructures for Dye Sensitized Solar Cells

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The dye sensitized solar cell (DSSC) is an emerging alternative for the production of electricity from solar energy. It is based on a junction between a n-type wide gap semiconductor and a p-type light absorbing material. The selected material for the first one, in most cases, corresponds to TiO₂ nanoparticles, while the second one consists on an organic or inorganic dye. The open-circuit voltage generated in the cell corresponds to the difference between the Fermi level of the electron in the solid and the redox potential of the electrolyte used in order to regenerate the dye molecule. Thus, the electronic structure, and in particular the band gap of the n-type nanoparticles, influence the efficiency of the cell [1]. In this work we present structural and electronic properties study for bulk polymorphs of TiO₂, and related nanostructures simulated by slabs. All of them are based on: Rutile, Anatase and Monoclinic TiO₂(B). We report band gaps and surface energies, discussing the geometrical reconstruction in each case. TiO₂(B) is included due to experimental results, in which it appears during the thermal annealing of H₃Ti₃O₇ nanostructures obtained by hydrothermal synthesis [2], which

was also verified by our group. Since there is no much work on this polymorph nanostructure, our findings could contribute to the state of art of TiO₂ for DSSC purposes. The simulations were performed using the DFT-GGA, using SIESTA code [3], Quantum Espresso [4] and WIEN2k [5]. SIESTA calculations were used for the structural optimization of bulk and slab models. After this surface energy were determined by Quantum Espresso, which adopts a plane-wave basis set. Finally, for the bulk structures, we performed all-electron-full-potential-plane-wave code WIEN2k, in order to apply the recent modified-Becke-Johnson exchange potential + LDA-correlation [6], which allows better estimation for band gaps, closer to experimental ones. The comparison between these models is also based on the corresponding band gaps, and surface energy [7-8].

[1] M. Grätzel, *Journal of Photochemistry and Photobiology C: Photochemistry Reviews* 4, 145 (2003)
 [2] Y. V. Kolen'ko et al, *J. Phys. Chem. B* 110, 4030 (2006) [3] Soler, J. M. et al, *J. Phys.: Condens. Matter* 14, 2745 (2002) [4] Giannozzi, P. et al, *J. Phys.: Condens. Matter* 21, 395502 (2009) [5] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka and J. Luitz, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universität Wien, Austria), 2001. ISBN 3-9501031-1-2 [6] F. Tran, and P. Blaha, *Phys. Rev. Lett.* 102, 226401 (2009). [7] O.V. Prezhdo et al, *Progress in Surface Science* 84, 30 (2009). [8] M. Casarin et al, *ACS Nano* 3 (2), 317 (2009).

2 - 22 – Density Functional Theory applied to the study of Au atom and dimer on MgO(001) surface

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The most important catalytic reactions in the chemical industry are those that take place on metals, mainly transition metals. However, some metal oxides have electronic and physical properties that can induce catalytic properties of metals. Among the wide variety of oxides available for the application in catalytic systems, magnesium oxide has particularly been used in both theoretical and experimental basic research due to its apparent structural simplicity and facility of synthesis. It has been found that the most important properties of the MgO are directly or indirectly related to the presence of defects, particularly of defective points. The most important defects in magnesium oxide are those created by oxygen vacancies. It is well known that defects not only can act as catalytic

centers for chemisorption of small species but also as nucleation centers for growing metal clusters and can modify the catalytic activity of these adsorbed metal particles via the metal-support interaction at the interface. In the present work, we carried out a systematic study using Density Functional Theory (DFT) to analyze the adsorption energy and chemical reactivity of one Au atom and the Au₂ dimer on regular site and neutral oxygen vacancies (Fs sites) of MgO(001) surface. The molecular electrostatic potential (MEPs) have been used to determine how the reactivity of a particular site on MgO(001) surface changes during the adsorption of Au_n (n=1-2). Our results indicate that the neutral oxygen vacancies is more reactive than regular sites of MgO surface and does not promote dimerization of gold.

2 - 23 – Anisotropy and relaxation processes of uniaxially oriented CoFe₂O₄ nanoparticles dispersed in PDMS

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When a uniaxial magnetic field is applied to a non-magnetic dispersive medium filled with magnetic nanoparticles, they auto-assemble into thin needles parallel to the field direction, due to the strong dipolar interaction among them. We have prepared in this way magnetically oriented nanocomposites of nanometer-size CoFe₂O₄ particles in a PDMS polymer matrix, with 5 and 10 % w/w of magnetic particles. In this work, we present the characteristic magnetization and magnetic relaxation curves measured with applied magnetic fields forming an angle α with respect to the needle direction. In both experiments, a small magnetic anisotropy is present. We show that the magnetic viscosity (calculated from the logarithmic relaxation curves) as a function of α presents a minimum at $\alpha=0$, indicating slower relaxation processes associated with this configuration of fields. The results seem to point out that the local magnetic anisotropy of the nanoparticles is oriented along the needles, resulting in the macroscopic magnetic anisotropy observed in our measurements.

2 - 24 – On Local Temperatures for Quantum Driven Systems and Heat Flow

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We introduce thermometers to define the local temperature of an electronic system driven out-of-equilibrium by local AC fields. We also define the effective temperature in terms of a local fluctuation-dissipation-relation. We show that within the weak driving regime these two temperatures coincide. We also discuss the behavior of the local temperature along the sample. We show that it exhibits spatial fluctuations following an oscillatory pattern. We also show that the local temperature is the correct indicator for heat flow and its use allows for a generalization of the Wiedemann-Franz law.

2 - 25 – Magnetization reversal in Ni and Co nanowire arrays: simulations and measurements

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The study of magnetic nanostructured systems is a topic that attracted considerable interest due to their interesting physical properties and potential technological applications. In particular, highly ordered arrays of magnetic nanowires produced inside the pores of anodic alumina membranes by electrochemical deposition have been the focus of intense research. Different groups have investigated the stable magnetic configurations as a function of the aspect ratio of the magnetic cylinders, the reversion mechanisms of the magnetization in nanowires, the influence of magnetostatic interactions among nanowires, and in general, the behavior of the magnetic properties as a function of different parameters.

In this work, we perform a study of the magnetic properties (reversal mode, coercivity and remanence) as a function of the angle existing between the applied field and the nanowire axis through micromagnetic simulations and measurements. Arrays of Ni and Co nanowires have been prepared by electrodeposition into nanopores of alumina membranes which were prepared from an ultra pure aluminum foil by the two-step anodization technique. The morphological characterization of this system was performed by Transmission Electron Microscopy (TEM) which reveals an ordered hexagonal structure. Magnetic properties were studied in a Vibrating Sample Magne-

tometer (VSM) with the external magnetic field applied at different angles. The magnetization reversal has been investigated using the three-dimensional Object Oriented MicroMagnetic Framework software (OOMMF). In this work we investigate the magnetic properties of Ni and Co nanowires characterized by 1 μm of length and 25 nm of radii. In order to study the effect of the magnetostatic interactions between the wires, we have simulated a hexagonal cell of seven nanowires with a 100 nm center-to-center distance. We have used the exchange coupling $A = 30 \times 10^{-12}$ J/m ($A = 9 \times 10^{-12}$ J/m) and saturated magnetization $M_s = 5.2 \times 10^5$ A/m ($M_s = 4.9 \times 10^5$ A/m) for Co (Ni) nanowires. Besides, we have used a size mesh of 5 nm in which magnetization is free to rotate in three dimensions. In all the cases the damping constant is 0.5. The magnetostatic interaction between the nanowires reduces the coercivity, in contrast to the remanence which is not affected. Finally, the simulation results are compared with the measurements at Ni and Co nanowire arrays.

2 - 26 – Study of the magnetic properties of Ni granular films

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In this work, we perform a study of the magnetic and morphological properties of the granular $\text{Ni}(\text{SiO}_2)$ films which were prepared in a magnetron co-sputtering system, with the transition metal and SiO_2 (or Ag) targets mounted on two separate guns. The glass substrates were rotated during sputtering, to ensure composition uniformity. The metal volume fraction was controlled by the relative sputtering rates, and then determined by energy-dispersive X-ray spectroscopy using a Philips EDAX XL30 on films deposited in the same run on Kapton. The samples deposited on Kapton were used for magnetic measurements. The morphological characterization of this system was performed by Transmission Electron Microscopy (TEM) and High Resolution Transmission Electron Microscopy (HRTEM) which reveal a structure with extremely fine dispersion of Ni metal nanoparticles embedded in an insulating matrix. Magnetic properties were studied in a Superconducting Quantum Interference Device (SQUID) and a Quantum Design MPMS XL7 system in the temperature range 5-300 K showing that these Ni nanoparticles are superparamagnetic.

In order to have a more detailed picture of the magnetic characteristics of this system at 5 K, we have performed a detailed magnetic characterization by means

of First Order Reversal Curves (FORC) and FORC diagrams. The major hysteresis loops, delineated by the outer boundaries of the FORCs, correspond exactly to the hysteresis curves of the sample. The Ni nanoparticles show a regular hysteresis loop with a coercivity of 850 Oe at 5 K, in contrast with the superparamagnetic hysteresis loop at 300 K. In the FORC diagram of the sample at 5 K one can observe the presence of a narrow ridge centered around 0 Oe, that is the reversible component of the magnetization, and only one narrow ridge along the coercivity axis corresponding to the irreversible component of magnetization, this ridge is peaked at 817 Oe, near the major hysteresis loop coercivity value of 850 Oe. This pattern is characteristic of a set of noninteracting single-domain particles as is expected for this sample. Finally, the distribution of coercivity of the FORC diagram at 5 K is related to the size distribution of the Ni nanoparticles.

2 - 27 – Microwave absorption behavior of a polyaniline magnetic composite in the X- band

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The development of nanosized materials is a subject of considerable interest both for understanding of the fundamental properties of magnetic materials, and for new technological applications. Polyaniline (PANI) / Fe₃O₄, Fe₂O₃ composites with conducting, magnetic and electromagnetic properties were successfully prepared with various amounts of Fe₃O₄, Fe₂O₃. The samples were characterized structurally by scanning electron microscopy and x ray diffraction and magnetically with a vibrating sample magnetometer. In order to explore microwave-absorbing properties in X-band, composite nanoparticles were mixed with an epoxy resin to be converted into a microwave-absorbing composite. Microwave behavior with different Polyaniline (PANI) / Fe₃O₄, Fe₂O₃ ratio (9, 14 and 18%w/w) were studied using a microwave vector network analyzer from 7.5 to 13.5GHz. Absorption increases when sample ratio increases for a constant thickness of 2 mm. Magnetite contents increase sample absorption. Preliminary results on samples prepared under a moderate magnetic field are presented.

2 - 28 – Four terminal resistance of an interacting quantum wire with a back-scattering impurity.

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We investigate the behaviour of the four-terminal resistance R_{4pt} in an interacting quantum wire described by a Luttinger liquid in the presence of a single impurity within the wire. Results are discussed at zero and finite temperature, as well as the effects of the relative magnitudes of the coupling parameters involved in the system.

2 - 29 – Graphene on epitaxial ferroelectric BaTiO₃: an atomistic study

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The exceptional electrical properties of graphene have made it a promising material for device applications, such as field effect transistors. However its intrinsic high mobility can be degraded when it is supported on a dielectric substrate, as the widely used SiO₂, due to the substrate surface properties. Recently it was reported that graphene mobility increases when SiO₂ is replaced by a ferroelectric material, which is characterized by a reversible nonvolatile electric polarization. Here we study the interaction of a graphene nanodot with the film surface of the prototypical ferroelectric BaTiO₃ using atomistic modeling through Molecular Dynamics simulations performed at room temperature. The ferroelectric film is under bi-axial compressive strain presenting a tetragonal (001)-oriented phase, and domains with electric polarization pointing towards and inwards the surface. Binding energies for graphene dots of different sizes depending on the polarizations and boundaries of the domains are reported.

2 - 30 – Adsorption of Mn and V on BN nanotubes: a theoretical study

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Boron nitride nanotubes (BNNts) have extraordinary chemical and physical properties that suggest a large number of nanotechnological applications. In particular, the study about adsorption of transition-metal atoms on BNNts is interesting for the changes that it produced in nanotube's properties. Previous studies have found that transition-metal atoms like V, Mn and Cr are adsorbed on the walls of BNNts and cause a net magnetic moment ($4.39 \mu_B$ with an atom of V, $4.99 \mu_B$ with Mn y $4.08 \mu_B$ for the Cr) [1]. These results suggest their use on spintronics and molecular electronic. By means of calculations based on Density Functional Theory (DFT) within ultrasoft pseudopotential approximation [2], we study the adsorption of atoms of Mn and V on (8,0) zigzag and (5,0) arm-chair BNNts. In each case, we found adsorption energies of most stable configurations (0.04 eV for Mn and 0.47 eV for V). This, in contrast with previous results reported by Wu et. al. (0.4 eV for Mn and 0.83 eV for V) [1]. In this work, we study changes in electronic properties of systems (band structures, densities of states and charge densities) produced by the adsorption. This study reveals important aspects about potential bonds on external walls of BNNts.

[1] Xiaojun Wu and X. C. Zeng. *J. Chem. Phys.*, 125 (2006) 044711. [2] K. Laasonen, A. Pasquarello, R. Car, C. Lee, D. Vanderbilt, *Phys. Rev. B*. 47 (1993) 10142. [3] P.N. D'yachkov, D.V. Maskaev, *J. Phys. and Chem. Sol.*, 70, (2009) 180-185.

2 - 31 – Characterization of Platinum clusters through chemical reactivity descriptors and vibrational spectroscopy: a theoretical study .

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Metallic clusters have been the object of many studies, due to the novel properties that they present at

bulk level. Transition metal clusters have been studied for its potential use as catalysers and in the production of electronic nanodevices. In particular, platinum clusters are used as catalysers in chemical industry, in CO, NO reduction and play an important role in fuel cells to produce energy from Hydrogen, as an alternative source of clean energy. Theoretical computations by means of density functional theory (DFT) were performed to study structural evolution, electronic properties and vibrational spectroscopy of Pt_n ($n=2-13$) clusters. Here we present the characterization of such clusters through global reactivity descriptors, chemical potential, chemical hardness and electrophilicity index, computed using vertical electronic affinities and ionization potentials. Our results show that platinum clusters tend to stabilize in high spin configurations, as reactivity and size increase. All computations were performed with B3PW91 exchange and correlation functional and Gaussian 03 suite of programmes.

2 - 32 – Large surface anisotropy in Fe-doped NiO nanoparticles

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Nanoparticles (NP's) have been subject of several studies due to the new properties that these materials present when crystallite size is reduced. In case particular of the magnetic nanoparticles, your properties are modified when NPs have size lower than 10 nm [1]. These magnetic properties are related to the finite size effects and/or high surface/volume ratio [1,2]. Besides the interface effects can present magnetic properties different of the superparamagnetic behavior observed in these systems. Surface and interface driven properties play a dominant role in all applications of magnetic nanoparticles [2]. In this sense, the main challenge is the control of the size, size distribution and morphology of NP's. In this work, we have used the co-precipitation method [3] to obtain $Ni_{1-x}Fe_xO$ nanoparticles with different particle sizes and doping concentrations ($1\% \leq x \leq 10\%$) in the presence of organic precursor to study the magnetic and structural properties. X-ray diffraction (XRD) results show that all samples present NiO cubic crystallographic phases without presence impurities phases. Our analysis XRD using Rietveld refinement and Scherrer equation show a decreasing in the particle size as function of synthesis temperature and of the doping amount. ZFC-FC magnetization curves carried out on a superconducting quantum interference device (SQUID) magnetometer point out a non-homogeneous distribution of particle size and a large surface effect for 10% Fe-doped samples at low temperature region. We believe that this behavior can be associated to the bro-

ken exchange bond resulting of freezing of disordered surface spins caused by Fe ions.

[1] R.H. Kodama, S.A. Makhlof and A.E. Berkowitz, Phys. Rev. Lett. **78**, 1393 (1997).

[2] D. Fiorani, Surface Effects in Magnetic Nanoparticles, Ottawa, Springer, 2005.

[3] C.T. Meneses, W.H. Flores, F. Garcia and J.M. Sasaki, J. Nanoparticle Res. **9**, 501 (2007).

2 - 33 – CT-AFM Electrical Transport Studies in Patterned Silver-Mesoporous Titania Nanocomposite Thin Films

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The unique electronic, optical catalytic and chemical properties of metallic nanoparticles (NP) embedded in oxide thin films represent a great promise for advanced applications such as nanoelectronics, bioanalysis and optoelectronics. For the development of NP-based electronics, it is desirable to engineer three-dimensional arrays of metal nanoparticles that can be used as highly controlled wires, circuits and/or electrodes. Embedding NP within thin films permits to exploit their properties derived from size or confinement and protect them from the environment. Mesoporous thin films (MTF) provide restricted chemical environments and grant accessibility to ions or molecules due to their controlled pore size domains, constituting ideal matrices for metallic NP inclusion. In this work, we explore the 3D electronic conductive properties of patterned nanocomposites formed by TiO_2 MTF loaded with Ag NP by the Photocatalysis-Assisted Mesopore Patterned Array (PAMPA) lithography procedure previously *developed*¹ We performed conductive tip atomic force microscopy (CT-AFM) measurements to study for the first time the localized electrical properties of the NP-MTF patterned nanocomposite, A remarkable conductivity dependence on the film mesostructure and metal NP loading was observed, confirming a three-dimensional current flow throughout the nanocomposite.

[1] E.D. Martínez, M.G. Bellino, G.J.A.A. Soler-Illia, ACS Appl. Materials & Interfaces, 2009, 1, 746.

2 - 34 – Characterization structural, morphological and optoelectrical of Bi_2S_3 thin films grown by co-evaporation

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This work presents results concerning the synthesis and characterization of polycrystalline n-type Bi_2S_3 thin films. The films were grown by a chemical reaction of their precursor elements which are co-evaporated on a soda-lime glass substrate, and later will be used as an buffer layer in solar cells based in Cu_3BiS_3 . The effect of the preparation conditions on the optical, morphological and structural properties, as well as on the electrical conductivity (σ) was studied through spectral transmittance, X-ray diffraction (XRD), atomic force microscopy (AFM) and σ versus T measurements, respectively. The results revealed that, independently of the deposition conditions, the films grow only in the orthorhombic Bi_2S_3 bismuthinite phase. It was also found that the Bi_2S_3 films present an energy band gap E_g of about 1.38 eV, regardless of the thickness of the samples. It was also found that the electrical conductivity of the Bi_2S_3 films is affected by the transport of free carriers in extended states of the conduction band as well as for variable range hopping transport mechanisms, each one predominating in a different temperature range

2 - 35 – Impurity-assisted chain creation in transition-metal break junction experiments studied from first principles

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In the last few years, one-dimensional systems were experimentally realized as suspended monoatomic chains in mechanically controllable break junctions (MCBJs). In these experiments the chains under consideration are not at their equilibrium interatomic distance due to mechanical stress. Using first-principles calculations, we extended a stability and producibility

criteria for chain formation to zig-zag and dimerization and applied it successfully to Cu, Ag, Au, Ir and Pt atomic chains.

It has been shown experimentally that oxidization of chains can trigger the formation of significantly longer chains. The improvement of our model for chain formation enables us to take a detailed look into impurity assisted chain formation, where zig-zag bonds can play an important role. In particular we focus on O, N, C and H assisted noble metal as well as magnetic Ir and Pt chains. For simplicity, we assumed that the presence of impurity atoms in experiments results in ..M-X-M-X... (M:metal, X:impurity) chain structure in between the metal leads.

2 - 36 – Synthesis and characterization of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3/\text{SiO}_2$ core-shell nanoparticles

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$\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($x=0.22, 0.3$ and 0.33) nanoparticles (NP) were synthesized using liquid-mix method, starting from metallic nitrates and adding citric acid to obtain cation complexes and ethylenglycol to polymerize. The powder obtained after a thermal treatment at 700°C was dispersed in isopropyl alcohol and SiO_2 coated using the Stöber method. An aqueous ferrofluid of $\text{La}_{0.78}\text{Sr}_{0.22}\text{MnO}_3$ (0.6mg/ml) and gels from $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($x=0.3$ y 0.22) NP and oil-wax gel (Gelwax®) were prepared. X Ray diffraction analysis, scanning and transmission electron microscopy, infrared spectroscopy and magnetic measurements were used to characterize the samples.

The thermal response of a ferrofluid containing $\text{La}_{0.78}\text{Sr}_{0.22}\text{MnO}_3$ (NP) suspended in aqueous solution of chondroitin 6-sulfate sodium salt (3mg/ml), and a gel containing $\text{La}_{0.75}\text{Sr}_{0.3}\text{MnO}_3$ NP were studied, while exposing the samples to a RF magnetic field (41 kA/m, 260kHz). The temperature vs. time curves were recorded and the gel's Specific Loss Power (SLP) was obtained from the initial slope of such curves. SLP values around 3W/g were obtained. The relationship of SLP to the variable AC field was studied.

The order temperature of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($x=0.22$ and 0.33) NP, was determined by Magnetic-Thermo-Gravimetry, leading values of about 334K and 368K, respectively. From the comparison of ac susceptibility measurements on coated and uncoated samples ($x=0.33$), the thickness of the SiO_2 layer was estimated to be of the order of 4 nm. M vs H curves have a

Langevin-like shape, however displaying a small coercivity of about 30 Oe ($x=0.22$). From these curves magnetic cores of 14 to 21 nm diameter were estimated.

2 - 37 – Charge localization in Co doped Ceria with oxygen vacancies

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The search and development of novel materials, ferromagnetic beyond room temperature, is currently a subject of intense work with the driving force of its potential technological applications. In this regard, Cerium oxide with diluted magnetic impurities is a natural candidate for spintronics as it offers a good integrability with the current electronic devices. However, this material still poses several questions being the main one to find a widely acceptable explanation for the observed room temperature ferromagnetism. There is experimental evidence supporting the idea that the free electrons left behind by oxygen vacancies localize themselves in specific Cobalt and Cerium atoms, changing their oxidation states ($\text{Co}^{4+} \rightarrow \text{Co}^{2+}$ and $\text{Ce}^{4+} \rightarrow \text{Ce}^{3+}$, respectively) and turning the Cerium atoms into magnetic ones. The study of this charge localization is crucial to approach an understanding of the magnetic properties in these materials. Using the framework of the density functional theory, we study the relative stability of different Oxygen vacancies and we show that they tend to locate close to the Co impurities. In addition, we address the issue of charge localization in these materials for different concentrations of both Co impurities and Oxygen vacancies.

2 - 38 – Structural and magnetic properties of FeGa alloy grown as thin film

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The FeGa (iron gallium) alloy has the particularity of being magnetostrictive, i.e., it modifies its lattice parameter when its magnetic state is changed. This property allows us to think about possible applications

in the field of nanotechnology, due to the possibility of controlling the magnetism of devices without applying external magnetic fields. The previous studies have been made on FeGa bulk; however, future applications, as nanodevices, require that FeGa were grown as thin films.

The samples studied are epitaxied $\text{Fe}_{1-x}\text{Ga}_x$ thin films (grown by MBE) with x from $\sim 10\%$ to $\sim 30\%$ and different thickness. X-ray diffraction shows that there is a coexistence of two crystalline phases, one of which is tetragonal and whose base and height ratio increases monotonically with the Ga concentration. The other phase is cubic and its lattice parameter also increases with Ga concentration. We have also determined the thickness of these samples by small angle x-ray reflectometry.

We have performed the magnetic characterization of these samples by mean of magnetometry and ferromagnetic resonance. The results show changes in the magnetic structure as a function of the Ga concentration and the film thickness. When $x > 0.2$ the in-plane uniaxial hard axis turns from the $[0-11]$ direction to $[100]$. Furthermore, when the film thickness is varied, changes in anisotropy directions are observed, indicating the strong influence of the interface magnetic structure on the magnetic behavior of the film.

2 - 39 – “p”-orbitals’ mediated magnetic interaction: the case of Mn chains

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Molecular layers grown on metallic surfaces constitute adequate substrates to study the nature of mediated magnetic interactions. The case of Mn chains deposited on a copper nitride molecular monolayer grown on $\text{Cu}(001)$ has already been addressed in the literature, both, theoretically as well as experimentally. Different deposition sites for the chains have been considered appearing clear differences in the mechanisms which give rise to the magnetic ground state. In this contribution, we are interested in the role played by different “p” orbitals in the mediation of magnetic interactions among Mn atoms. We consider, thereafter, Mn chains deposited on $\text{Cu}(001)$ with $\frac{1}{4}$ monolayer Oxygen and $\frac{1}{4}$ monolayer Nitrogen coverage, which build non reconstructed surfaces with (2×2) unit cells, and perform calculations within the frame of Density Functional Theory.

2 - 40 – A ferromagnetic resonance study of Fe/MnAs bilayers: magnetic anisotropies and interlayer coupling

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In this work we present a ferromagnetic resonance (FMR) study of Fe/MnAs bilayers epitaxially grown on GaAs (100). Important Fe/MnAs interface effects are observed, i.e., the very weak exchange coupling between Fe/MnAs, and the addition of uniaxial anisotropy terms to the free energy density of the iron layer. Moreover, the general appearance of the FMR iron spectrum is highly temperature dependent. The resonance field, linewidth, and intensity of the Fe line are strongly altered in the alpha-beta phase coexistence region of the MnAs layer, where a severe drop of the resonance field is simultaneously observed. A complementary chemical profile analysis of the sample shows an important intermixing at the Fe/MnAs interface, which arises as a crucial factor for the understanding of the magnetic behavior of this system

2 - 41 – Influence to the spatial conformation of NT functionalized with different polymers according to their electronic distribution.

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The purpose of this work is to study the influence to the spatial conformation of a polymer grafted onto multi-walled carbon nanotubes (MWCNT) according to the differing electronic distribution of the polymer's repetitive unit. It is known that polymers with aromatic rings interact with the nanotube through pi-pi staking interactions, tending to wrap the MWCNT and propitiating a better dispersion of them in a solvent with affinity to the polymer or in the polymer itself, leading to a composite material with well dispersed MWCNT. On the other hand, if trying to anchor the MWNT to one of the phases of a block copolymer, it would be more efficient to have the MWCNT functionalized with a polymer that does not wrap the nanotube, thus allowing the anchorage by means of inter-diffusion of the polymer into the block with more affinity to it. In this work, we made a graft-from functionalization using as monomers: 4-vinylpyridine (monomer with an aromatic substituent) and acrylonitrile (monomer with a non aromatic, where the substituent is a nitrile group). The functionalization efficiency was studied by spectroscopic and thermal technique. The spacial conformations of the polymer around carbon nanotubes were studied by high resolution transmission electron microscopy (HRTEM). It was seen, in both cases, polymer wrapping the NT. However, for polymers with aromatic rings, this effect is predominant, while with polyacrylonitrile derivates what can be seen is polymer wrapped onto itself and bound to the MWCNT's wall.

2 - 42 – Influence in the optical response of the addition of multiwalled carbon nanotubes in films of epoxy resin and azobenzenes.

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Among many others, one of the applications of multi-walled carbon nanotubes (MWCNT) is to immerse them in a polymer matrix since new mechanical, electrical or thermal properties could be induced into the polymer. Azobenzene and its derivatives are widely known for undergoing a photoisomerization process when illuminated with light of the proper wavelength. When added to a hosted matrix, these nonlinear optical materials may give rise to certain degree of anisotropy when exposed to linear polarized light. The photoinduced trans-cis-trans cycles of these kinds of molecules end up when their dipole moment is normal to the polarization axis of the light. Maximum anisotropy is thus reached when molecules are all aligned in that direction and there is no coupling

with the electrical field of light. When the exposure light is turned off, some degree of anisotropy is lost. Moreover, anisotropy is totally lost when illuminating with circular polarized light. The fact that anisotropy loss occurs limits the capability of using these materials in data storage, optical switching or holographic recording and making this characteristic still a challenging subject of study. We recently demonstrated that MWCNT interact with an azobenzene derivative, Disperse Orange 3 (DO3) via π - π stacking interactions [1]. In this sense, it could be expected that MWCNT interacting with DO3 molecules partially inhibit the molecules trans-cis-trans cycles. Therefore a change in the rate of induced anisotropy as well as in the relaxation rate or in the percentage of anisotropy losses could also be expected. In this work, we studied the optical response of epoxy resin films filled with MWCNT non-covalent functionalized with DO3. Also films of epoxy resin and DO3 without MWCNT were done in order to see the effect of MWCNT in these films. We found that in the case of films containing MWCNT the process of reaching the maximum anisotropy is slower than the obtained for films without them. The anisotropy loss process is also different in both films indicating that a higher anisotropy would remain in the film with MWCNT.

[1] Díaz Costanzo, G.; Ledesma, S.; Mondragón, I.; Goyanes, S. J. Phys. Chem. C, 2010, **114** (34), pp 14347-14352

2 - 43 – Production of carbon nanotubes: influence of the catalyst on the yield

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Multi-wall carbon nanotubes (MWCNTs) were synthesized by chemical vapor deposition (CVD) on catalytic iron nanoparticles dispersed in a silica matrix, prepared by sol gel method. This work explores the influence of the variables of synthesis that rules the sol to xerogel transition on the catalytic activity of the iron nanoparticles. In particular, the variation of both iron precursor and hydrolysis-condensation catalyst agent on the matrix structure, and its influence on the yield of carbon nanotubes growth was studied. The

silica precursor utilized was tetraethyl-orthosilicate. As metal precursor, it was used iron (III) nitrate or iron (III) chloride. The hydrolysis-condensation catalysts used were hydrochloric, nitric or hydrofluoric acids. The sols were dried at two different temperatures in air (25 or 80°C) and then treated at 450°C for 10h. The catalyst was characterized by XRD and TPR. The xerogels were introduced into the CVD chamber and reduced in a hydrogen/nitrogen (10% v/v) atmosphere at 600°C. MWCNTs were formed by deposition of carbon atoms from decomposition of acetylene at 700°C. The samples were characterized by XRD, TGA, SEM and TEM. After calcination at 450°C, each system acquired different crystalline structure and degree of crystallinity. MWCNT yield was notably dependent on the Fe-matrix synthesis conditions, in spite that all the other variables (as Fe/Si ratio, gas flow, temperature, etc) were identical. The most active catalyst was that prepared with HF dried at 25°C, and the less active was that prepared with HNO₃. Carbon nanotubes displayed a diameter of about 25-40nm and several micron lengths. The growth mechanism of MWCNTs is base growth mode for all catalysts. The differences in MWCNT yield are discussed in terms of crystalline and iron nanoparticle sizes.

2 - 44 – Influence of filler alignment in the mechanical and electrical properties of carbon nanotubes/epoxy nanocomposites

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Current and projected markets for carbon nanotube based polymer composites are aimed at the exploitation of the high electrical conductivity of carbon nanotubes coupled to their unique geometry. Due to the low filler loading fractions required, the mechanical properties and the surface finish of the composite matrix can be maintained. In previous studies we have shown that the use of random disperse multi-wall carbon nanotubes (MWCNT) as a conductive filler in an epoxy matrix leads to an electrical conductivity exceeding 10^{-6} Sm^{-1} , sufficient for anti-static applications, at filler concentrations as low as 0.4 wt%. The present work investigated the influence of an alternating current (AC) electric field on dispersions of

MWCNT in an epoxy matrix during curing. The expectation was that an aligned network would form if the aggregation process was guided in this way, and that interesting anisotropic electrical conductivities and mechanical properties might emerge. The composite materials are disks of 30mm diameter and 3.6mm of thickness. The matrix is diglycidyl ether of bisphenol-A with isophorone-diamine as hardener and MWCNT with weight percentage between 0.04 and 0.2 wt% were used as filler. An AC electric field (250 ACV; 50 Hz) along thickness was applied before and through curing. The AC electric current through the sample, in the thickness direction, was measured during the whole cure cycle. The evolution of the electrical conductivity shows that MWCNT alignment begins at ambient temperature but goes to saturation during the gelification process (50 min at 60°C for this epoxy system). This result, novel in the literature, allows optimizing the time and the temperature during which is necessary to apply the electric field to achieve the maximum possible alignment. The DC conductivity was measured after cure cycle. The percolation threshold was around 0.06 wt% of MWCNT content with a conductivity of $1.4 \times 10^{-5} \text{ Sm}^{-1}$, this is one order less in the filler content than the composite with MWCNT dispersed at random. The Rockwell hardness of the nano-composites decreases but the wear resistance increases for both aligned and random MWCNT networks. The hardness fall is stronger for the composites with the aligned network. This could be explained by a “crack initiator” behavior of the carbon nanotubes due the weak interaction between nanotube wall and resin.

2 - 45 – Nanostructures titanium films grown with a plasma immersion ion implantation and deposition system: influence of the bias voltage on the crystalline structure

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Titanium films have been widely investigated in the last years because of their importance in a large variety of technological applications. Ti coatings have been employed as interlayer on steel to improve adhesion of hard coatings based on titanium compounds or to allow the diffusion of carbon from DLC coatings. Ti coatings on titanium alloys have been proposed to im-

prove the biocompatibility of the alloy, since a pure titanium barrier layer prevents harmful substances such as aluminum or vanadium from leaching into biological tissues. Methods based on plasmas, such as magnetron dc sputtering and vacuum arcs, have been employed to obtain titanium films. Plasma immersion ion implantation combined with deposition (PII&D) using cathodic arcs as plasma sources is a technique that has demonstrated to be useful for the fabrication of nanostructure coatings. Applying PII&D a substrate is immersed into the plasma plume produced with a cathodic arc and is biased with high-voltage pulses. When the high negative potential (typically many kilovolts) is on, a plasma sheath forms around the workpiece and ions are accelerated towards the surface and implanted. While the bias is off, ions condense on the surface resulting in the deposition of a coating or a film. The use of high voltage pulses to bias the substrate allows to obtain denser films and to relax internal stress improving the adhesion, tribological and mechanical properties. In this work the characteristics of Ti coatings on steel and on copper substrates obtained with a PII&D system were analyzed. The films were deposited varying the pulse amplitude from 2 to 12 kV, with a pulse frequency of 200 Hz and locating the substrate at two distances from the cathode, 20 and 40 cm. The film structure was studied by glancing-angle X-ray diffraction (GA-XRD). The morphology was observed with an atomic force microscope. Significant changes in GA-XRD spectra with the bias voltage were observed indicating important modifications on the film structure produced by the implantation of high energy ions.

2 - 46 – Magnetic states of Co- and Fe impurities on graphene

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We present ab-initio calculations of the stability and electronic structure of graphene mono- and bilayers systems. We study the magnetic behavior of Co and Fe impurities, substitutionally introduced in graphene monolayers, and substitutional and interstitially in bilayers. The behavior is completely different in each case. Particularly the stability of the graphene bilayer is pretty enhanced by the introduction of these impurities. We analyze the dependence of magnetic moments on Co-C or Fe-C distances, and on external applied electric field.

2 - 47 – Vortices in magnetic nanodots

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Nanodots of magnetic materials may present magnetic vortices in their ground state configuration. These are flux closure structures, with the magnetic moments generally confined to the plane, except at their cores[1]. Vortices in nanodots have many potential applications, such as magnetic memories (VRAM's) and spin transfer nano-oscillators (STNO's). The characteristics of these vortices, including the vortex core size can be controlled to suit these applications. This can be achieved making use of the interface interactions in multilayers, e.g., using a stack of Co/Pt bilayers[2]. The magnetization of the vortex cores can be inverted through the application of static, rotary, or pulsed magnetic fields; polarized currents have the same effect. Manipulation of the sign of the core magnetization is required for the application of nanodots as memory elements, or oscillators. In the present work we show recent results obtained with micromagnetic simulation of static and dynamic properties of vortices in magnetic multilayers.

[1] Guslienko J. *Nanosc. Nanotech.* **8**, 2745 (2008)

[2] Garcia et al. *Appl. Phys. Lett.* **97**, 022501 (2010).

Spintronics, dilute magnetic semiconductors, and semiconducting heterostructures

3 - 1 – Structural, optical and morphological properties of $\text{Ga}_{0.72}\text{Mn}_{0.28}\text{As}$ thin films deposited by magnetron sputtering for spintronic device applications

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In this work GaMnAs alloy materials were deposited on Corning glass 7059 and GaAs (001) substrates by RF magnetron sputtering technique. Concentration of Mn about 0.28 was obtained by Energy dispersive X-ray spectroscopy (EDS). The substrate temperature was changed from 440 C to 520 C and layer thickness between 172 nm and 428 nm were obtained. Characterization by atomic forced microscopy (AFM) and x-ray diffraction (XRD) were performed to determinate the surface morphology and crystal structure, respectively. From transmittance spectral measurements were determined the optical constants: Band gap energy (E_g), absorption coefficient, refraction index (n). A correlation between morphological properties and substrate type was studied too. Diluted magnetic semiconductor such as GaMnAs are considered one of the promising materials for the development of new spin-electronic devices.

3 - 2 – Relation between structural and magnetic properties in $(\text{Ti,Fe})\text{O}_2$ powders obtained by mechanical milling

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In previous works we have found a relationship between magnetism and oxygen vacancies in TiO_2 powders doped with hematite ($\alpha\text{-Fe}_2\text{O}_3$) by mechanical alloying [1]. Also we found a correspondence between oxygen vacancies and oxidation state of Fe (more Fe^{2+} more oxygen vacancies in the octahedron of coordination of Fe). Then, with the objective to investigate the role of oxygen vacancies and ions Fe^{2+} in the magnetism of diluted magnetic oxides (O-DMS) we doped TiO_2 with Fe by mechanical alloying of TiO_2 with different fractions of FeO (between 2.5 and 10 at. percent) in argon atmosphere. XRD, Mössbauer spectroscopy, X ray absorption spectroscopy (XAS), AC-susceptibility and magnetization measurements were employed in order to characterize the Fe-doped TiO_2

powders. A XAS results showed that Fe ions are incorporated into the rutile phase with oxygen coordination lower than that expected in this phase. The coordination number of oxygen decreases with the increase of Fe^{2+} ions as it was previously found in milled samples of TiO_2 doped with hematite. The RT Mössbauer spectra were reproduced using two paramagnetic interactions, one corresponding to Fe^{2+} (isomer shift 0.87 mms^{-1}) and the other to Fe^{3+} (0.31 mms^{-1}). Magnetometric measurements showed the presence of paramagnetic and ferromagnetic like interactions at room temperature. The relation between relative fraction of Fe^{2+} and the oxygen vacancies with magnetic behaviour will be discussed.

[1] A.M. Mudarra Navarro, V. Bilovol, A.F. Cabrera, C.E. Rodríguez Torres and F.H. Sánchez Physica B 404 (2009) 2838-2840.

3 - 3 – Ferromagnetism diluted in Zn- and Co-doped $\text{CeO}_{2-\sigma}$

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This work aims to study a new system that shows diluted magnetic with room-temperature ferromagnetism. It is known that zinc oxide and cerium have diluted magnetic properties and we believe obtaining the Zn- and Co-doped $\text{CeO}_{2-\sigma}$ that may open a new line of research in material for application in spin electronic with Tc above room temperature. A proteic sol was prepared by dissolving $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ and $(\text{NH}_4)_2\text{Ce}(\text{NO}_3)_6$ in filtered coconut water with $x = 0.01, 0.05$ and 0.1 to obtain the $\text{Ce}_{1-2x}\text{Zn}_x\text{Co}_x\text{O}_{2-\sigma}$. Afterwards, the sol was heated at 100°C for 24 h for gelification and calcined at 600 and 800°C for 1 h. The XRD patterns for both calcination temperatures, were identified using JCPDF #34-0394, which suggests a cubic symmetry belonging to the F_{m-3m} space group characteristic of CeO_2 without Zn or Co oxide phase. Except for $x = 0.1$, that showed spurious phase attributed to Co_3O_4 indicating that the maximum doping into CeO_2 is below 10%. Raman spectrum we observed a peak most pronounced feature for the CeO_2 samples, and it is localized at about 463 cm^{-1} to calcined temperature of 600°C and 467 cm^{-1} to 800°C . This mode ($F2g$) represents a symmetric "breathing" mode of the O atoms around each Ce. Besides peaks at about 250 and 600 cm^{-1} are also associated with CeO_2 due to the presence of defects in the resulting formation of oxygen vacancies. The M versus H (M(H)) at 2 and 300 K showed ferromagnetic behavior for $x = 0.01, 0.05$ and 0.1 for samples calcined at 600 and 800°C . The saturation magnetization (Ms) at room temperature for samples calcined at 600°C , showed values

of the 3.1×10^{-5} , 6.99×10^{-4} and 8.55×10^{-4} emu/g for concentrations of $x = 0.01$, 0.05 and 0.1 , respectively. However, the samples calcined at $800^\circ C$ happened an increase in saturation magnetization about twice higher for $x = 0.1$ and four times higher for $x = 0.05$ indicating that the increase of crystallinity and the generation of oxygen vacancies (confirmed by Raman spectroscopy), contributing to the ferromagnetism of $Ce_{1-2x}Zn_xCo_xO_{2-\sigma}$. The measures of M versus T were collected under ZFC and FC protocols (M(T)) between 2 and 300 K. The sample with $x = 0.1$ showed the highest value of magnetization (2×10^{-3} emu/g), followed $x = 0.05$ (1.6×10^{-3} emu/g) and $x = 0.01$ (1×10^{-3} emu/g) when calcined at $600^\circ C$. It was observed a increasing of the M(T) with increasing calcination temperature. The Zn- and Co-doped samples showed no irreversibility temperature or blocking temperature and we can infer that Currie temperature (T_C) is above room temperature.

3 - 4 – Saturation Magnetic Moments studies of Mn doped GaAs and GaN doped thin film

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GaAs and GaN thin films doped with Mn were grown by Reactive Sputtering method. We have studied films doped with different concentrations of Mn (0.5 – 18 %) by means of magnetic susceptibility and Electron Spin Resonance (ESR) experiments. A single nearly temperature independent $g \sim 2$ line is observed for the Mn-doped films. ESR intensity of this line roughly follows the paramagnetic Curie-law measured in the magnetic susceptibility. At low-T, we have observed ferromagnetic loops for $Ga_{1-x}Mn_xN$ ($x = 18\%$) thin films and followed the maximum saturation magnetic moment (M_S) as a function temperature for this film. However, no evidence for a ferromagnetic transition was verified on the ZFC and FC susceptibility curves, in contrast to the ferromagnetic ordering observed in crystalline films for at $T_C \sim 110$ K.

3 - 5 – Rare-earth doping induced exponential depletion the neutral dangling bonds (D^0) density in amorphous Si films

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In this work we study the effect reduction in the density of dangling bonds species D^0 states in a-Si films as function concentration for different Rare-Earth species. The amorphous silicon thin films doped with different concentrations of rare-earth ($a\text{-Si}_{1-x}\text{RE}_x$, RE = Y^{3+} , Gd^{3+} , Er^{3+} , Lu^{3+}) were prepared by co-sputtering and investigated by Electron Spin Resonance (ESR) and Raman scattering experiments. According to our data the RE-doping reduces the ESR signal intensity of the D^0 states with an exponential dependence on the rare-concentration. Furthermore, the reduction produced by the magnetic rare-earths Gd^{3+} and Er^{3+} is remarkably greater than that caused by Y^{3+} and Lu^{3+} , which led us to suggest an exchange-like coupling between the spin of the magnetic RE's³⁺ and the spin of silicon neutral dangling bonds.

3 - 6 – Structural and Magnetic Characterization of $Ce_{1-x}TM_xO_2$ Nanoparticles

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In last years the study of the so-called diluted magnetic semiconductors (DMS) has attracted the attention of the scientific community due the strong potential of their application on technological devices [1]. For practical applications, it is very important that DMS samples present magnetic order at room temperature. There are reports in the literature which state that the appearing of the magnetic order is sample dependent, that is, magnetic clusters can be grown inside the semiconductor host depend on the sample preparation and the doping level. On the other hand, the existence of the localized ferromagnetism has been observed via X-ray magnetic circular dichroism [2]. Then, the main challenge is to control the insertion of the magnetic ion inside the semiconductor host. In this work, we have used co-precipitation chemical method to synthesize the $Ce_{1-x}TM_xO_2$ ($0.01 \leq x \leq 0.1$) DMS system at nanometric scale (TM = Fe, Cr). The structural and magnetic properties have been investigated by means of

X-ray diffraction (XRD) and magnetization measurements. Rietveld refinement method is used in the analysis of the XRD pattern. The results show the presence of single crystalline phase with a crystalline structure that is isomorphous to the semiconductor host CeO_2 . Particle average sizes ranging between 4 and 7 nm were obtained from the Rietveld refinement results together with the Scherrer formula. This result was confirmed by transmission electronic microscopy images in case of Fe (0.01 in weight) doping sample. DC magnetization measurements performed at room temperature as a function of the field have shown a ferromagnetic behavior for all $Ce_{0.99}TM_{0.01}O_2$ samples (CNPq, FAPITEC).

[1] J.K. Furdyna, J Appl. Phys.(1998) 64, R29.

[2] M. Kobayashi, et al., Phys. Rev. B 72, 201201, 2006.

3 - 7 – Effects of Cr doping on the room temperature ferromagnetism of chemically synthesized $CeO_{2-\delta}$ nanoparticles

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In the last years, many works have been suggested cerium oxide (CeO_2) as a very interesting candidate to develop spintronic devices because its electronic configuration and structural properties are similar to silicon. In this work, we studied the synthesis of $Ce_{1-x}Cr_xO_{2-\delta}$ nanoparticles by the sol-gel method. The samples were prepared by adding $Ce(NO_3)_3 \cdot 6H_2O$ and $Cr(NO_3)_3 \cdot 9H_2O$ to de-ionized water to obtain a 2M solution with a molar ratio of $x = [Cr]/[Cr] + [Ce]$ with target ratios meant to obtain a systematic variation of x in the 0–0.05 range. Then, the mixture was polymerized to form the gel at 100°C for 24h. After that, the amorphous composite precursor obtained was calcinated at 400°C in air for 1h to produce the metal oxide nanoparticles. All samples showed only the cerianite cubic and the peaks of CeO_2 and were identified using JCPD 34–0394. The sizes of the crystallites estimated from the peaks of the XRD patterns are in the range 30–58 nm. It was observed that all samples showed the Raman vibrational frequency around 468 cm^{-1} , which is the value expected for the vibrational mode of the Ce-O. This observation suggests the absence of secondary phase and is in agreement with the findings obtained from XRD. SEM images showed that the surface topography of the $CeO_{2-\delta}$ sample has a porous and loosen structure, while the Cr doped samples exhibit a dense and compact structure. The morphology study by TEM showed that the pure and Cr doped $CeO_{2-\delta}$ particles present average diameter around 35 and 50 nm, respectively. The Cr content in the samples, determined by EDS, was about $x = 0, 0.018,$

0.037, and 0.051, which was consistent with the design of our experiment. The XPS spectra for Cr doped $CeO_{2-\delta}$ samples showed that a mixed oxidation state with Cr^{2+} and Cr^{3+} coexisting. Based on the Gauss fitting, the $Cr2p_{3/2}$ and $2p_{1/2}$ peaks positions were found at 576.1 eV and 587.2 eV respectively. These results exclude the possibility of the Cr cluster formation and indicates that a higher content of Cr^{3+} substitute Ce ions positions in the crystal. The Cr doped $CeO_{2-\delta}$ samples is found to be ferromagnetic. We verified that, at 300 K, samples had weak ferromagnetic behavior, with magnetization saturations of 5×10^{-3} and 3×10^{-2} emu/g for samples with 1% and 5% of Cr, respectively. The coercivity field also increases by six orders of magnitude from 95 Oe(1%Cr) to 101 Oe(5%Cr). The ZFC and FC magnetization curves exhibited the same small slope behavior, indicating a strong paramagnetic contribution. These results indicate that the weak ferromagnetic behavior observed in Cr doped $CeO_{2-\delta}$ nanoparticles are related with the dilute localized magnetic moments presence inside the semiconductor matrix.

3 - 8 – Effect of the thermal treatment in vacuum on Fe- doped SnO_2 powders

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On the last years an enormous activity has been directed to understand the origin of the magnetism in oxide diluted magnetic semiconductors. These kinds of material are produced doping a semiconductor oxide with a transition metal. Most reported models for the observed magnetic behaviour are based on the interaction among magnetic impurities mediated by oxygen or free carriers. Furthermore experimental works have shown that defects, like oxygen vacancies, could lead to ferromagnetism. Since oxygen vacancies concentration can be modified by adequate thermal treatment, in this work we study the influence of the thermal treatment (TT) in vacuum on SnO_2 doped with 10 at. % of Fe. The sample was prepared by mechanical alloying during 5h in air. The TT was carried out in vacuum during two hours at the 773K. It leads to an important change in the structure of the sample. Before TT from the structural point of view the sample is monophasic (rutile) with Fe substituting Sn in the lattice of semiconductor. After TT, iron ions migrate from SnO_2 lattice and recombine with tin and oxygen forming a new spinel type $Sn_xFe_{3-x}O_4$ phase. A fit of the diffractogram corresponding to TT sample shows that the 30 % of the intensity corresponds to the spinel type phase. The room temperature Mössbauer

spectrum reveals about 93 % of irons in magnetically ordered state in contrast with the paramagnetic order observed in the non treated sample. Magnetization vs applied magnetic field (M vs. H) curve shows hysteresis loop, typical of soft ferrimagnet. So, we ascribe the magnetic behavior detected after the TT to the formation of the $\text{Sn}_x\text{Fe}_3 - x\text{O}_4$ phase.

3 - 9 – Size and doping effect on structural and magnetical properties of $\text{Sn}_{1-x}\text{TM}_x\text{O}_2$ nanoparticles (TM = Fe, Cr, Mn and Ni)

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Diluted magnetic semiconductors (DMS) have attracted many researchers at areas different because its potential in applications at optoelectronic devices, in which one seeks to control both the charge and spin degrees of freedom of the electron [1-4]. In the last years some works have been reported to present ferromagnetic order close to room temperature. Some groups defend the idea of the existence of magnetic clusters, but for others groups this ordering is related to localized impurity magnetic moments induced by indirect exchange (RKKY) interaction mediated through free carriers (either electrons or holes) [2,4]. So, the control in preparation of these materials is extremely important for appearing of both properties. In this sense we have studied the magnetic and structural properties of Mn-doped SnO_2 and ZnO for different doping concentrations obtained by coprecipitation method. These samples were prepared such in bulk and nanostructure form. X-ray diffraction results show that all samples present isomorphous phase to the host structure without presence impurities phases for concentrations up to $x = 0.10$. For nanostructured samples, analysis of Rietveld refinement show that particles have average size of 4-25 nm for SnO_2 . These results also confirm the presence of high microstrain in the samples with size very small. Magnetization results as function field at room temperature show that the ferromagnetic origin in these samples appears only for doping concentration higher than 0.1. Other result interesting is the dependence on magnetic properties as function of the particles sizes showing the intermediary limit of appearance of weak ferromagnetism in these systems. (FAPITEC-SE, CNPq)

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[3] D. Karmakar et al., Phys. Rev. B 77 (2008) 245208.

[4] B.D. Yuhas et al., Nano Letters 7 (2007) 905.

3 - 10 – DFT study of the structural, electronic and optical properties of the LiF and $\text{Li}_{0.75}\text{M}_{0.25}\text{F}$ (M=Mn, Mg, Ti)

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Structural, electronic, and optical properties of the lithium fluoride LiF, and the doped compounds $\text{Li}_{0.75}\text{M}_{0.25}\text{F}$ (M=Mn, Mg, Ti), are studied using the full-potential linearized augmented plane wave method (FP-LAPW) in the framework of density functional theory (DFT). The exchange-correlation potential is treated by the generalized gradient approximation within the scheme of Perdew, Burke and Ernzerhof (GGA-PBE). The calculated bulk properties, including lattice constants, bulk moduli and their pressure derivatives are in great agreement with the available data for the LiF, data are not available for the $\text{Li}_{0.75}\text{X}_{0.25}\text{F}$. Energy band structures show that the LiF is direct energy band gap insulator material and the doped systems are metallic. Analysis of the density of states and the energy vs. volume graphics, allowed us to understand the effect of the impurities in the LiF structural and electronic behavior. the energy dependent refractive index, reflectivity and the absorption spectrum are calculated for all compounds within the random phase approximation (RPA) using Kohn Sham orbitals. Based on our results we postulate the $\text{Li}_{1-x}\text{M}_x\text{F}$ (with $x < 0.25$) systems as a potential diluted magnetic semiconductors.

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3 - 11 – ELECTRICAL TRANSPORT PROPERTIES OF AgInS₂ THIN FILMS PREPARED BY CO-EVAPORATION

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This work presents results regarding the influence of preparation conditions on the electrical transport properties of AgInSi₂ (AIS) films, grown by co-evaporation of precursors in a two-stage process. For this, the AIS films were investigated by conductivity and Hall-voltage measurements. This measurements as a function of temperature, carried out in the range between 90K and 600K revealed that the electrical transport in AIS films is affected by two different mechanisms. At temperatures greater than 350K, the conductivity is predominantly affected by hole transport in extended states of the valence band, whereas at temperatures below 250K the conductivity is mainly determined by the variable range hopping (VRH) transport mechanism. These results were correlated with XRD measurements.

3 - 12 – Substrate dependence of the optical and structural properties of GaSb layers

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In this work, we report the optical and structural properties of GaSb layers grown on Si(100) and GaAs (100) substrates by using magnetron sputtering R.F technique in an argon atmosphere. We varied the substrate temperature ($300\text{ }^{\circ}\text{C} < T_s < 600\text{ }^{\circ}\text{C}$), and the Ar pressure ($10^{-3}\text{ Torr} < P < 10^{-2}\text{ Torr}$) in order to correlates with the microstructure, morphology and vibrational modes of the GaSb layers. We observed an improvement of the structural ordering of the GaSb layer by X-ray diffraction when increasing the growth temperature and decreasing the residual Ar pressure. The optical properties were analyzed from FTIR spectroscopy and micro-Raman spectrum taken at room temperature by using the line 479 nm of an argon laser as excitation source. The results show a strong influence of the growth condition and the substrate orientation on the microstructure and TO and LO vibrational modes associated to GaSb.

3 - 13 – Optical, structural and magnetic characterization of AlN/Mn Multilayers

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The AlN/Mn multilayers were deposited by magnetron sputtering on Si (100) and glass substrates in atmospheres of Ar and Ar+N mixture, respectively. The power supplies applied to the Mn and Al targets were fixed at 30 watt and 150 watt. The optical and structural properties were studied from X-ray diffraction and Fourier Transform Infrared spectroscopy (FTIR) spectrum. The crystal structure of the AlN/Mn multilayer's obtained from x-ray spectrum show peaks associated of the cubic phase of the each layer, respectively. FTIR spectra evidenced vibrational active Raman modes of AlN located at 500 cm^{-1} and 900 cm^{-1} , identified as $E_1(\text{TO})$, and $E_1(\text{LO})$. Vibrating sample magnetometry and AC susceptibility were used to explore the magnetic behavior of the layers at different temperatures. The layers show ferromagnetic behavior beyond room temperature.

3 - 14 – Spin relaxation mechanisms in the impurity band of semiconductors

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We explore spin-relaxation mechanisms of the electronic spin in the impurity band of n-doped semiconductors. We propose two spin relaxation mechanisms made possible by the spin-orbit interaction of electrons in the impurity band, which are analogous to the Rashba and Dresselhaus couplings that are present in semiconductor nanostructures. The spin relaxation time is obtained by means of numerical calculation of the time evolutions of initially pure spin states. We find that both the Rashba and Dresselhaus interactions are relevant in terms of spin relaxation, but surprisingly the latter dominates over the former. The spin relaxation times found are slightly shorter than the experimental ones available in the literature, which shows the relevance of the mechanisms studied here. The quantitative disagreement could be explained by the simplifications made in our model calculations, like for example the neglect of electron-electron and electron-phonon interactions.

3 - 15 – Interaction of solids with twisted light

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We study the interaction of solids and nanostructures with light carrying orbital angular momentum (twisted light). We find the selection rules that regulate the optical transitions induced by twisted light in bulk semiconductors, and quantum wells, dots and rings. We describe the electrical currents generated in these material systems and the transference of angular momentum from light to matter. For bulk, quantum wells, and quantum rings we developed equations of motion which describe the quantum dynamics of the photo-excited electrons and solve them analytically up to first order in the applied twisted-light field.

3 - 16 – Lateral confinement effects on the magnetic domains arrangement of MnAs micrometric bars

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One of the major challenges of spintronics development nowadays is the capability of integrating semiconductors and ferromagnetic materials in multifunctional devices. In this field, the MnAs alloy is a promising material due to the facts that it presents ferromagnetism until 314K and grows epitaxially on GaAs. The typical size of a magnetoelectronic device is 50-1000 nm, so it is important to look at the physical properties of MnAs in the nanoscale. Previous studies performed on MnAs thin films indicate that the structural and magnetic properties of these materials differ from those of the bulk. A magneto-structural phase coexistence is observed in a broad temperature range just below the Curie temperature, formed by an hexagonal ferromagnetic phase (α) and an orthorhombic paramagnetic phase (β). This phenomenon is explained in terms of substrate-induced strains. The α and β phases are organized in a regular pattern of stripes when the film is deposited onto GaAs[100] while they are randomly organized when the film is grown on GaAs[111]. In this work we present a study of the magnetic properties

of MnAs(120nm)/GaAs[100] micrometric bars. Samples of different width and constant length were fabricated by electron lithography. The bars were oriented parallel and perpendicular to the hard-magnetic axis of the system, i.e. c -axis. The magnetic imaging of the micrometric bars was made by magnetic force microscopy between 24°C and 11°C. Our results indicate that the α/β phase coexistence and the magnetic domain arrangement depend on the size and the orientation of the bars, while the alignment of the striped parallel to the axis is preserved in both orientation of confinement.

3 - 17 – Highly anisotropic domain wall velocity in MnAs/GaAs (001) thin films

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In most of the commercial magnetic storage available devices, the magnetization is still controlled by applying short magnetic field pulses supplied by a current line located above the magnetic cell. Nevertheless, this technique is still subject to severe impediments, like the influence of stray fields over the adjacent cells or the large power required for switching the magnetic state, which limit the device scalability. One alternative method would be to store information on magnetic domains separated by domain walls along a magnetic track[1]. Moving the domain walls by a current using the spin transfer process would allow for information retrieval by a fixed reading head. For that purpose hybrid heterostructures based in the (III,Mn)V family, which combine magnetic and transport properties, have proved to be of great interest. Moreover, these films present a strong in plane uniaxial anisotropy, which is an advantage taking into account that the out-of-plane geometry might limit the domain wall velocity[2]. Up to now there has been very few studies of domain structure and domain wall propagation in (III,Mn)V heterostructures with in-plane magnetization[3]. The first step is to investigate the domain structure and domain wall propagation in an applied magnetic field, which can provide the key parameters for current-driven propagation[4]. We combine magneto optical imaging and magnetic pulse technique to study the domain wall dynamics in MnAs/GaAs (001) thin films with in plain magnetization. The domain wall velocity is found to be highly anisotropic, and, surprisingly enough, does not seem to depend on temperature, even in the interval where both ferromagnetic α and paramagnetic β phases coexist [1]. This fact suggests different magnetization reversal mechanisms in both easy and hard magnetic axes and rises the question of which is the role of the beta phase in the domain wall pinning. Several features of the domain wall nucleation and propagation

recently predicted[6] for this system were contrasted in our experiments, showing a good agreement with the model for the domain dynamics.

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Intermetallic compounds

4 - 1 – Synthesis and thermoelectric properties of polycrystalline Zn_4Sb_3 compounds prepared by hot pressing method

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Single phase $\beta - Zn_4Sb_3$ samples were prepared by using hot pressing method. Their structural and morphological properties were studied by x-ray diffraction analysis (XRD) and Scanning Electron Microscopy (SEM), respectively. The transport properties were evaluated from Seebeck coefficient $S(T)$ and electrical resistivity $\rho(T)$ measurements in the temperature range between 100 and 290K. $S(T)$ shows positive values suggesting a p-type material, its magnitude increases with the processing time, reaching maximum values close to 300 $\mu V/K$. The electrical resistivity, measured by four D.C. probe method, increases with processing time, however its magnitude is less than 25 $m\Omega\cdot cm$. An order-disorder transition was observed in the transport properties around 240K, which is a characteristic property of pure single crystals of $\beta - Zn_4Sb_3$. From $S(T)$ and $\rho(T)$ experimental data the thermoelectric power factor PF was calculated, this performance parameter reaches maximum values close to 100 $\mu W/K^2\cdot cm$, which make this kind of compounds promising materials for thermoelectric applications.

4 - 2 – Metallic cathode surface modification by using low pressure pulsed vacuum arc discharge

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Electrical discharges in a pulsed vacuum arc system at low pressure were produced, using a peak current of 100 A with pulses of 30 ms. Discharges were carried out applying a voltage of 104 V between the electrodes. Materials used as cathode were Ti, Zr, Ni, Cu, Mo and W. The cathodes morphology after the discharges production was studied by using the scanning electron microscopy (SEM) technique. Ti and Zr presented the highest erosion. Moreover, circular craters on Ni and Mo cathodes were observed and a region of the Zr cathode, with high erosion and great quantity of craters was analyzed. The discharge voltage for each material was measured, obtaining arc voltage values. Finally, relationships between arc voltages and

some material characteristics as melting point, boiling point, electrical and thermal conductivity were observed.

Keywords: Morphology, Spots, Arc voltage, Metallic cathodes.

4 - 3 – Microstructural evolution in TiZrN thin films varying the substrate temperature during deposition

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Materials microstructure is considered as one of the most relevant characteristics for defining their performance and specific applications. For this reason, the microstructure becomes an important factor in material science. In this work the development of the microstructure as a function of substrate temperature in Titanium-Zirconium Nitride thin films is studied. The films were grown by the cathodic pulsed vacuum arc technique on stainless steel 316L substrates varying the temperature values of 20, 50, 100, 150 and 200°C. For the films growth, four pulses were applied; each 30 ms and time between these pulses was 40 s. X-ray diffraction was used to identify the crystallographic phase present in the films evaluating the lattice parameter. By using Scherrer equation, microstructure characterization was carried out depending on the lattice strain and crystallite size analyzing the influence of the substrate temperature. Other important measurement for elucidating important films structure characteristics were rocking curves in order to obtain the dislocations density in the material, presenting a substantial broadening and asymmetry. Surface analysis was carried out by scanning probe microscopy in atomic force microscope mode, obtaining values for roughness and grain size depending on the parameter substrate temperature.

4 - 4 – Effect of annealing process on TiN/TiC bilayers grown by pulsed arc discharge

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In this work, a study of annealing process effect on TiN/TiC bilayer is presented. The annealing temperature was varied between 0 and 500 °C. The materials were produced by plasma-assisted pulsed arc discharge. In order to grow the films, a target of Ti with 99.9999 purity and stainless-steel 304 substrate were used. For the production of TiN layer, the reaction chamber was filled up with nitrogen gas until reaching a 2.5 mbar and the discharge was performed at 310 V. The TiC layer was grown in a methane atmosphere at 3.0 mbar and 270 V. Both films were grown at a substrate temperature of 150 °C. The microstructure evolution was study by means of XRD. At 400 °C, TiO₂ phase begun to appear and it was well observed at 500 °C. Crystallite size and microstrain was obtained as a function of the annealing temperature. XPS technique was employed for analyzing the bilayers before and after the annealing process. Narrow spectra of Ti2p, N1s and O1s were obtained, presenting TiO phases.

4 - 5 – Study of Cohesive, Electronic, and Magnetic Properties of the Ni-In Intermetallic System

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Cohesive, electronic and magnetic properties of the intermetallic system Ni-In, specifically the stable phases Ni₃In-hP8, Ni₂In-hP6, NiIn-hP6 y Ni₂In₃-hP5, have been investigated. Presently, these materials are of great interest in connection to the application of the In-Sn alloys as lead-free micro-soldering alloys, and considering Ni as the contact material. In spite of this, scarce literature regarding basic thermodynamic properties of the Ni-In intermetallic phases has been found. Full-Potential Linear Augmented Plane Wave method (FP-LAPW) within the framework of the Density Functional Theory (DFT) with exchange and correlation effects in the Generalized Gradient (GGA) and Local Density (LDA) approximations is used. All

calculations include spin polarization. Structural parameters, formation energies and cohesive properties of different phases are studied through minimization of internal parameters. Density of states (DOS) is analyzed for each optimized structure. We found that the NiIn-hP6 phase is the most stable one and only the Ni₃In-hP8 phase exhibits magnetic properties.

4 - 6 – (Fe, Si)₂Mo Laves phase solid solution

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Silicon plays an outstanding role in C14 Laves phase Fe₂Mo stability. However, only a few early works have been devoted to study silicon solubility. Experimental studies established the existence of C14 phase at three compositions in the ternary system Fe–Mo–Si along a constant 0.66 at %Mo content. A semi empirical approach to describe phases stabilities in the ternary system was recently enhanced by the incorporation to the data base of FeSiMo formation energy calculated with first principles methods. Some of the authors of the present work have presented in a previous paper the first fully first principles calculation of the ground state and thermodynamic functions at finite temperatures of the pseudo binary system Fe₂Mo – Si₂Mo. A cluster expansion based on first principles calculation of formation energies and Monte Carlo simulations for finite temperatures have been implemented. A miscibility gap that had not been experimentally reported has been predicted. We present in this work a different approach to random (Fe, Si)₂Mo solid solution by means of special quasirandom structures (sqs) as a proven technique to simulate random alloys. The ATAT package was used to generate sqs and the SIESTA code based on pseudo potentials was used to calculate formation energies. The previous results were confirmed.

4 - 7 – Density Functional Theory applied to study of the chemical reactivity of Mg and Mg₂Ni alloy

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Hydrogen is an excellent energy carrier to be used in both fuel cells and combustion engines as a clean fuel. However, the success of a hydrogen economy relies on our ability to store hydrogen safely and economically under ambient conditions and with large gravimetric and volumetric density. Magnesium-based alloys are considered to be the most promising materials for hydrogen storage because of their high storage capacity, the abundance of magnesium in the Earth's crust and low cost compared to alternative systems. Of all the magnesium-based alloys, the intermetallic compound Mg₂Ni can be easily synthesized and it reacts readily with gaseous hydrogen to form reversibly the stable hydride Mg₂NiH₄, which, from the engineering point of view, is considered to be a very convenient material for hydrogen storage purposes. Using a density functional approach calculation, the energetic, electronic and reactivity properties of Mg and Mg₂Ni alloy are systematically investigated. Our results indicate that pure magnesium is more reactive than Mg₂Ni alloy against hydrogen adsorption and the molecular electrostatic potentials show us the sites most susceptible to electrophilic attack.

4 - 8 – Electrical resistivity of pressurized iron and Fe-Ru alloys

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The $p - T$ phase diagram of iron is complex, displaying at least four solid phases with different magnetic properties. Hexagonal iron is the stable phase above 13 GPa and its magnetic state, thought to be antiferromagnetic, is still the object of debate. Notably, between 13 GPa and 31 GPa an unconventional superconducting state develops.

Iron-ruthenium alloys, Fe_{1-x}Ru_x, have a hexagonal structure for $x > 0.3$. The magnetic ground state of these alloys is also under debate, and superconductivity has been reported only for very low Fe-content (i.e., $x \sim 1$). We will discuss differences and similarities of the pressure- and alloying-induced hexagonal phases of iron as probed by low temperature electrical resistivity measurements.

4 - 9 – Atomistic modeling of ternary additions to NiTi and quaternary additions to NiTiPd, NiTiPt and NiTiHf shape memory alloys

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Development of new NiTi-based high temperature shape memory alloys (SMA) relies mainly on the ability to identify the appropriate alloying additions that introduce the desired changes in the austenite-martensite transition temperature. Experimental work has been done in this direction, and several elements have been studied that have that effect but, as is often the case in alloy development programs, ternary or higher order additions introduce changes in properties, some of them critical enough to invalidate their use for specific applications. It is also common that a variety of practical considerations, such as costs, processing, environmental effect, and others, introduce additional difficulties, making the search of the appropriate candidates a lengthy and costly process. In spite of the enormous progress and the inherent difficulties of performing systematic studies of new compositions, no single picture has emerged yet to systematically deal with the different variables that should be taken into account for any given application. This is the case with ternary additions such as Pd, Pt and Au, in alloys Ti₅₀Ni_{50-x}Y_x (Y = Pd, Pt, Hf), which are among the most promising candidates for high temperature shape memory alloys (HTSMA), but due to the costs associated with precious metals, other alternatives must be considered. In addition, while several studies can be cited on specific ternary systems, basic information on the quaternary cases is, in comparison, lacking. Modeling focusing on the basic properties of large numbers of ternary and quaternary cases could then be helpful in the process of downselecting compositions that meet desired criteria in terms of strength, density, phase structure, etc. As a first step in this direction, this work provides a systematic study of a large number of additions to NiTi, some known and some never tried before: X = Au, Pt, Ir, Os, Re, W, Ta, Hf, Ag, Pd, Rh, Ru, Tc, Mo, Nb, Zr, Zn, Cu, Co, Fe, Mn, V, Sc, Si, Al and Mg. In addition, we extend this work to the study of the physical properties of quaternary alloys Ni-Ti-Pd-X, Ni-Ti-Pt-X and Ni-Ti-Hf-X, with the same options for X, and compare their changes relative to the ternary base alloy. The atomistic modeling work is made using the Bozzolo-Ferrante-Smith (BFS) method for alloys for the energetics. Bulk properties such as lattice parameter, energy of formation, and bulk modulus of the B2 alloys are studied for variations due to the presence of one or more additives, thus developing a database for

HTSMA candidates that could aid in current and future experimental work towards the development of HTSMA for specific applications.

4 - 10 – Investigation on the oscillatory behaviour of the lattice parameter in ternary iron-nitrogen compounds

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In the last years, many theoretical and experimental studies have been reported on TM-Fe₃N alloys (TM, 3d transition metal), due to the potential technological applications on derivatives of Fe₄N in very important magnetic properties, ie. high density magnetic recording. These compounds have a perovskite-type structure, where the TM atom is located at the corner of the cube, the Fe atom in the center of the faces and the N atom in the center of the cube, corresponding to the 1a, 3c and 1b Wyckoff position, respectively. In the present work, using ab-initio calculations (Wien2k code), we show that the lattice parameter have an oscillatory behaviour. The oscillations of these parameters are decreasing with increasing of the atomic number Z of the TM-Fe₃N compound. The oscillations of the lattice parameter are strongly related with the type of TM in the compound and the charge distribution of the d-orbitals of the atoms in the sites 1a (TM) and 3c (Fe). The magnetic properties of compound changes with the 3d metal, i.e., it is non magnetic for TM=Sc, ferrimagnetic for TM=Ti, V and Cr, and ferromagnetic for TM= Mn, Fe, Co, Ni, Cu and Zn, in the case of Cu and Zn the ferromagnetism is due only to the Fe atoms in 3c sites. It is worth to mention that some authors do not consider Zn in the 3d series; in the present work we have included it in our series for completeness.

4 - 11 – A first-principles study of hydrogen storage in saline hydrides. Lithium hydride series.

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The problem in extending the application of hydrogen as a clean energy source is based on storage and portability. In this regard, saline hydrides such as lithium hydride appear as new alternatives to this, owing to their properties, their high reactivity and reversibility. In addition to experimental studies, theoretical research can provide extensive information about these types of systems. The first principles calculations based on density functional theory

(DFT) have been used to study the physical properties of Li-H compounds. The crystal structure, electronic properties and internal optimization parameters are treated by the LAPW method implemented in the WIEN2k code. In the present study we show the comparison of two different phases of lithium hydride compounds, in four different crystal structures, with the purpose of comparing the formation energies in all cases, and determine which is the structure with the best structural properties for applications in energy reservoir. The comparisons between the results obtained in the structures of lithium-hydride are discussed in this work.

4 - 12 – Ab-initio modeling of phase stability and thermodynamic properties of Cu-In and Cu-Sn intermetallics. Calculation of energy parameters involved in the thermodynamic assessment of the Cu-In-Sn system using sublattice models

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The In-48at.%Sn eutectic alloy is an attractive candidate for the development of Pb-free solders within the diffusion soldering method. In order to understand the phase formation between the soldering alloy and the Cu substrate, the knowledge of the physico-chemical properties of the formed intermetallic phases (IPs) and the phase equilibrium properties of the Cu-In-Sn system are of great importance. Previous attempts to investigate the phase stability of the IPs of the Cu-In-Sn system were based on combining the experimental information available, with thermodynamic models for the Gibbs free energy of the ternary and binaries phases. In this way using methods like the CALPHAD method ("Calculation of Phase Diagrams") it is possible to get useful predictions for the phase relations on the ternary field, starting from information of the binary subsystems. Extensions of the binary phases to the ternary field can be modeled by the Compound Energy Formalism, in which varying amounts of the third element are added substitutionally to the binary phase. Certain IPs of the Cu-In-Sn system can be treated with models of the type $(\text{Cu})_a(\text{In},\text{Sn})_b$, while others non-stoichiometric Cu-In and Cu-Sn binary phases, with models of the type $(\text{Cu})_a(\text{In},\text{Sn})_b(\text{In})_c$ o $(\text{Cu})_a(\text{In},\text{Sn})_b(\text{Sn})_c$, respectively. In this work we perform *ab-initio* calculations

using the Vasp Code to determine the energy parameters involved in the application of CEF to various IPs of the Cu-In-Sn system. We use the projector augmented wave potentials (PAW) and the exchange-correlation functions of Perdew and Wang in the generalized gradient approximation. We study the end-member compounds involved in the CEF treatment of the ternary phases generated by adding In to the binaries ϵ -Cu₃Sn (oP8) and ξ -Cu₁₀Sn₃ (hP26), and adding Sn to the CuIn₂ phase (tI12). This work extends a recent research performed for the end members associated to δ -Cu₇In₃ (aP40), η -Cu₂In (hP6) and η -Cu₆Sn₅ (mC44) phases. All these results are considered to establish trends in the relative stability and thermodynamic properties of the IPs of the Cu-In and Cu-Sn subsystems. We critically compare the calculated formation energies for the CEFs compounds with data previously obtained by phenomenological Cu-In-Sn CALPHAD analysis.

Highly correlated systems and general field theory applications

5 - 1 – von Neumann entropy of the Bose-Hubbard model at half-integer densities

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Using the Density Matrix Renormalization Group (DMRG) method, we investigated the entanglement in a one-dimensional boson chain with nearest-neighbors interactions. The measures of entanglement calculated were: one-site, two-site and block von Neumann entropy in order to investigate the quantum phase transition of the Charge Density Wave (CDW) to the Superfluid phase (SF) for half-integer densities. It was observed that the behavior of the block entropy as a function of the number of sites changes from a critical value of the hopping parameter (t), which represents the kinetic energy of the bosons. For values above this critical point, the block entropy tends to behave logarithmically, which agrees with the mean field theory and shows us the presence of the Superfluid phase. For values below that critical hopping this entropy shows an increasing behavior which saturates near the last sites of the chain and therefore represents the Charge Density Wave phase. The one-site entropy as a function of the number of sites also give us information about the quantum phase transition. For the superfluid phase this entropy saturates rapidly while the CDW phase grows smoothly until it reaches a maximum value. Finally we studied the two-site entropy which did not give us information about the phase transition. We found that the von Neumann entropy is a useful quantity to determine the CWD-SF quantum phase transition, which happens at $t_c = 0.1$.

5 - 2 – Quantum Phase Transitions and Kondo Effect in Parallel Double Quantum Dots.

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Semiconductor quantum dots offer the possibility to explore strongly correlated phenomena as well as

quantum phase transitions in a highly controllable system. A double quantum dot geometry, in which dot 1 is in the Kondo regime and dot 2 acts as a non-interacting resonant level, can be tuned to access a quantum phase transition between Kondo-screened and free-local-moment phases [1]. Using the numerical renormalization-group technique, we explore the effect of nonzero Coulomb interactions U_2 in dot 2, taking into account two different configurations. In the first one, the dot-2 on-site energy ε_2 is fixed at the Fermi energy. For this instance, a critical value of U_2 separates local-moment and Kondo-screened phases. In the second configuration, the value of U_2 is changed in such a way that dot 2 is always at particle-hole symmetry. In this case, as U_2 is increased, the system evolves from a local-moment to an underscreened spin-1 regime. In both configurations, the on-site energy in dot 1 can be tuned to access a quantum phase transition of the Kosterlitz-Thouless type. Signatures of these behaviors are also reflected in the linear conductance of the system. By calculating the spin-spin correlation functions between the dots and between each dot and the leads, we are able to identify how the Kondo effect develops in each dot and how the spin-spin interactions are distributed throughout the system [2].

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5 - 3 – The solution of the nonlinear Schrödinger equation using Lattice-Boltzmann

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We present the solution of the nonlinear Schrödinger equation using the lattice Boltzmann method. We show results for one and two dimensions, with several kinds of nonlinear terms. To implement the expansion B.G.K. (Bhatnagar-Gross-Krook), we assume the distribution function as a complex function that satisfies the Boltzmann equation. Moreover, we contrast our simulation results with previous theoretical developments, finding good results.

5 - 4 - 1/2-spin Anderson Model out of equilibrium: conductance and Kondo's Temperature

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We calculate conductance through a quantum dot weak coupled to metallic contacts by means of Keldysh out of equilibrium formalism. We model the quantum dot with 1/2-spin Anderson Model and consider the limit of infinite Coulomb repulsion. We solve the interacting system with the numerical diagrammatic Non-crossing Approximation (NCA) and its extension out of equilibrium. We obtain conductance as a function of temperature and gate voltage, from differential conductance (dI/dV) curves. We discuss this results in comparison with those from the linear response approach which can be performed directly in equilibrium conditions. Comparison shows that out of equilibrium numerical results are in good agreement with the ones from linear response regime supporting reliability to the method employed. The discussion becomes relevant when dealing with general transport models through interacting regions. Left and right couplings could be not proportional preventing the application of linear response approach. We also analyze the dependence of conductance vs gate voltage curve with temperature. We find that it presents a plateau for low temperatures as a consequence of Kondo Effect. Related to this, we discuss different ways to determine Kondo's temperature and compare the values obtained in and out of equilibrium.

5 - 5 - Transport phenomena in a mesoscopic ring threaded by a harmonically time-dependent magnetic flux

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We consider a mesoscopic ring threaded by a harmonically time-dependent magnetic flux in contact to particle reservoirs. We study the behavior of the induced currents between the ring and the reservoirs, as well as the influence of the magnetic flux in the conductance when a small bias is introduced by different chemical potentials of the two reservoirs. We consider a model of non-interacting electrons and solve the problem by recourse to non-equilibrium Green functions.

5 - 6 - Transition between SU(4) and SU(2) Anderson models

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Motivated by experiments in nanoscopic systems, we study a generalized Anderson, which consists of two spin degenerate doublets hybridized to a singlet by promotion of an electron to two conduction bands, as a function of the energy separation δ between both doublets. For $\delta = 0$ or very large, the model is equivalent to an SU(4) or SU(2) Anderson model respectively. We study the evolution of the spectral density and its width in the Kondo limit, for several values of δ using the non-crossing approximation (NCA). As δ increases, the Kondo peaks splits and the Kondo temperature (determined by the half width at half maximum of the peak at the Fermi energy in the spectral density) decreases dramatically.

Soft Condensed Matter

6 - 1 – Thermally stimulated conductivity (TSC) IN Cu_3BiS_3 thin films deposited by co-evaporation: determination of trap parameters related with defects in the gap

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Thin films of Cu_3BiS_3 were produced by evaporating of precursor species of Cu and Bi in atmosphere of sulfur through a process that includes two stages. Thermally stimulated current (TSC) measurements are carried out on as-grown Cu_3BiS_3 crystals in the temperature range of 150-300 K. The measurements were performed while increasing the temperature at a rate of 5 K-min. Analysis of X-ray diffraction and thermal power measures to room temperature enabled the phase and the type of conductivity of the material respectively. The spectra obtained from the TSC showed the presence of trapping centers associated with the peaks in the currents curves as a function of temperature. Transport mechanisms as hopping and thermally active carriers were identified for low and high temperature regions, respectively. Three trapping levels around 1.04 eV were detected from the TSC spectra. These levels in Cu_3BiS_3 crystals may be associated with the presence of structural defects and-or unintentional impurities during preparation process. The trap parameters were determined by various methods of analysis, and they agree well with each other. A correlation between electrical properties and defects in the material were also studied.

6 - 2 – Percolation in insulating-conducting composites: modeling the conductance-strain dependence.

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One of the most interesting issues in theoretical and experimental studies of disordered insulator-conductor composites is the effect on the transport properties of external perturbations, like electric and magnetic fields, mechanical stress or molecular adsorption (1,2). We focus in the present work on composites of conducting particles embedded in an insulating elastomer matrix. The matrix is compressed by

the action of an externally applied uni-axial pressure keeping constant the amount of conducting particles, a process that increases the electrical conductance of the composite, which can be used for obtaining a pressure sensor. These systems are usually considered as isotropic percolating networks where the dependence of transport properties, like the dc-electrical conductance, G , is expressed as function of the percolation probability between neighboring particles

Here a model for the dependence of the electrical conductance, G , with the strain induced by external mechanical stress in conducting particles-polymer composites is presented. The model assumes that the percolation probability between neighboring particles must depart from a scale-invariant behavior but saturate at moderated-high strains, reaching percolation path's saturation, with sigmoid dependence. This dependence is obtained by proposing a dynamic picture where contacts or bonds between neighboring particles are created but also destructed when a stress is applied and relatively moderated or high strains are produced in the composite. The electrical conductance of prepared graphite-poly-dimethylsiloxane composites were measured as function of the applied pressure and fitted by the presented model. The elastic response to the uni-axial compression was studied using a texture analyzer. The possibility of non-universal effects in the conduction critical exponent, t , was taken into account. It is concluded that the saturation of the response in the G vs. strain plots can not be assigned to non-universal behavior of the exponent t , or to saturation of the elastic response. On the other hand the presented model accounts for all the main experimental features observed in these systems and for previously reported data of elastomer composites. The simulated behavior of the piezoresistivity coefficient is also in qualitative agreement with previous reports.

(1) N. Johner, C.Grimaldi, T. Maeder, and Peter Ryser, Phys. Rev. E, 79, 20104 (2009). (2) I. Balberg, J. Phys. D: Appl. Phys. 42, 64003 (2009).

6 - 3 – Ab initio study of Cd in bulk and at the (001) surface of metallic Indium: structural, electronic and hyperfine properties

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Nuclear techniques, such as Perturbed-Angular-Correlation spectroscopy (PAC), have proven to be versatile tools for the study of a broad set of phenomena in condensed matter physics and in many other fields. Through the detection of electric-field gradients (EFG), e.g., it is possible to obtain a fingerprint of the electronic structure near and at the site of a given probe-nucleus. In the last decade, ab-initio calculations have assumed an important role in supporting, improving or confuting the interpretation of experimental data. Especially for such very sensitive properties such as the EFG, the availability of these accurate and external-parameter-free calculations has opened new possibilities. For instance, by a combination of experiments and calculations, the systematic of the EFG at different impurities sites in oxides could be understood [1]. The structural and electronic properties of layers at and near surfaces are important to understand the interaction of atoms under these special boundary conditions. The reconstructions and surface states and changes of the electronic properties between different atomic layers (or even between atoms in the same layer) are of fundamental interest for both basic and technological reasons. Using PAC, monolayer-resolved studies are possible [2] and the measured EFG could give structural and electronic information of the system that cannot be obtained by other methods, but their interpretation is not straightforward. In the present work we present a study of the EFG at isolated Cd impurities in bulk and at the (001) surface of metallic In. Our study shows that the combination PAC - ab initio calculations gives a complete description of the surface reconstruction and the changes induced by the presence of the Cd probe with respect to the bulk undoped structure.

[1] See, for example, L.A. Errico, M. Rentería, and H.M. Petrilli, *Phys. Rev. B* 75, 155209, 2007. [2] W. Körner, W. Keppner, B. Lehnorff-Junges, and G. Schatz, *Phys. Rev. Lett.* 49, 1735, 1982.

6 - 4 – Electrical properties of AgGeSe films used in ion selective electrodes

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Chalcogenide glasses have been used as sensitive membranes in ion selective electrodes (ISEs) for more than three decades. Their chemical stability ensures high endurance even in aggressive acidic media and their remarkable glass forming ability enables the use of these materials, either as bulk or as thin films, in the development of sensitive membranes for micro-sensors or multi-sensor arrays. In order to understand the sensing properties of these materials it is necessary to know first its electrical properties.

The bulk chalcogenide glasses $Ag_x(Ge_{0.25}Se_{0.75})_{100-x}$ ($0 \text{ at.}\% \leq x \leq 25 \text{ at.}\%$) have been studied as sensitive materials for ISEs. For $x \geq 8 \text{ at.}\%$ the glasses exhibit sensibility to Ag^+ and Cu^{2+} ions in aqueous solutions. For $x < 8 \text{ at.}\%$ the electrode's response was poor with almost no sensibility. On the other hand, this system behaves as ionic conductor (10^{-5} S/cm) for $x \geq 8 \text{ at.}\%$ and as insulator ($< 10^{-13} \text{ S/cm}$) for $x < 8 \text{ at.}\%$.

Membranes with smaller resistance were prepared in order to study whether the sensibility of these materials is determined by the ionic conductivity exclusively or by the total electrical resistance of the membrane. Thin films of compositions $Ag_x(Ge_{0.25}Se_{0.75})_{100-x}$ ($0 \text{ at.}\% \leq x \leq 25 \text{ at.}\%$) were deposited by PLD and the electrical transport of the films was analyzed by measuring the surface and bulk DC conductivity.

6 - 5 – Renormalized charge in spherical colloids with various boundary conditions

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The electrostatic force, long-range force is the principal responsible for phenomena in complex fluids. Complex fluids such as proteins and colloids in solutions presents a great variety of properties that make such an important and extensive field research at the industry in obtaining: aerosols, gels, foams, medicines and food, and the field of science in the description of colloids through the scattering of light, prediction of phases and structures.

The colloidal particles are of the order of micron size, sizes larger than atomic or molecular dimensions, in a solvent considered as a continuum, unstructured and characterized by a dielectric constant (ϵ). The charge of the colloids in an ionic solution (solvent)

is screened by the adherence of the micro-ions of opposite sign (screening cloud) from the solvent, thus changing the electrostatic interactions between colloids described by the nonlinear Poisson- Boltzmann equation (PB)

$$\Delta\Psi(r) = \kappa^2 \text{Sinh}[\Psi]$$

or linearization, approximation of Debye-Hückel (DH)

$$\Delta\Psi(r) = \kappa^2\Psi$$

where $\Psi(r)$ is the potential, κ is the inverse screening length.

DH approximation approach becomes inadequate to describe highly charged colloids, but using the concept of charge renormalization (Z^*) this linear equation is valid at great distances from colloid (distances greater than the Debye length). This parameter that takes into account the colloidal charge (Z) as the screening due to the micro-ions (κ). We calculated renormalized charge of spherical colloids with different boundary conditions such as: colloids with constant density and colloid charge that allow the entry of ions inside, and we compare the potential obtained by the DH approach and PB equation.

6 - 6 – Thermal and magnetic behavior of *Angustifolia Kunth* bamboo fibers covered with Fe_3O_4 particles

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Several *Angustifolia Kunth* bamboo fibers, which have been previously treatment with an alkaline solution, were coated with magnetite particles. The coating of the fibers was achieved by an in-situ coprecipitation method with Fe^{2+} and Fe^{3+} in NaOH or NH_4OH . The fibers were evaluated by chemical analysis using atomic absorption (A.A.) technique, structural characterization by X-ray diffraction (XRD), morphology by scanning electron microscopy (SEM), thermal stability with thermo-gravimetric analysis (TGA) in nitrogen at temperature range between 23 °C to 800 °C, and magnetic behavior using vibrating sample magnetometry (VSM) applying a magnetic field between -27 KOe and 27 KOe at room temperature. We found that the thermal stability and magnetization depend of the synthesis method used to cover the *Angustifolia Kunth* bamboo fibers. In addition, it was observed an improved magnetic response when NaOH solution is used to generate the magnetite coating on the fiber surface.

6 - 7 – Thermomechanical behaviour of SBR reinforced with carbon nanotubes functionalized with polyvinylpyridine.

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SBR is a so called statistical polymer of styrene/butadiene (SBR) (75% butadiene in weight). SBR is superior to natural rubber regarding less ageing and greater resistance to heat and wear. The greatest limitation of SBR for industrial applications is in its high heat generation when subjected to cyclic loads. This is caused by its great plastic phase, which generates a high hysteresis. This disadvantage of SBR is critical when considering rubber products with great thickness subjected to repetitive stresses due to the poor thermal conductivity of rubber and its consequent inefficiency at heat dissipation, being this one of the most important points to be resolved with this material. One possible solution to this problem is the addition of carbon nanotubes (NT). In particular, if these NT are functionalized with a polymer akin to the styrene phase, they will position themselves in it, improving the response compared to the non functionalized NT. The purpose of this work was to study the mechanical and thermal response of SBR reinforced with different concentrations of NTs, functionalized and non functionalized. We used polyvinyl pyridine (PVP) because of its compatibility with the PS in SBR and having the extra benefit of being a conductor polymer. The influence of the addition of NT, functionalized or not, was studied at the temperature and energy associated to the cure of SBR by Differential Scanning Calorimetry (DSC). The composites, once cured at the temperature determined by DSC, were mechanical and thermally characterized.

6 - 8 – About the cure kinetics in Natural Rubber/Styrene Butadiene Rubber blends at 433 K

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Vulcanized blends of elastomers are employed in several goods mainly to improve physical properties and reduce costs. One of the most used blends of this kind are those composed by natural rubber (NR) and styrene butadiene rubber (SBR). The cure kinetic of these blends depends mainly on the compound formulation and the cure temperature and time. The preparation method of the blends can influence the mechanical properties of the vulcanized compounds. In this work the cure kinetic at 433 K of NR/SBR blends vulcanized with the system sulphur/TBBS is analyzed in samples prepared by mechanical mixing and solution mixing. The two methods produce elastomer domains of NR and SBR which present different microstructure due to the cure level attained during vulcanization. The cure kinetics is studied by means of rheometer tests and the model proposed by Kamal and Sourour. The analysis of the cure rate is presented and is related to the structure obtained during the vulcanization process.

6 - 9 – Metastability of the vortex lattice in superconducting films containing competitive artificial and intrinsic pinning centers

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The vortex lattice (VL) in type II superconductors is known to model numerous other elastic systems in interaction with pinning landscapes. In most cases, pinning centers largely outnumber the vortex lines, and provide random weak potentials that give rise to complex dynamics, metastability and history effects. A new generation of patterned samples containing artificial arrays of strong pinning centers reveals new VL dynamics. The fingerprint of strong periodic pinning centers is an anomalous increase in critical current which generally occurs for applied "matching fields" producing a number of vortex lines equal to the number of artificial pinning sites. An open question is the effect of competing random defects on the matching anomaly. In this context we have studied the VL mobility in patterned Nb films containing periodic arrays

of sub-50nm magnetic nanodots or holes, by means of *ac* susceptibility measurements. Nb films are chosen because compared to other unpatterned films, show quite strong random disorder and may lead to competing interactions. We observe matching effects in the patterned films within a wide temperature range, determined by the periodicity of the strong artificial pinning potential. In addition to these effects, we find a novel hysteretic behavior. Below a crossover temperature $t^* \simeq 0.75T_C$, the "matching field" not only depends on the geometry of the pinning array but depends on the sample thermo-magnetic history. This hysteretic response is examined in detail and we have consistently ascribed it to metastable VL configurations that arise from the competition between pinning by random intrinsic and periodic artificial arrays. By means of different measuring protocols, including small magnetic field loops, field cooling procedures or the application of a perturbation as an *ac* "shaking" field, we examine the response of the different VL configurations that are accessible with these pinning landscapes.

6 - 10 – Thermodynamic Behavior Above the Critical Temperature

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In this work, it was studied the thermodynamic properties above of the critical temperature of a magnetic bilayer (thim film), when submitted the actions of the interactions of exchange, the dipolar anisotropy (long range) and of a external magnetic field. The interaction of exchange between spins next neighbors is ferromagnetic. It was found numerically the magnetization in function of the temperature, and the relation of dispersion of the thim film. We use the Green's function theory dependents of two times and temperature, wich is a method very adysted for systems of many interagents bodies. The results showed that the system presents long-range order until a critical value of parameter of dipolar anisotropy. The behaviors of the magnetization and the relation of dispersion in the presence and the absence of a external magnetic field for diverse values of dipolar anisotropy have been showed.

6 - 11 – Transition from a dilute to a very dense liquid

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Adsorption on single planar walls and filling of slits with identical walls are investigated in the frame of a density functional theory. It was found that when for a given adsorbate-substrate combination the adsorption on a single wall exhibits a first-order wetting transition then asymmetric profiles always appear in the filling of an equivalent slit. Moreover, both these features terminate at the same temperature. The behavior is analyzed by varying the strength of the adsorbate-substrate attraction, the temperature T , and the coverage Γ_ℓ . It is shown that for a rather strongly attractive surfaces the adsorbed liquid becomes very dense and reaching densities characteristic of solids.

Development of Experimental and Computational techniques

7 - 1 – Numerical ab-initio approach to study hydrogen diffusion in 9Cr steels

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Recently, Hurtado Noreña et al [1] have studied the hydrogen (H) diffusion effects on 9Cr steels, candidates to futures conventional thermal power plants. Based on the numerical resolution of Fick's equations in presence of trapping sites, and from the fit of electrochemical H detection curves, these authors provided quantitative information about the binding energy between H and trapping sites during diffusion process. In the present work, we calculate the equilibrium configurations and migration barriers of H for soft-martensitic steels. We have used a new theoretical approach based on ab-initio technique, employing the Monomer method [2] adapted to the SIESTA code as in Refs.[3,4]. Martensitic steel of BCT structure, containing 9%Cr in weight, is a complex system to be simulated. Our main difficulty arise in modeling such a system. For this purpose, we have considered an incremental approach, namely: the effect of c/a is not as relevant as the effect of substitutional Cr [5], then i) we start our calculation with a BCC-Fe structure in presence of an adequate environment of Cr; finally, ii) we calculate the migration barriers of H through BCC-FeCr crystallite relevant to diffusion process.

[1] Hutado Noreña, C; Bruzzoni, P.; Mat. Sci. and Eng. A 527, 3, 410-416 (2010).

[2] Ramunni, V.P.; Alurralde, M.A.; Pasianot, R.C.; Phys. Rev. B 74, 054113 (2006).

[3] Ramunni, V.P.; Pasianot, R.C.; Bruzzoni, P.; Phys. B 404, 18, 2880-2882 (2009).

[4] Pasianot, R.C.; Pérez, R.; Ramunni, V.P.; Weissmann, M.; J. Nuc. Matt. 392, 1; 100-104 (2009).

7 - 2 – Experimental and theoretical interface interaction analysis of TiN/TiC bilayers

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TiN/TiC bilayers were grown by using the cathode vacuum arc technique. In order to study the interface interaction, depth profiles were obtained by XPS (X-ray photoelectron spectroscopy). An inter diffusion between TiN and TiC at the interface showing the formation of Ti-C-N bonds. For understanding the physical process present in such an interface, simulations employed the Gaussian 98W software, observing the interface behavior, using quantum mechanics tools as first order perturbation theory. Simulations showed the formation of several bonds in the TiN-TiC interface because of the existence of internal stress as those observed in the diffraction patterns. The atomic density at the interface is high. It implies bonds formation and destruction in order to stabilizing the system. Moreover, atomic reaccommodation is appreciated as a way of releasing stress.

7 - 3 – Simulation of the magnetic field influence on the magnetocaloric properties in $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ thin films

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In this work, the magnetocaloric effect of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ as thin films varying the stoichiometry was calculated. For this aim, classical Monte Carlo simulations used in order to consider the interaction between nearest neighbors were implemented. Ions with valence Mn^{3+} and Mn^{4+} interacting with La^{3+} and Ca^{2+} respectively were considered. Terms like Zeeman effect and magnetocrystalline anisotropy were included in the Hamiltonian. Moreover, Heisenberg hamiltonian was employed for obtaining a more realistic model. Curves of specific heat and entropy, ΔS and ΔT were obtained varying the external magnetic applied field for different values of x. Results show the magnetic, lattice and electron contributions to the total specific heat and entropy.

7 - 4 – Modeling Voltage Rectification Effects on Mesoscopic Superconducting Devices

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The general and central idea that motivates this work is the recent technological progress allowing the observation of ratchet effects in very complex systems such as cold atoms, electrons in semiconductors, vortices in superconductors just to mention a few. But the main question on this field is that “is not simple” in each case to know feasibly which are the mechanisms underlying these many bodies complex effects in condensed matter. In particular, motivated for recent experiments reporting voltage rectification effects in mesoscopic superconducting triangles [Schildermans *et al*, PRB **76**, 224501, 2007] we simulated an improved model for such a system. We studied thermal fluctuations effects and capacitive effects on a Small Josephson Junction Closed Loop that mimics the rectification phenomena observed experimentally due to the superposition of a field induced persistent current with the bias current. At finite temperature we predicted that the amplitude of the rectified signal depends strongly on the current contacts configuration on the Josephson Junction Ring (weak link type junctions), in coincidence with the observations on the mesoscopic superconducting triangle sample. In addition we analyze the range of parameters where a closed loop of capacitive junctions is an appropriate model to explain the experimental observation. In short, in this work we conclude that the closed loop of SNS Josephson Junctions is a good and robust enough model in a considerable range of thermal fluctuations to explain the observed voltage rectification effects on mesoscopic superconducting samples.

7 - 5 – Numerical simulation of Ge solar cells using D-AMPS-1D code

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A solar cell is a solid state device that converts the energy of sunlight directly into electricity by the photovoltaic effect. When light with photon energy

greater than the band gap is absorbed by a semiconductor material, free electrons and free holes are generated by optical excitation in the material. The main characteristic of a photovoltaic device is the presence of internal electric field able to separate the free electrons and holes so they can pass out of the material to the external circuit before they recombine. Numerical simulation of photovoltaic devices plays a crucial role in their design, performance prediction, and comprehension of the fundamental phenomena ruling their operation. The electrical transport and the optical behaviour of the solar cells discussed in this work were studied with the simulation code D-AMPS-1D. This software is an updated version of the one-dimensional (1D) simulation program AMPS (Analysis of Microelectronic and Photonic Devices) that was developed at The Penn State University, USA, during the years 1988-1993. In AMPS the technique of finite differences and the Newton-Raphson iteration method are used to solve the Poisson and the continuity equations that are subjected to appropriate boundary conditions. The three unknowns were chosen as the quasi-Fermi levels and the electron potential. The letter D stands for new developments that were introduced in recent years. Structures such as homojunctions, heterojunctions, multijunctions, etc., resulting from stacking layers of different materials can be studied by appropriately selecting characteristic parameters such as the gap energy, carrier mobilities, absorption coefficients among others. The code evaluates the external device characteristic curves such as the current density-voltage (J-V) under dark and under illumination, the quantum efficiency (EQ), the reflectivity, and internal quantities such as the electric field, the free and trapped carrier concentrations, the recombination and generation rates, etc.. In this paper, examples of cells simulation made with D-AMPS-1D are shown. Particularly, results of InGaP and Ge photovoltaic devices are presented. It is important to mention that these structures can be use both in homojunction and multijunction devices. For the Ge cell, an example of the first scenario is the case of devices for thermophotovoltaics applications and an example of the second one is the triple junction InGaP-GaAs-Ge cells for space or terrestrial applications. In this work, numerical simulation of single junction n-p InGaP-Ge solar cells was performed. The optical reflectivity, the EQ and the role of the InGaP buffer on the device were studied. Moreover, a comparison of the simulated electrical parameters with experimental results was performed.

7 - 6 – Lattice Bhatnagar-Gross-Krook Model for Anomalous Subdiffusion

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A new lattice Boltzmann (LB) model is proposed for solving the anomalous subdiffusion equation, mathematical development is shown from the BGK model that extends the simulation method for the normal diffusion equation, considering that the development of the Chapman-Enskog expansion of this model is based on some approximations and properties formulated from fractional calculus, this result is clearly discussed due to mean square displacement is not linearly dependent on time. The computational implementation shows that the method can be used to simulate the anomalous diffusion equation.

7 - 7 – Lattice Boltzmann Model for Fractional KdV Equation

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We propose a lattice Boltzmann model (LB) which simulates the fractional Korteweg-de Vries (FkdV) equation by using a method of higher moments of the lattice Boltzmann equation. For this model we developed the fractional Chapman-Enskog expansion, obtaining a series of lattice Boltzmann equations on different time scales, which recover exactly the macroscopic fractional KdV equation, taking into account the conservation law for t_0 , we obtained the equilibrium distribution function. The numerical examples show that the method can be used to simulate the fractional KdV equation.

7 - 8 – Non equilibrium Thermodynamics and Entropy Production in Dielectric Breakdown process for polymer materials

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In the present paper we applied the non equilibrium thermodynamic theory in the analysis of the dielectric breakdown process. From the thermodynamic viewpoint all phenomena in nature have a tendency to reduce their energy, is the case of the propagation of electrical tree structure. As the tree channel

front moves, the intense field near the front moves electrons and ions irreversibly in the region beyond the tree channel tips where electromechanical, thermal and chemical effects cause irreversible damage and from the non equilibrium thermodynamic viewpoint: entropy production. We choose the capacitive model (CDBM) to simulate the dielectric breakdown process. We select CDBM based on the special characteristics of the model: 1) Two different protocols are presented to select the capacitor that will be broken out of the set that meet breakdown conditions: 2) Protocol 1 is associated with the entropic contribution of the electrical tree growth process 3) Protocol 2 is identified with the corresponding internal energy contribution. 4) In the CDBM the dependence of the fractal dimension on the applied voltage has its thermodynamics origin in the interplay between energy injection and space charge formation process 5) The CDBM is also capable of qualitatively reproducing the temporal dependence of the breakdown process All of these combined give us an excellent framework for the entropy production evaluation in the tree growth process.

7 - 9 – Monte Carlo Studies of Critical and Dynamic Phenomena in Mixed Bond Ising Model

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The Hamiltonian of spin with mixed bond interactions [1] is used commonly to model several composed, such as $\text{Co}(\text{S}_p\text{Se}_{(1-p)})$ in the which atoms of Co interact amongst themselves through atoms either of S or Se [2], in that way, the interaction among the atoms of Co is modeled by two different exchange interaction. The mixed-bond Ising model also has been used to model composed that present modulated magnetic structures as the case of $\text{Fe}_p\text{Au}_{(1-p)}$, $\text{Eu}_p\text{Sr}_{(1-p)}\text{S}$ and $\text{Fe}_p\text{Al}_{(1-p)}$ [3]. In this work, we studied the thermodynamic properties and of our analysis we determined the critical exponents and we constructed the phase diagram for mixed-bond Ising model. The model was studied by means Monte Carlo simulation applied for cubic lattice by using Metropolis and Wolff algorithm with histogram technique and finite size scaling theory [4].

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[2] T.J. SATO, T.J. et al. *Phys. Rev. B.* 68 (2003) 214411.

[3] S. ABIKO; S. NIIDERA; F. MATSUBARA, *Phys. Rev. Lett.* 94 (2005) 227202.

[4] C. BERCHE, B.B. P CHATELAIN, W. JANKE, *Eur. Phys. J. B* 38 (2004) 463-474

7 - 10 – Modeling of high entropy alloys of refractory elements

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Reverting the traditional process of developing new alloys based on one or two single elements with minority additions, the study of high entropy alloys (HEA) (equimolar combinations of many elements) has become a relevant and interesting new field of research due to their tendency to form solid solutions with particular properties in the absence of intermetallic phases. To date, very few cases have been studied, but all show that the study of HEA is a promising and perhaps revolutionary area of growth in materials science. There are currently no theoretical or modeling studies of specific HEA which explain the formation, structure, and properties of these alloys, mostly due to the large number of constituents involved. In this work we focus on the HEA with refractory elements. While there is abundant experimental work concentrating on fcc-based HEA, there is only one experimental case that has been studied where all the constituents are refractory elements. To aid in the development of new compositions, as well as understanding the intricate details during the alloy formation process and the transition to what could be addressed as the high entropy regime, we show atomistic modeling results for W-Nb-Mo-Ta and W-Nb-Mo-Ta-V HEA for which experimental background exists. Such work indicates that these alloys exhibit unusual properties but the complexity of the system introduced unavoidable limitations in determining the role of each element, the transition to the high entropy regime characterized by the formation of extended solid solutions and, more importantly, limits the ability to identify the interactions and features responsible for such transition. We achieve this goal by means of atomistic modeling using the BFS method for alloys for the energetics. We show results for equimolar alloys of 4 and 5 elements (W, Nb, Ta, Mo, V), for which experimental results exist, and provide a straightforward algorithm for the determination of the features responsible for the characteristic HEA behavior.

7 - 11 – A potential for Th from inversion of cohesive energy: elastic constants

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An interatomic pair potential for fcc Th was derived by using the Chen-Mobius lattice inversion method. The cohesive energy vs lattice parameter relation required by this method was derived from first principles electronic structure calculations. Based on this potential the elastic constants of fcc Th were calculated by applying three different types of strain to the starting crystal. In order to improve the accuracy of the validity of the potential a Salter-Kirkwood type non-additive three body correction was implemented. The computed elastic constants are found to be in a very good agreement with experiments.

7 - 12 – Magnetocaloric effect observed by differential thermal analysis

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The magnetocaloric effect (MCE) is the isothermal change of magnetic entropy and the adiabatic temperature change induced in a magnetic material when an external magnetic field is applied.

In this work, we study this effect using the differential thermal analysis technique (DTA), which consists in measuring simultaneously the temperatures of the sample of interest and a reference one while an external magnetic field ramp is applied. We calculate the temperature difference (ΔT) from these values.

By using this method, we study the MCE in $\text{La}_{0.305}\text{Pr}_{0.32}\text{Ca}_{0.375}\text{MnO}_3$, which presents phase separation effects at low temperatures (< 200 K).

We obtain ΔT vs H and ΔT vs t curves, and analyze how the MCE varies by changing the external pressure and the rate of the magnetic field ramp. Our results show that the effect is amplified by working at lower pressures ($< 10^{-4}$ Torr) and at high velocity. However, at high vacuum a temperature gradient appears and makes it difficult to set the temperature properly. Also, self-heating of the sensor becomes relevant at this condition. Therefore, we decide to work at pressures of the order of 1 Torr. We also measured MCE at different temperatures, finding an inverse MCE, characterized by a $\Delta T < 0$ on increasing magnetic field, in the region between 140 K and 180 K.

Then, from DTA measurements of samples with different masses and a description of the thermal coupling of our system, we obtain the effective specific heat of the system. With this analysis, we are able to describe the influence of the environment and subtract it to calculate the adiabatic temperature change of the sample.

Finally, we propose a thermodynamic model which allows us to relate the DTA results with magnetization measurements.

7 - 13 – Microstructure and hard magnetic properties in bulk rods of Nd₆₀Fe₃₀Al₁₀ glass forming alloy

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The Nd₆₀Fe₃₀Al₁₀ alloy exhibits a large glass forming ability which allows to obtain relatively thick cast rods containing large volume fractions of amorphous phases. In this work the microstructure and the hard magnetic properties of as-cast rods are characterized. The alloy is processed by suction casting onto chilled copper mould to obtain cylinders 5 mm diameter and 50 mm length. This diameter is selected because it is an upper limit for this processing route, beyond which the hard properties largely deteriorate. A room temperature coercivity of 0,34 T is obtained. The sample microstructure is heterogeneous, with very different size scales near the surface and along the central zone. However, in both regions a large fraction of an amorphous ferromagnetic phase is observed; it is found that paramagnetic nanocrystalline phases - mainly Nd or Nd-rich particles, embedded in the amorphous matrix - are somewhat coarser in the central zone. These larger nanocrystals, less efficient to pin domain walls, are proposed to be responsible for the lower coercive fields observed, as compared with those found in cylinders 1-3 mm diameter where no inhomogeneities are found. This conclusion is supported by microstructure, calorimetric and magnetic domain observations.

7 - 14 – Simulation of magnetorheological fluids to a magnetic field

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A magnetorheological fluid (MR) is a liquid with a density greater than water, which passes an oily state to a quasi-solid to be exposed to a magnetic field. Currently, the use of MR fluids is extended to different industries, engineering, medicine, etc., Depending on the scope.

The mathematical program to use is a computer simulation technique that uses a numerical system called finite element method (FEM) or finite-difference numerical procedure to obtain approximate solutions for problems can be represented by a system of equations differentials, these programs lead to better products at lower costs, improve existing processes, to study the structural component failure or a computer, widely used in engineering and physics.

In this research, a mineral magnetite, which were determined by percentage of iron using two methods: physical test (magnetic separation) and chemical testing (chemical gear), the first we worked with two grain sizes (100 mesh and mesh 200), with a score of 78.26% and 86.63% respectively and magnetite in the second we worked with 200 mesh, resulting in an average of 94.1% magnetite, which were found very high content of magnetite. Then he prepared another part of the magnetite mesh sizes 400 and 500, which are derived magnetorheological fluid 8 which has a variation in the concentration (30:70 and 50:50), also working with two liquids different (SAE 20 and SAE 50) finding the best behaved fluid to the applied magnetic field in the final design team and determining the value of the variables that are at stake.

As a final result expected from a model and simulation of a magnetorheological fluid to a magnetic field.

7 - 15 – Point defect properties in the vicinity of an Al/U interface

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The static and dynamic properties of vacancies and interstitials have been studied in the neighborhood of an Al/ α -U interface using classical atomistic techniques. A suitable interatomic EAM potential for uranium and aluminum have been used for this purpose. First, a bicrystalline Al(fcc)/ α -U(A20) simulation block is built in such a way that the two compact planes and two directions are correspondingly parallel, i.e., (111)Al// $(001)\alpha$ U and $[110]$ Al// $[100]\alpha$ -U. Vacancies and interstitials are generated in the proximity of this planar defect to study properties and interaction with the interface as a function of distance. To characterize their properties far from the interface, the same defects have also been studied in bulk Al and α -U. We observed that the vacancy is stable in the first (001) U interfacial layer and unstable up to the second layer on each phase. Regarding interstitials, the final configurations depend both on the initial unrelaxed position chosen and on atomic species. They can take the form of mixed crowdions or simple interstitials. Point defects generated beyond around the third plane of each phase recover their corresponding bulk value. Taking into account the previous formation studies, only point defect jumps in the first layers of the interface are studied. We have applied the monomer method, a recently developed static calculation technique, to find point defect migration energy barriers in the same Al/ α -U interface structure. The advantage of this new calculation methodology over other more familiar techniques resides in which, given an initial equilibrium position of the jumping defect, no assumption is made upon the final equilibrium position. Results show that in both bulk and interface α -U the presence of an Al impurity decreases the vacancy jumping barrier. On the other hand, the interchange between a vacancy and a first neighbor U impurity in Al is not favorable with respect to other jumps. These results suggest a faster diffusion of Al in α -U than viceversa.

Bicentennial Symposium

8 - 1 – The Solid State Theory group in Bariloche

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I will do a brief chronicle about the evolution of the Solid State Theory group in Bariloche with special emphasis in its beginnings (1964-1980).

I will describe, from a very personal point of view, some of the research subjects at that time and the ambience we experienced as physicists.

Finally, I will also tell about the role of the group in the lectures at Instituto Balseiro and in the training of researchers in the area of Solid State Physics.

8 - 2 – Science and Physics in Argentina and Latin America in the Last Decades

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The bicentenary of the Argentinean first independent government is an excellent opportunity to meditate, to reflect once more, about the importance that education, science and technology have to consolidate what symbolically was the road initiated by Argentineans two hundred years ago. In this interdependent world, the capacity to formulate, in an autonomous way, social and economic policies depends very much in the articulation, in our Latin- American region, of a creative, intelligent and effective scientific and technological development. Condensed matter physics is a fascinating area from the scientific point of view. It is as well an area of physics closely related to the present more advanced productive activities. It has not only a cultural importance, it is fundamental because it is on the base of the third industrial revolution. This symposium, with the contribution of the personal experiences of the invited speakers, will be a place where to compare and shine light to the difficulties and successes that the process of scientific development, in particular condensed matter physics, have had in Argentina and other Latin-American countries. I will refer to this problematic in my talk.

8 - 3 – The National Synchrotron Light Laboratory, Brazil. Past, present and future

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The Brazilian Synchrotron Radiation Project started its development in 1981 at the Brazilian Center Physical Research (CBPF) in Rio de Janeiro. The subject was thoroughly discussed, from 1981 to 1986, involving most of the Brazilian scientific societies. During that period, the project was also presented at a meeting of the Argentinian Physical Society, in La Plata, and at the SLAFES held in Mar del Plata. When the project reached its maturity, in 1986, the Brazilian CNPq organized an open competition to decide on the location site of the future National Laboratory. Four proposals were submitted by institutions at Rio de Janeiro, Niteroi, Campinas and San Carlos. Campinas was selected and so, in January 1987, the National Synchrotron Light Laboratory (LNLS) started its activities.

Ten years were needed for the LNLS (1987-1996) to complete its basic infrastructure, to develop the technical design and to build a second-generation light source (UVX), consisting of an electron storage ring of 1.37 GeV and a linac injector of 120 MeV. In parallel, seven beam lines were designed and built, which started to be used in July 1997. The number of users of LNLS grew from 200 in 1997 to 2400 in 2009, with approximately 45

LNLS launched recently a project to develop a new third-generation light source (Sirius), comprising an electron storage ring of 3.0 GeV with permanent magnet dipoles, a booster and a linac. The optical quality of this new light source will be considerably higher than that of the current UVX storage ring, and comparable to, and in many ways better than, that of light sources recently constructed in first world countries.

Argentinian users met in November 2010 at INIFTA, La Plata, with representative members of LNLS, Argentinian Physical Society (AFA), Argentinian Crystallography Association (AAC) and Ministry of Science of Argentina (MinCyT) to discuss preliminary issues concerning the possibility of constructing one or two argentinian beam lines to be installed at LNLS, in the new facility, Sirius. This initiative is particularly interesting, since it would allow for greater participation of Argentina's user community and would include some share of responsibility for the operation of LNLS. If this project were approved, the argentinian beam lines would be defined and built in parallel with the construction of the future Sirius light source.

Finally I will briefly describe several experimental investigations developed at the LNLS, some of them in collaboration with research groups in Argentina.

8 - 4 – Low Temperature Laboratory and Superconductivity in Bariloche

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In 1958 a relevant outcome took place in Bariloche. Jose A. Balseiro opened the academic ceremony introducing new 13 "licenciados" in Physics of the first promotion of the today Instituto Balseiro with an unforgettable commencement address. This was a qualitative as well as quantitative breakthrough in Argentina as a result of the distinctive project initiated three years before. It was time to consolidate the endeavor: Some of the new licenciados should be sent abroad to complete their training as researchers, some should stay to help teaching new students and, more important, new research facilities had to be created looking for excellence to consolidate the research center. My life experience in physics started that year as a student in Bariloche and ended a couple of years ago when I retired as a professor and researcher in the same center. I will try to describe the challenge of assembling the Low Temperature Laboratory and later on the how the laboratory addressed the research on High Temperature Superconductors.

8 - 5 – Science and political Institutions: development of Physics in Argentina, 1940-2000

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The foundation of the Argentine Physical Association (AFA in spanish) in 1944, helped the small group of local physicists to launch different projects aiming at consolidating physics research activities and teaching in the country. Since then, most of the Argentine senior physicists - Enrique Gaviola, Teófilo Isnardi José Balseiro, Juan José Giambiagi, Jorge Sabato, among others- had leading roles within the scientific system and contributed not only to set the basis of the new research institutions and scientific careers but also to give a social and economical content to physics research in Argentina and Latin America.

The aim of this talk is to go through some landmarks of the argentinean research institutions, focusing on conflicts, tensions, and discussions which took place among physicists, military , and politicians, and besides making a balance out of the historical path followed by Physics in Argentina.

8 - 6 – Half a century of condensed matter physics in Latin America: a personal perspective

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Condensed matter (or solid state) physics in Latin America has seen an impressive development during the last half century. From a relatively small and inexperienced community we have grown into a mature one which contributes, at a very competitive level, to the development of the field worldwide. For our region these have been difficult years, from the economic, social and political perspective. Nevertheless, the progress of condensed matter physics has been much larger than the wildest expectations we had five decades ago. Acceptedly, it shows a degree of development that varies strongly from one country of the region to another, but the average is more than satisfactory. I will review general trends and focus on some particular events, specially those in which for better or worse I participated in, and that have also marked me as a person and scientist.

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8 - 7 – The Development of the Study of Magnetism in Brazil

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As in most Latin American countries, scientific research had a late start in Brazil. The studies of Condensed Matter were initiated at the National Institute of Technology in Rio de Janeiro in the 1930s, through the initiative of a German physicist, Bernard Gross. In the 1960s, the first studies of Magnetism were made, in Rio, Porto Alegre and São Paulo. Initially, most of the studies used hyperfine interactions; among the pioneers were Jacques Danon in Rio and John D. Rogers at Porto Alegre. The development of the area of Magnetism was stimulated by Schools organized every other year, beginning in 1998. Other milestones were the organization in Recife of the International Conference on Magnetism (ICM) in 2000 and the inauguration of the synchrotron light source (LNLS) at Campinas in 1997.

8 - 8 – The troubled beginnings of solid state physics in Buenos Aires

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Memories and anecdotes of 50 years work. A personal and of course, incomplete point of view telling how this field, at that time new, followed the political scenario of Argentina.

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