1 – Kondo Resonance in Magnetic Molecule Spintronics

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It has been shown that magnetic molecules adsorbed on metallic surfaces can be a very effective implementation of quantum gates. Within this perspective, we discuss the role played by many body effects in these magnetic molecules to study spin dependent phenomena. We show that the physics associated to the Kondo regime is fundamental to understand the transport properties of these systems and that this regime can be a very effective scenario to read the system spin configuration with important implications for quantum information.

2 – Graphene viewed through STM and transport experiments

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Graphene, a one-atom thick form of crystalline-carbon possesses extraordinary electronic properties making it a prime-candidate for novel nano-electronic devices, at the same time raising the prospect to observe phenomena hitherto unseen in condensed-matter physics such as Klein tunneling. These unusual properties, arising from a unique type of charge-carriers that behave like massless Dirac fermions, are most prominent near the Dirac point where their density vanishes. I will present STM and transport experiments on graphene samples decoupled from the supporting substrate which demonstrate the existence of the Dirac point and the Dirac fermions. In the presence of a magnetic field a sequence of discrete Landau energy levels carrying the distinctive signatures of long lived massless Dirac-fermions is observed. The Dirac-fermions are slowed down by electron-phonon interactions and acquire a small mass, seen as a gap in the tunneling spectrum.

3 – Localized spins in graphene

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Graphene is a two dimensional material with a low energy electronic structure corresponding to massless, chiral, fermionic quasiparticles described by the Dirac equation. It is a semimetal that can be globally or locally doped with electrons or holes using gate electrodes. The peculiar electronic properties of this system lead to a number of new and interesting effects. We study the problem of magnetic impurities, atomic or molecular, adsorbed on clean graphene [1]. Using the numerical renormalization group we calculate the spectral, thermodynamic, and scattering properties of the impurities and discuss their potential use to inject and generate spin polarized currents. We show that with a small magnetic field the scattering due to impurities becomes strongly spin dependent and predict new magnetotranspot effects.

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4 – Multifunctional oxides for spintronics

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The wealth of physical phenomena exhibited by transition metal oxides constitutes an exciting playground for solid state scientists and a world of opportunities for novel devices. Their range of functionalities spans from superconductivity to ferromagnetism in the bulk and can be further broadened by considering their interfaces [1]. There, novel electronic phases may appear such as the metallic state found at the interface between a Mott insulator and a band insulator [2].

In this talk, I will try to illustrate how multifunctional oxides can bring novel degrees of freedom to spintronics [3]. After reviewing briefly the potential of halfmetallic oxides for spin based studies and devices, I will present results on the use of ferroic (ferromagnetic, ferroelectric) and multiferroic oxides as tunnel barriers and magnetic pinning layers in spintronics heterostructures. Notable results include the realization of four resistance state memory elements through the combination of tunnel electroresistance and magnetoresistance [4], and the ferroelectric control of exchange bias [5,6].

I will also discuss recent progress on the physics of the metallic electron gas that appears in epitaxial heterostructures combining two band insulators, namely $LaAlO_3$ and $SrTiO_3$ [7]. Finally I will propose some directions to add ferroic degrees of freedom to such low dimensional interface phases.

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5 – Unique spin-spiral structures in low dimensional magnets

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Magnetic nanostructures are often complex, multicomposite materials with low symmetry, non-collinearity and strong spin-orbit coupling effects. In the last years we could establish first-principles methods to describe accurately the underlying magnetic interactions, i.e. the symmetric and antisymmetric exchange, the magnetocrystalline anisotropy and their dependence on dimensionality and structure in realistic materials. This talk will focus on low-dimensional magnetic systems and the importance of relativistic effects for the magnetic properties: due to the lack of inversion symmetry at the surface, the Dzyaloshinskii-Moriya interaction can induce non-collinear spin structures of a particular rotational sense in ultrathin magnetic films. This behavior will be discussed in three different examples, domain walls in two monolayers Fe on W(110) [1], an antiferromagnetic monolayer Mn of W(110) [2], and the ferromagnetic Mn on W(100) [3]. A related phenomenon, the Rashba-effect on magnetic surfaces, will be demonstrated on Lanthanide surfaces [4,5].

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6 – From Spin Ice to Kagome Ice in $Dy_2Ti_2O_7$

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Water is special in that it exists at usual temperatures and pressures in the three basic states. Maybe due to this, together with its ubiquity and importance, the first notions of the concept of phases and changes of state are usually given using water as an example. Very recently, the analogy between the phases of water and the many other forms of order existing in nature has been focused on the lower temperature range of the phase diagram, in what has now been called *SpinIce*.

SpinIces are crystalline solids ($Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$) whose magnetic degrees of freedom below $\sim$1K can be mapped into those describing the proton (dis)order in normal ice. The frustration present leads to a degeneracy of the fundamental state similar to that predicted by Pauling in 1935 to account for the residual entropy in water ice. Aside from being a realisation of a "magnetic ice", the magnetic properties of Spin Ice compounds, conferred by their special structure and composition, makes these systems a unique arena to study the possible consequences of competing interactions.

One important difference with water is that in the magnetic case it is relatively easy to perturb and measure the relevant properties. A magnetic field of the order of 1T is enough to completely raise the degeneracy of the fundamental state. A smaller field along the (111) crystalline direction can order one fourth of the spins in the lattice. The disorder of the remaining magnetic moments, arranged in a set of parallel Kagome planes perpendicular to the field, still holds a macroscopic entropy at T = 0K. This constitutes the so called *KagomeIce*.

In this talk we will firstly discuss more deeply some general equilibrium aspects of these systems. We will then see very recent experiments showing peculiarities on the actual magnetisation process below 600 mK, when the system is driven by an external magnetic field from the Spin Ice state into the Kagome Ice.

7 – Static and dynamic properties of FCC FePt ferromagnetic films

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We have studied the static and dynamic properties of FePt thin films as a function of film thickness in the range 10 nm $\leq t \leq$ 100 nm. These films, that are ferromagnetic at room temperature, have been deposited by magnetron sputtering on oxidized Si (100) substrates. As deposited films are polycrystalline and grow in a disordered FCC phase with a moderate texture along the [111] direction.

All magnetic properties are considerably different for thinner ($t \leq$ 30 nm) than for thicker ($t \geq$ 60 nm) films. In the thinner films the in-plane magnetic hysteresis loops are almost square with a large remanent magnetization and a relatively small coercivity. Thicker films, on the contrary, reverse magnetization in a two step process and have larger coercivities. Isothermal remanent magnetization, DC demagnetization and magnetic viscosity measurements also show a different behavior in the two thickness ranges. Magnetic force microscopy revealed that thicker films have a stripe-like domain structure with a period of 200 nm. This domain structure is not observed in the thinner samples.

The dynamic response of the films was studied by ferromagnetic resonance measurements at 9.5 GHz (X-band) and 34 GHz (Q-band). In the thinner films we have observed a single resonance line which is related to the uniform precession of the magnetization vector. Thicker films show an additional resonance line when the magnetic field is applied close to the film normal.

All the above results are consistent with the presence of a perpendicular anisotropy field that favors a small out of plane component of the magnetization. In the case of thicker films it is energetically favorable to form domains with a perpendicular magnetization component of varying sign.

8 – Pressure induced superconductor quantum critical point in multi-band systems

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In multi-band superconductors where quasi-particles arising from different orbitals coexist at a common Fermi surface, external parameters which affect the mismatch of the Fermi wave vectors associated with these distinct quasi-particles can destroy superconductivity even at zero temperature. This problem has a wide interest in physics ranging from cold atom systems to color superconductivity in neutron stars. In condensed matter this is relevant for inter-metallic systems and heavy fermions where external pressure can reduce the critical temperature and eventually drive these systems to the normal state. In many cases this transition is continuous and is associated with a superconductor quantum critical point (SQCP). In this work we study a two-band superconductor in the presence of hybridization V. This one-body mixing term is due to the overlap of the different wave-functions and directly determines the mismatch of the bands. Since it can be tuned by external pressure, it turns out as an important control parameter to study the phase diagram and the nature of the phase transitions. We use a BCS approximation and include both inter and intra-band attractive interactions. For negligible inter-band interactions, as hybridization (pressure) increases we find a SQCP separating a superconductor from a normal state at a critical value of the hybridization Vc. We show that in the case inter-bands interactions are dominant the transition to the normal state is discontinuous. We obtain the behavior of the electronic specific heat close to the SQCP and the shape of the critical line as V approaches Vc.

9 – Unforeseen properties of MnAs epilayers grown on GaAs semiconductor

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MnAs epilayers grown on GaAs substrates offer spin-polarized source for spin injection in GaAs-based spintronics devices [1]. Moreover MnAs films grown on GaAs(001) display, at room temperature, a self-organized pattern of submicron-wide stripes, alternating the ferromagnetic hexagonal α-MnAs phase with the paramagnetic orthorhombic β-MnAs phase [2]. The stripes are aligned parallel to the c axis of the α-MnAs phase, whose easy magnetization direction is perpendicular to the stripes. The film thickness controls both the period and the height of the stripes. For a given thickness, i.e., for a given period, the sample temperature T determines the relative width of α and β stripes. With its regular pattern of submicron wide stripes with a nanometric corrugation, MnAs/GaAs(001) can be considered also as a self-organized template for the growth of nanometer-thick magnetic layers, whose magnetic properties can be controlled by changing the temperature. In this talk, I will introduce the intriguing use of this template to modify the magnetic behaviour of iron epilayers deposited on it [3-5]. I will also present our findings on giant magnetocaloric effect (MCE) displayed by MnAs epilayers. This effect is also associated with the magneto-structural α-MnAs / β-MnAs first-order phase transition. We have successfully demonstrated the possibility to control the MCE behaviour by selecting the epitaxial relation between MnAs and GaAs substrate [6].

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10 – Nanotribology and hard hydrophobic coatings

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Water, not necessarily in ice form, is a good lubricant in everyday life, making it "slippery when wet". It also acts as a lubricant in numerous industrial and biological settings, where it keeps sliding surfaces apart from each other and allows easy shearing. However, it is not necessarily true at nanometer scale. In this work we will review some basic aspects of the effects of the humidity and their relations with the friction and wear at nanometer scale. We will also present some results on the tribology of hard hydrophobic coatings (diamondlike carbon and carbon-fluorine films) together with some potential applications for these materials.

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11 – Half-metallic ferromagnetic transition metal oxides: Correlated electronic structure of bulk CrO_2 from hard X-ray photoemission

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CrO_2 has theoretically been predicted to be a half-metallic ferromagnet [1], i.e. a metal for one spin component and an insulator for the other one. The motivation for the recent very intense experimental investigations of this material has been its potential use as spin injector in spintronics for, e.g., tunnel magnetoresistance [2] and spin-momentum transfer torque switching of magnetizations [3]. The original experimental test of the electronic structure by spin- and angle-resolved photoelectron spectroscopy (SPAR-PES) [4] using a photon energy of $h\nu = 21.2$ eV (i.e. small photoelectron escape depth) yielded a spin polarization of 90%, but not a well pronounced Fermi edge. It was conjectured whether the material is closer to a Mott insulator rather than a metal obeying a $\rho \sim T^2$ law [5]. Hence, there is an ultimate need about getting experimental information of the bulk electronic structure of CrO_2 , like for many other oxide materials [6].

We present the first comprehensive investigation of electronic core states and valence band states of CrO_2 by means of hard X-ray photoelectron spectroscopy (HAX-PES) using photon energies of $h\nu \sim 8$ keV [7]. The use of HAXPES with a relatively large photoelectron escape depth yields a first real bulk-sensitive investigation of the electronic structure of CrO_2. However, while we observe a pronounced metal-type Fermi edge for $h\nu = 700$ eV, it is almost absent in HAX-PES. This fact is attributed to a recoil effect of the photoelectrons, shifting spectral weight from near EF to below it. In addition, a well screened feature is found in the Cr $2p_{3/2}$ core level, consistent with the metallicity of CrO_2. The lower and upper Hubbard band could be identified by HAX-PES and inverse PES, respectively, resulting in an experimental value of Hubbard $U \sim 3.5$ eV, which is in good agreement with $U = 3.0$ eV in LSDA + U calculations [8]. In HAX-PES the intensity near EF is rather small, but finite and temperature independent. This excludes an enhanced density of states at EF as conjectured in the framework of an orbital Kondo effect using LDA + DMFT calculations [9].

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12 – How to reveal atomic-scale magnetic order with scanning probe microscopes

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In recent years, spin-polarized scanning tunneling microscopy (SP-STM) has been established as a technique to resolve magnetic nanostructures down to the atomic scale [1-4]. Very recently, it has even become possible to measure the exchange interactions between tip and sample by magnetic exchange force microscopy (MExFM) [5,6]. However, the interpretation of such measurements is non-trivial, especially on the atomic scale. For SP-STM there are various contributions to the tunneling current from structural, electronic, chemical, and magnetic sample properties. For MExFM there are many basic open questions concerning e.g. the influence of tip material, structure, and sample systems on the size, sign, and distance dependence of exchange forces. Successful interpretation approaches for both techniques rely on an accurate description of the electronic structure of tip and sample and their interaction making density functional theory (DFT) an indispensable tool.

Here, I will present the theory of SP-STM and explain how one can reveal collinear and non-collinear magnetic order on the atomic scale [1-4]. This allows us to verify theoretical predictions based on DFT such as two-dimensional antiferromagnetism [1] or spin-spiral structures driven by the Dzyaloshinskii-Moriya interaction [3,4]. Surprisingly, it is even possible to image non-collinear atomic-scale magnetic order using a non-magnetic tip as the electronic structure changes slightly from atom to atom due to spin-orbit coupling. Finally, I will show how the antiferromagnetic order of Fe on W(001) can be resolved by MExFM and discuss how the structure and chemical composition of the tip influence the measured forces [6,7].

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13 – STM Atom/Molecule Manipulation: Realizing Single Molecule Switches and Devices

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Scanning tunneling microscope (STM) manipulation of single atoms and molecules on surfaces have enabled construction of novel quantum structures on an atom-by-atom basis and demonstration of single molecule devices on a one molecule at-a-time basis. STM is not only an instrument used to '*see*' individual atoms by means of imaging, but also a tool used to '*touch*' and '*take*' atoms/molecules or to '*hear*' their vibration by manipulations. Therefore, STM can be considered as the '*eyes*', '*hands*' and '*ears*' of the scientists connecting our macroscopic world to the exciting atomic and nanoscopic world. In our research projects, we combine STM manipulation schemes with a variety of tunneling spectroscopy measurements to investigate properties specific to the type of atoms/molecules. These innovative experiments are tailored to address several critical issues covering both fundamental understanding of atom manipulation mechanisms, and realization of monomolecular switches and devices. In this talk, our recent results of single atom/molecule manipulations using a low-temperature STM will be presented.

The atomic scale interaction is a fundamental subject of materials. Just by approaching the STM tip over a silver cluster on a Ag(111) surface, the binding of the top cluster atom is greatly reduced due to the perturbation of the tip. By tuning tip-cluster interactions, individual atoms from the silver cluster could be repeatedly and reproducibly extracted on an atom-by-atom basis [3]. This process involves extraction of individual atoms and a subsequent manipulation of atoms on the rough terrain of a 3-D cluster surface. One of the visions of nanotechnology is the development of nanoscale electronic and mechanical devices using individual molecules or molecular components [1,2]. A monomolecular switch can be operated by changing either the conformation or electronic state of a molecule between two or more levels. By injecting tunneling electrons into a molecule, rotation or conformation changes can be performed with a single bond precision. Three types of single molecule switches; a Kondo switch and manipulation of Kondo resonance [4], a multi-step chlorophylla switch [5], and a molecular charge transfer switch will be presented.

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14 – Resistance switching: what lurks at the root?

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Charge-storage memories as represented by the flash memory [1] are dominating commercial markets of storage media. However, there is an emergent anxiety that they face a miniaturisation limit (currently estimated 20 nm) in a few years. The so-called resistance-change memory is considered to be an emerging candidate of scalable replacement for flash; three types of the resistance-change memories are now under development [2]. Those are the phase-change memory (PCM), the programmable metallisation cell (PMC), and the resistive random-access memory (RRAM). The third one uses "electroformed"[3] metal/oxide/metal sandwiches, which are reviewed in this talk from a viewpoint of understanding the mechanism of the weird resistance change phenomenon.

Recent intensive and worldwide researches of RRAM have clarified that the current flows inhomogeneously through the oxide in the low-resistance state, even when it does rather homogeneously in the high-resistance state. This indicates that there appears a current constriction structure, most probably at the interface. Thanks to the constriction, the current density becomes extremely large especially when the resistance state changes from low to high. This current constriction structure is the most essential matter of the resistance change phenomenon, and we call it a "faucet" [4, 5].

In several combinations of the oxide and metal electrode, the averaged free enthalpy of oxygen segregation is close to the free reaction enthalpy of oxide precipitation from the metal [6]. Then, the large current density can easily drive local chemical reactions such as electro-oxidation and electro-reduction, and the reactions can be drastically accelerated by a local Joule heating due to the current concentration. In addition, a possible direct effect of the oxygen and/or cation electromigration [7] may play an important role. It has been actually demonstrated that the current density of 10^7 A/cm^2 induces intriguing local oxidation on thin titanium strip [8]. I would like to review and discuss the essential faucet structure, as well as the possibility of those local chemical reactions at the non-equilibrium interface between the metal electrode and the oxide matrix, suggesting what is necessary to realise the resistance-change memory.

Financial supports are provided by New Energy and Industrial Technology Development Organization (NEDO), and Grant-in-Aid for Scientific Research from MEXT, Japan.

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15 – High magnetic field frontiers in Superconductors, Heavy Fermions, Multiferroics, and Quantum Magnets reveal exotic states of matter.

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Advances in the production of high magnetic fields with clean electromagnetic environments, and substantial progress in the electronics and experimental techniques, have now made entirely new frontiers of condensed matter (T,H) phase diagrams available and amenable to direct observation in the laboratory. Research efforts at the National High Magnetic Field Laboratory in the area of high temperature superconductors have uncovered intriguing details of their Fermi surface that suggest a condensate that lives on a corrugated magnetic landscape. The very existence of a Fermi surface in these unusual materials, questioned by some until recently, is now well established and its details scrutinized to shed new light on the superconducting pairing mechanism. Heavy fermion systems $Ce_3Pt_4In_3$, URu_2Si_2, $CeIn_3$, and $YbInCu_4$, lent themselves to the first specific heat experiments in fields up to 60 Tesla (a million times Earth´s field on the surface), giving us access to metal-insulator transitions, quantum critical points, Fermi surface reconstruction and metamagnetism, phenomena that can be fine tuned with a magnetic field knob. These results have put an enormous pressure in the theorists to properly model strongly correlated electrons, a phenomenally complex task still in early stages of development. Low dimensional and frustrated quantum magnets as well as multiferroics brought back a sense of relief and sanity to the community, since in these systems calculated phase boundary critical exponents, dimensional reduction, magnetization plateaus and spin lattice correlations can be contrasted directly with experiment. Time permitting, I will discuss some remarkable examples of the most exiting condensed matter phenomena observed by my team and close collaborators at high magnetic fields.

16 – 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 complementary effect where the contact resistance of electrodes at opposite ends -a non volatile memory device- exhibit variations of opposite sign, These reversible variations are further studied using different electric protocols, to show differences at each electrode. We discuss the mechanism driving the effect both on LaPrCaMnO and TiO samples contacted with Ag electrodes.

17 – Non-local transport and entangled Andreev pairs in hybrid superconducting nanostructures

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Nanoscale superconductors connected to normal metallic electrodes provide a potential source of entangled electron pairs. Such states would arise from the splitting of Cooper pairs in the superconductor into two electrons with opposite spins, which then tunnel into different leads, by means of a process known as crossed Andreev reflection (CAR). In an actual system, the detection of these entangled pairs is hindered by the elastic co-tunneling (EC) of individual electrons between the leads, which yields an opposite contribution to the non-local conductance. The simplest theory in fact predicts a complete cancellation between these contributions for a BCS superconductor weakly coupled to non-magnetic leads. In this talk I would present some recent theoretical work which demonstrates that the balance between CAR and EC processes can be broken in several situations:

• When the superconductor is coupled to normal electrodes by small capacitance tunnel junctions and electron interactions have an important influence [1].

• In the case of high-Tc superconductors, where the d-wave character of the order parameter can lead to long-range CAR processes along certain crystal orientations [2]

• At the interface between a BCS superconductor and graphene, where specular Andreev reflections can take place [3]. These findings may help to clarify some intriguing experimental results and provide future strategies for the detection of entangled pairs in solid-state devices.

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[3] P. Burset, W. Herrera and A. Levy Yeyati, in preparation.

18 – Proximity effect between superconductors and ferromagnets: from thin films to nanostructures

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Recently, a new set of experiments has revived interest in the proximity effect. One of the major break-through was the prediction and experimental verification of -junctions comprised of superconductor/ferromagnet (S/F) sandwiches [1]. Superconductors can be employed to probe the ferromagnetism of metals by virtue Andreev reflection. Using nanocontacts defined by e-beam lithography, the spin-polarization P of the current across the S/F interface can be determined reliably [2]. We recently observed a systematic decrease of P with increasing contact size, which is attributed to spin-orbit scattering [3]. Particularly intriguing is the non-local Andreev reflection, i.e. an incident electron from a ferromagnetic nanocontact is retroreflected as a hole in an adjacent contact forming a spatially separated but entangled Einstein-Podolski-Rosen pair [4]. Finally, the proximity-induced superconductivity can be probed by magnetization measurements. We report on the fate of normal metal (Ag) squeezed between a superconductor and a ferromagnet [5].

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19 – A Novel Approach to Study Highly Correlated Nanostructures: The Logarithmic Discretization Embedded Cluster Approximation (LDECA).

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This talk will present a new approach to study transport properties of highly correlated local structures. The method, dubbed the Logarithmic Discretization Embedded Cluster Approximation (LDECA) [1], consists of diagonalizing a finite cluster containing the many body terms of the Hamiltonian and embedding it into the rest of the system, combined with Wilson's idea of a logarithmic discretization of the representation of the Hamiltonian. The physics associated with both one embedded dot and a double dot side coupled to leads is discussed in detail. In the former case, the results perfectly agree with Bethe ansatz data, while in the latter, the physics obtained is framed in the conceptual background of a two-stage Kondo problem. In addition, a many body formalism provides a solid theoretical foundation to the method. Results for other systems will also be presented and a new version of the method, where the Lanczos exact diagonalization step is replaced by a Density Matrix Renormalization Group (DMRG) procedure will be introduced.

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20 – Magnetoelectric effects in oxide heterostructures and multilayer capacitors

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Magnetoelectric effects in condensed-matter systems permit the interconversion of magnetic and electrical signals. I will report strain-mediated electrically driven magnetic switching in an eptiaxial manganite film of $La_{0.67}Sr_{0.33}MnO_3$ on a ferroelectric-ferroelastic substrate of $BaTiO_3$ [1]. The large magnetoelectric effects are attributed to the use of an interface that is both planar and epitaxial. I will also report that magnetoelectric effects may be observed in multilayer capacitors [2]. These are standard cheap electronic components based on $BaTiO_3$ in which the interdigitating electrodes are now based on Ni rather than Ag-Pd to cut cost. Strain-mediated magnetoelectric effects arise after poling due to magnetostriction in the Ni and piezoelectricity in the $BaTiO_3$.

[1] Giant sharp and persistent converse magnetoelectric effects in multiferroic epitaxial heterostructures, W Eerenstein, M Wiora, JL Prieto, JF Scott and ND Mathur, Nature Materials **6** (2007) 348

[2] A one-cent room-temperature magnetoelectric sensor, C Israel, ND Mathur and JF Scott, Nature Materials **7** (2008) 93

21 − Electric transport and Raman Spectroscopy Measurements in Graphene Devices

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One of the most important recent developments in the physics of low dimensional systems was the demonstration that high quality, few layer graphene flakes could be produced, either by micromechanical exfoliation of graphite or by surface graphitization of SiC. This novel two dimensional system presents high room temperature mobilities and a set of interesting electric transport phenomena such as anomalous integer quantum hall effect observed even at room temperature and non vanishing conductivity when the density of charge carriers approaches zero. For instance, in single layer graphene, the electric transport can be described by considering that the carriers behave as two dimensional massless Fermions. For monolayer graphene this is a consequence of the peculiar linear dispersion relation in the vicinity of the K and K' points of the band structure, where the minima of the conduction band and the maxima of the valence band occur. In bilayer graphene the conduction and valence band are parabolic near the K and K' and a tunable band gap can be generated by the application of an electric field between the layer. One of the major challenges to explore the physics of graphene is the reliable fabrication of multiterminal devices with well defined geometries. The flakes obtained by micromechanical exfoliation are difficult to observe by optical microscopy, have irregular and unpredictable shapes and are randomly distributed over the oxidized Silicon substrate. In order to make devices first the flakes must be found and their position indexed with respect to alignment marks and then a well defined geometry is defined usually by a combination of e-beam lithography and reactive plasma etching. In this talk we will address fabrication methods of graphene devices using laser beam lithography where monolayer and bilayer graphene flakes can be observed and their position precisely found using a builtin infrared illumination, with the photoresist already on top of the substrate. We will address our recent results on the use of Raman spectroscopy to study the phonons and electronic structure of graphene, make an overview of our ongoing work in electric transport in graphene devices fabricated at UFMG and also of the future propects and developments that we expect to achieve.

22 − Ab initio simulations at the surface of halfmetallic manganites

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A good understanding of the surface physical properties in colossal magnetoresistant hole doped manganese oxides is highly desirable for future spintronic applications of these promising materials. In this talk we will revisit the relevant electronic properties of the (001) surface, discuss the presence of a ferrodistortive instability and its effect on the magnetic properties of the surface. The role of oxygen vacancies and strain in thin films manganites will also be addressed.

23 – Myths and truths about magnetism in semiconductor oxides

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Dilute magnetic semiconductor oxides (ODMS) are envisioned as sources of spin polarized carriers for future semiconductor devices which would simultaneously utilize the spin and charge of the carriers. Among the most studied oxides are ZnO, TiO_2 and SnO_2 systems, pure and doped (with several transition metals), prepared in the form of powders and films, the latter being grown by different deposition techniques. A great deal of theoretical work has been also devoted to this topic. Claims of room temperature ferromagnetism, or of the absence of it, have been made by both experimentalists and theorists. Here, a review of the more recent results on the subject will be presented and discussed, along with the report on some sources of extrinsic ferromagnetism which have been identified in film samples. Our own results in ODMS powders and films where a main paramagnetic behaviour was observed, it will be presented.

24 – Physics of graphene nanoribbons

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Graphene, the single layer form of crystalline carbon, has been the focus of tremendous scientific activity since its isolation in 2004. Besides its remarkable properties of good conductivity and structural flexibility, the low-temperature/energy properties can be obtained by modeling the material with Dirac-type Hamiltonians, opening the possibility of studying QED phenomena in a condensed matter system. Numerical models based on tight-binding calculations for semi-infinite geometries revealed the relevance of edge termination on graphene properties: armchair edges produce either metallic or insulating ribbons while zigzag only produce metallic ones. Furthermore, zigzag ribbons are expected to exhibit a new insulating phase of matter, the Quantum Spin Hall (QSH) phase, when intrinsic-spin orbit (I-SO) interactions are considered[2]. The QSH phase is characterized by the presence of chiral edge states, with electron momentum coupled to its spin. Although much theoretical work has been carried out on graphene, questions on the role of enhanced Coulomb interactions resulting from confined geometries remain opened. The aim of this talk is to provide insight into these issues by studying tight-binding and Dirac-type model Hamiltonians that include the I-SO and unscreened Coulomb interactions for ribbons with both edge terminations. Our results indicate that metallic armchair ribbons, with no Coulomb interaction, retain their conducting properties in the presence of the I-SO interaction regardless the strength of the coupling. In the presence of an unscreened Coulomb interaction, the small-momentum electron-electron scattering opens a width (W)-dependent charge gap in the spectrum of half-filled (neutral) ribbons that vanishes in the limit of infinite width as 1/W, in agreement with recent experimental observations. The gap survives in the presence of realistic I-SO interactions. Calculated correlation functions, reveal an incipient magnetic order along the edges analogous to the one predicted in the QSH phase for zigzag ribbons. In zigzag ribbons, the character of localized edge wavefunctions for non-interacting electrons changes from a strong localization to a damped oscillatory behavior as the I-SO coupling is changed. Unscreened Coulomb interactions open a charge gap and destroy the chiral property of the edge states, thus rendering the QSH phase instable. A numerical analysis of the width-dependent gap suggests an exponential vanishing with W in contrast with results for armchair ribbons.

25 – Nanophases in Thin Manganites Films: Electronic soft matter?

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The formation and the length scales of electronic nanophases in thin films of manganites are given. In addition we present data for electric field induced resistance changes observed at grain boundaries in thin film bridges. The results are discussed in the context of possible electronic soft matter behaviour.

26 – Nonvolatile resistive switching at perovskite oxide interfaces

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Recently, reversible resistive switching between two or multilevel resistance states has been found in capacitor like devices composed of a wide variety of insulating or semiconducting transition metal oxides [1]. The resistive switching attracts considerable attention due to the potential for device application such as resistance random access memory (ReRAM). The resistive switching behavior reported so far seems to differ depending on the materials consisting of the devices. Therefore, one can expect that the driving mechanism involved in the resistive switching depends on the materials. Some possible mechanisms have been proposed through detailed experimental and theoretical studies, and the proposed mechanisms can be classified into two types: filament or interface types [1].

In this talk, we focus on interface type resistive switching and describe recent advances in our understanding of the mechanism obtained from the study of devices composed of p-type and n-type semiconducting oxides such as $Pr_{0.7}Ca_{0.3}MnO_3$ (PCMO) [2,3] and Nb-doped $SrTiO_3$ (Nb:STO) [4,5], respectively. We demonstrated that the resistive switching takes place at the Schottky like interface between metal electrode and perovskite oxides, and that the density of oxygen vacancies plays an important role in the bistability in the resistance. A possible mechanism is electrochemical migration of oxygen vacancies in the vicinity of the interface.

This is a collaboration work with T. Fujii, M, Kawasaki, and Y. Tokura. This work was supported in part by Industrial Technology Research Grant Program in 2005 from New Energy and Industrial Technology Development Organization (NEDO) of Japan.

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27 − Charge, spin, orbital and lattice degrees of freedom in manganites

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The rich phase diagram of $La_{1-x}Ca_xMnO_3$ (LCMO) exhibiting several magnetic phases, orbital order, spin canting, charge order, Jahn-Teller distortions and phase separation is the consequence of the interplay of charge, spin, orbital and lattice degrees of freedom.

The manganese ions are in a mixed valent state of two magnetic configurations, Mn^{4+} and Mn^{3+}. Each Mn ion has three localized $3d$ electrons in t_{2g} orbitals with their spins ferromagnetically coupled to form a spin $S = 3/2$. The Mn^{3+} ions have an additional $3d$-e_g electron to form a total spin ($S = 1/2$) via Hund's rule coupling. The e_g electrons hop between Mn sites with amplitude t with a multiple occupancy of the e_g levels being excluded at each site by a large Coulomb energy. The hopping of the e_g electrons gives rise to the ferromagnetic *double-exchange*, which competes with the antiferromagnetic *superexchange* J between the t_{2g} spins of the ions. The two e_g-orbitals also couple to the lattice degrees of freedom via the *Jahn-Teller* effect.

Using a mean-field slave-boson formulation we calculate the ground state energy of the system for classical spins S oriented in the magnetic configurations of the A, B, C and G phases as a function of x and one model parameter, J/t. The experimental sequence of crossovers between ground states for LCMO was reproduced as a function of x for $J/t \approx 0.02$ [1].

Only the A, C and CE phases exhibit a Jahn-Teller distortion [2], leading to a contraction (expansion) of the c-axis for the A phase (C phase) and to long range orbital order. The effects of canting of the spins on the stability of the A and B phases and on phase separation is discussed. The model has been extended to electron-doping [3].

Preliminary results for the checkerboard charge and the orbital order of the CE-phase will be presented. There are 32 e_g bands (16 Mn ions in the unit cell) in the Brillouin zone of the CE phase which are grouped into two sets of 16 bands separated by a charge order gap. The charge gap does not directly affect the properties of the compound. If long-range orbital order is included an additional gap opens at the Fermi level. The support by the Department of Energy under grant DE-FG02-98ER45707 is acknowledged.

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28 − Application of scanning probe microscopy for the development and study of nanostructures

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Scanning probe microscopy (SPM) has become a useful tool for a wide spectrum of applications, including magnetic force microscopy (MFM), conductive atomic force microscopy (CAFM) and nanolithography. In this talk we will present several studied systems to discuss some of these applications. The CAFM was used to study the influence of low angle ion etching to improve the quality of high Tc superconductor's surface for technological applications. Electrically controlled nanoindentation (ECNI) was used to develop AFM nanotemplates which allows us to contact a single nanoobject, to fabricate nanojunctions (i.e. magnetic tunnel junctions, spin filters, etc) or to fabricate nanocontacts in order to study mesoscopic transport. Gold-gold nanocontacts were fabricated by using ECNI trying to achieve the smallest contact size. In this limit, the indentation process is stochastic. In spite of their high resistance (from 100 Ω to 1000 Ω). nanocontacts show a metallic like behavior, indicating their small size.

29 – Investigating the Atomic Layer Structure of Manganese Atoms on Nitrogen-polar Wurtzite Gallium Nitride Surface

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The investigation of magnetic or spintronic structures on wide band-gap semiconductors is important for future novel device applications. Gallium nitride is interesting because of its band-gap (blue-UV spectral range) and robust optoelectronic properties. And while the possibility for room-temperature dilute ferromagnetism in this system -as predicted by Dietl *et al.* [1]- is still intriguing, we have shown previously that ferromagnetic manganese gallium (MnGa) is almost perfectly lattice-matched to *c*-plane wurtzite GaN [2]. In the current work, we find that Mn atoms themselves form an ordered monolayer (ML) on N-polar wurtzite GaN [3]. We deposit sub-ML quantities of Mn on the GaN $(000\bar{1})$ surface and monitor the structure using reflection high energy electron diffraction (RHEED). By monitoring the RHEED diffraction streak intensities versus time, we deduce the surface ordering as a function of coverage. Within a fraction of a ML, the surface shows $3\times$ structure along $[1\ 0\ \bar{1}\ 0]$ but only $1\times$ structure along $[\bar{1}\ \bar{1}\ 2\ 0]$. In addition, the $1/3^{\text{rd}}$- and $2/3^{\text{rd}}$-order diffraction streaks differ in intensity by about a factor of three. The structure is optimized at a deposition of $\sim$0.86 ML Mn. These observations rule out the simple hexagonal $1/3^{\text{rd}}$ ML $\sqrt{3} \times \sqrt{3}$ R30^o reconstruction. To explain the RHEED periodicities and intensities, we postulate a Mn linear chain-type reconstruction having $2/3^{\text{rd}}$ ML Mn coverage with a spacing of $\sqrt{3}\times\sqrt{2}$ along the chains and 3a/2 between chains, and a surface sticking coefficient of $\sim$0.78. The arrangement of the Mn chain reconstruction on the w-GaN surface is also suggestive of an atomic template for MnGa film growth on w-GaN surfaces.

This work is supported by the U.S. Dept. of Energy, Office of Basic Energy Sciences (Grant No. DE-FG02-06ER46317) and the U.S. National Science Foundation (Grant No. 0730257).

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30 – Bottom-up approaches towards complex nanomaterials: combining tools for the construction of multiscale nanosystems

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Current "bottom-up" techniques for nanomaterials synthesis permit to produce an impressive palette of nanometric objects: nanoparticles, nanorods, nanotubes, block copolymers, dendrimers, nanostructured films, etc. These "Nano-Building Blocks" (NBB) can be currently produced in a reproducible way with a great variety of tuned features, including composition, dimensions, anisotropy and surface modification. Properties derived from structure, size or surface can be therefore accurately controlled or even designed.

In the last years, there is an increasing interest in combining these NBB into more complex functional structures that present properties at different length scales: nanoscopic, mesoscopic and micrometric. The possibility of accurately controlling the NBB properties, and combining soft chemistry approaches permits to create complex integrated materials, where different NBB are coassembled in space. The properties of these systems are derived from the properties of the NBB that form them, but also in their synergy. This "build-and-assemble" paradigm is "biomimetic", similar to the processes that take place in naturally occurring materials such as nacre, shell, bone and teeth.

In this work, several strategies will be presented that lead to complex nanomaterials formed by the combination of inorganic and organic NBBs. In particular, mesoporous materials derived from the combination of solgel chemistry and selfassembly of surfactants will be described. Mesoporous materials with amorphous or nanocrystalline inorganic frameworks present high surface area (100-1000m$^2g^{-1}$), and ordered arrays of monodisperse pores with tailored size in the mesoscale (250nm). Mesoporous Thin Films (MPTF) with oxide, phosphate, carbon or hybrid organicinorganic frameworks present interesting sensing, catalytic, electrical and optical properties, tuned by the pore size and geometry, wall composition, crystalline or amorphous character and surface features. Well defined monodisperse sized pores act as nanocavities with controlled environment and behaviour.

We have explored the production of accessible MPTF with their pore surface or interior modified by organic functional groups or nanoparticles. The presence of organic functional group leads to new sorption or controlled transport properties, opening the way to nanofiltering membranes. Ordered mesopores were used as an array of nanoreactors, permitting the inclusion of nanoparticles (NP), leading to tunable optical properties. Multilayer MPTF systems present a great variety of new properties: localized chemical.

31 – Superconductivity and Quantum Criticality in Heavy Fermions

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Soon after the discovery of heavy-fermion (HF) superconductivity (SC) in $CeCu_2Si_2$ (1979), UBe_{13} [Ott et al. (1983)], UPt_3 [Stewart et al.(1984)] and URu_2Si_2 [Schlabitz et al. (1984)], these materials were considered prime candidates for showing SC mediated by antiferromagnetic (AF) paramagnons [see, e.g., Schmitt-Rink et al. (1986), Scalapino et al. (1986)]. $CeCu_2Si_2$ was found to have a complex chemical phase diagram that can be transformed into a complex generic physical phase diagram (1996). The latter contains "phase A", an ordinary incommensurate spin-density wave (SDW) with very small ordered moment (2004). While moderate lattice expansion as achieved by low doping with Ge stabilizes "phase A", application of a tiny pressure weakens AF order and establishes a quantum critical point (QCP), presumably being of the (3D) SDW-type (1998). In the T-p phase diagram of $CeCu_2Si_{1.8}Ge_{0.2}$, a narrow superconducting dome centered around this QCP exists (2003), similar to the one found earlier for $CePd_2Si_2$ at the critical pressure $p_c \approx 2.8$ GPa [Mathur et al. (1998)]. Unique to $CeCu_2Si_{1.8}Ge_{0.2}$, however, is the occurrence of a second dome of SC that coincides with a weak valence transition near $p = 5$ GPa (2003).

We discuss evidence for HFSC under the *low-p* dome being mediated by extended AF quantum critical spin fluctuations, as first proposed for $CePd_2Si_2$. Interestingly, for the isostructural quantum critical compound $YbRh_2Si_2$ (2000), no superconductivity exists, at least above $T = 10$ mK. For this material, a number of experimental results, e.g., of the thermal (2003) and magnetic (2008) Grüneisen ratios, are presented. They highlight an unconventional nature of the QCP, at which an AF instability seems to coincide with a Mott transition in the subsystem of the 4f electrons.

Work done in collaboration with J. Arndt, M. Brando, S. Friedemann, P. Gegenwart, C. Geibel, C. Krellner, R. Kuechler, M. Loewenhaupt, N. Oeschler, Q. Si, O. Stockert, Y. Tokiwa, T. Westerkamp, S. Wirth and G. Zwicknagl.

32 – The Spin Reorientation Transition and Phase Diagram of Ultrathin Ferromagnetic Films

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Magnetic order in ultrathin ferromagnetic films is very complex due to the competition between exchange and dipolar interactions on different length scales, together with a strong influence of shape and magnetocrystalline anisotropy of the sample. In view of this complexity, theoretical work on simplified models and computer simulations are essential for rationalizing and guiding new experimental work.

In this talk we present recent Monte Carlo results of a two dimensional Heisenberg model for ultrathin films with perpendicular anisotropy. A complete phase diagram is obtained as a function of anisotropy and temperature, spanning a wide range of behaviors. We also observe and characterize a line of Spin Reorientation Transitions. These results are discussed in relation with experimental findings in different ultrathin films.

33 – Dynamics of Ordering of Block copolymer Thin Films Constrained to lie on a Curved Substrate

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In the last decade there has been a growing interest in the process of phase separation in selforganized thin films, mainly driven by their nanotechnological applications. Although important advances have been made to obtain ordered patterns into the nanoscale, the slow kinetics of ordering prevents the use of thermal treatments to obtain patterns with long range order [Gómez et al., Phys. Rev. Lett. 97, 188302 (2006)]. Then, different experimental methods have been employed to control the degree of order. Recently, there has been an increasing interest in the study of 2D modulated phases on curved surfaces [D. R. Nelson, Nano Lett. 2, 1125 (2002)]. One of the main differences between planar and curved 2D modulated phases is the nature of topological defects. On flat backgrounds, at low temperatures, the topological defects are nontrivial excitations of the ground equilibrium state. On the other hand, the curvature of the substrate can impose a topological requirement that includes defects in the ground state. In this talk we discuss the process of phase separation in thin film systems of cylinder forming block copolymers confined to lie on a curved substrate. We observe a coupling between defects and geometry that induces unbinding and self organization of disclination pairs. This open the possibility of a robust mechanism for an accurate control of smectic textures with potential applications to nanotechnology.

34 – Realistic Modeling of Materials with Strong Electronic Correlations

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Several characteristic properties of materials with strong electronic correlations will be described and microscopically explained within LDA+DMFT, a combination of ab initio band structure methods and the dynamical mean-field theory [1]. In particular, I will discuss

- the strong spectral transfer in (Sr,Ca)VO3 leading to a characteristic three-peak structure of the spectral function [2],
- the correlated band structure of the charge-transfer insulator NiO [3],
- the correlation-induced structural relaxation in the paramagnetic Jahn-Teller system KCuF3 [4],
- a generic mechanism explaining the appearance of kinks in the effective dispersion of correlated electron materials [5].

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