Spintronics, dilute magnetic semiconductors, and semiconducting heterostructures

3 - 1 – Thermoelectric transport properties of a quantum dot, immersed in a quantum wire

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The thermoelectrical effects in nanoestructures have gained renewed interest in recent years [1-3,5]. It happens due to the possibility of using nanoscopic systems to enhance the efficiency of macroscopic de-vices through the control of the energy transport on a microscopic scale. Recently, it was reported the experimental realization of nanoscopic thermal rectifiers [2], as well as the Coulombian control over a refrigeration process in a mesoscopic system [3]. In this work we study thermoelectric properties of a gate-defined quantum dot, with a very strong Coulomb repulsion inside the dot, immersed in a quantum wire, modelled by a tight-binding linear chain. We employ the X-boson approach for the impurity Anderson model [4], the localized state in this model is linked to the quantum dot and the conduction channel in the model is associated to the quantum wire. The thermoelectric transport coefficients were obtained in the presence of a chemical potential and temperature gradients, with the Onsager relation in the linear regime automatically satisfied, within the frame work of the Keldysh nonequilibrium Green's functions. We compute the linear thermopower, the thermal conductance and the thermoelectric figure of merit. Our results show a change in the sign of the thermopower as function of the energy level of the quantum dot (gate voltage in experimental works [5]), which is associated with an oscillatory behaviour and a suppression of the thermopower magnitude at low temperatures. We identify two relevant energy scales: a low tempera-ture scale dominated by the Kondo effect and a temperature scale characterized by charge fluctuations, where the thermoelectric figure of merit, that is a measure of the usefulness of materials or devices as thermopower generators or cooling systems indicates that this regime of temperature should be interesting for exploring practical applications. We also discuss the Wiedemann-Franz relation in this system. Our results are in qualitative agreement with recent experimental reports [5] and other theoretical works [1].

[1] R. Franco et. al. J. Appl. Phys. **103**, 07B726 (2008); M. Krawieck et. al. Phys. Rev. B **75**, 155330 (2007); R. Sakano et. al. J. Phys. Soc. Jpn. **76**, 074709 (2007); B. Dong et. al J. Phys. Condens. Matter **14**, 11747 (2002).

[2] C.W. Chang et. al. Science **314**, 1121 (2006); R. Scheibner et. al. cond-mat 0703514 (2007).

[3] Olli-Pentti Saira et. al. Phys. Rev. Lett. **99**, 027203 (2007).

[4] R. Franco et. al. Phys. Rev. B **73**, 195305 (2006); Phys. Rev. B **67**, 155301 (2003); Phys. Rev. B **66**, 045112 (2002).

[5] R. Scheibner et. al. Phys. Rev. B **75**, 041301 (2007); Phys. Rev. Lett. **95**, 176602 (2005).

3 - 2 – Electronic and magnetic properties of GaVN compounds as function of the pressure

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We report an ab-initio study about the pressure effects on the electronic and the magnetic properties of $Ga_xV_{1-x}N$ compounds (x=0.25, 0.50 and 0.75) in wurtzite-derived structures. We use the full-potential linearized augmented plane wave plus local orbitals method (LAPW+lo) within the spin density functional theory framework. The lattice constant depends linearly with Ga-concentration. The magnetic moment changes for a critical pressure. At x=0.75, a rather abrupt onset of the magnetic moment from 0 to 2 μ_B at P_{cr} ∼22.8 GPa is observed. For 0.25 and 0.50 Ga concentrations, the magnetic moment increases gradually when the pressure decreases toward the equilibrium value. The calculation of the density of states with Ga concentration is carried out considering two spin polarizations. The results reveal that for x=0.75 the compound behaves as a conductor for the spin-up polarization and that the density of states for spin-down polarization is zero at the Fermi level. At this concentration the compound presents a half metallic behavior; therefore this material could be potentially useful as spin injector. At high pressures $P > P_{cr}$ the compounds exhibit a metallic behavior.

3 - 3 – Ab initio calculations of the electronic and magnetic properties of Co_2FeSi-Au interface

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In this work, we first review the electronic and magnetic properties of the bulk Heusler alloy Co_2FeSi, in order to establish a reference baseline for a computational study of its interface with gold. We perform calculations using two different structural models, and applying both ASA and FP-LMTO, and FP-LAPW approaches with and without the inclusion of a Coulomb-exchange interaction, confirming previous results found for the bulk Co_2FeSi and moving on to explore the electronic and magnetic properties of the interface at issue. We found a change of sign of the spin polarization of both the density of states and the ballistic conductance at the Fermi energy, at the interface; suggesting the tunneling of minority electrons. We compare our results with the experimental data on point contact Andreev reflection of Co_2FeSi-Au structures.

3 - 4 – Confinement effects in magnetism of thin MnAs ribbons

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Thin films of MnAs grown on GaAs substrates have been intensively studied during the last ten years. The coexistence of two different phases, hexagonal (α-MnAs) and orthorhombic (β-MnAs) was reported for these films at room temperature, despite not being observed in bulk material. A periodic arrangement of these two phases in microscopic stripes is observed when the MnAs films are grown on GaAs (100) substrates. Many recent works show the effects of the lateral nanostructuration of the films, particularly, on the magnetic domain arrangement in MnAs dots of different sizes. In this work we present a systematic analysis of MnAs ribbons of different sizes and orientations fabricated by electron lithography from monocrystaline films of MnAs grown on GaAs. The topography and the magnetic domain behaviour of the ribbons were characterised by atomic and magnetic force microscopy. This characterisation is focused in the reversal mechanisms of the stripes magnetisation and the effects of lateral confinement on the coexistence of both phases (magnetic α and non-magnetic β) present in MnAs films.

3 - 5 – Magnetic and structural study of Fe doped tin dioxide

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The study of diluted magnetic semiconductors (DMS), like transition metal doped SnO_2, is of actual interest in magnetism because of their possible use in spintronics technology. In this work we present samples of SnO_2/Fe_2O_3 with 10 at % of Fe prepared by mechanosynthesis. Several samples were produced by milling the starting materials during different times. We report here on their magnetic and structural properties which have been investigated by magnetization measurements and XAFS (EXAFS- Extended X-ray Absorption Fine Structure and XANES- X-ray Absorption Near Edge Structure). The magnetic measurements (M vs H and M vs T) were carried out between 10 and 300 K. The M vs T ones were recorded under an applied field of 20 Oe (curves). We shall demonstrate the evolution of the magnetic properties of samples with milling time and its behaviour within different temperature ranges. It was noted that the sample with higher magnetization is the 1.5 h milled one which contains the major amount of bcc-Fe phase. It was observed that the hysteresis cycles of all the samples showed ferromagnetic (FM) plus paramagnetic (PM) behaviour within the whole temperature interval. In the case of the 10 h and 15 h milled samples measured at 10 K, the magnetization curves were reproduced with two FM components (only one FM component was needed for the rest of the samples). Fe K-edge XAFS analysis of $Sn_{0.9}Fe_{0.1}O_2$ in transmission mode indicate that Fe ions exhibit a 2+ oxidation state in the samples milled 0.25 and 0.5 h, while for 1, 1.5, 2, 5 and 10h they show an intermediate valence state between 2+ and 3+ values. We shall compare these results with the ones obtained by XRD and Mössbauer spectroscopy techniques.

3 - 6 – Structural and magnetic characterization of $Ti_{1-x}Fe_xO_2$ ($2.5 \leq x \leq 15$ at.%) nanoparticles

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TiO_2 is a semiconductor oxide that doped with transition metals can present ferromagnetism at room temperature, making it an interesting material for potential technological applications. In recent years, much attention has been given to iron-doped TiO_2. The Fe substitution Ti in the TiO_2 structure depends on multiple factors such as iron-loading, preparation method, calcination temperatures, etc. In this work, we report a magnetic and structural characterization of $Ti_{1-x}Fe_xO_2$ (x= 2.5, 5, 7, 10, 12.5 and 15 at. %) powders, prepared by mechano-synthesis using TiO_2 and Fe_2O_3 as starting materials. XAS (x-ray absorption spectroscopy) measurements performed at Fe K-edge showed that Fe ions are in 3+ oxidation state in 7 at. % Fe doped sample and in a mixture of 2+ and 3+ oxidation states for the others. EXAFS results show a good incorporation of Fe ions substituting Ti sites in TiO_2 rutile structure. It was observed from hysteresis cycles that all samples showed ferromagnetic (FM) and paramagnetic (PM) behavior from temperatures between 10 and 300 K. Magnetic measurements reveal a correlation between Fe^{2+} presence and magnetic behavior.

3 - 7 – Modeling the magnetic tunnel conductance at interdiffused interfaces in Fe/ZnSe/Fe junctions

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Electronic transport measurements in Fe/ZnSe/Fe magnetic tunnel junctions show that the tunnel magnetoresistance (TMR) is lower than the theoretical value estimated for sharp interfaces. However, several experiments suggest that interfaces are actually not perfect and that could be the reason for the lower TMR observed.

In this work, by means of electronic structure calculations (Wien2k and Siesta codes), we study different possible junctions analysing the effect of interdiffusion and reconstruction at the interface.

We propose a simple model for the conductance using ab initio potential profiles, which reveal that the effect of the reconstruction is to increase the kinetic energy of the conduction electrons, independently of their spin orientation. This, in turn, increases the conductivity and could explain the observed TMR behaviour.

3 - 8 – Paramagnetism in Co doped ZnO films deposited by pulsed laser ablation

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Diluted Magnetic Semiconductors (DMS), where a fraction of component ions of semiconductors are replaced by transition metal atoms, have recently attracted increasing attention because of their potential use in spintronic devices. Since the theoretical predictions of ferromagnetism in Co-doped ZnO [Dietl et al; Science, 287, 2000] this material is being intensively studied. In this work, we present a structural, magnetic and electrical transport characterization of $Zn_{0.9}OCo_{0.1}$ and $Zn_{0.85}OCo_{0.15}$ films deposited on Si/SiO_2 substrates in N_2 or O_2 atmospheres by pulsed laser ablation. X ray absorption spectroscopy results showed that Co ions are in 2+ state, substituting Zn in the ZnO structure. The magnetic results showed the lack of ferromagnetism. The M vs H loops taken at 5 K showed the characteristics of paramagnetic behaviour. These curves were well fitted with the Brillouin function using L = 1.3 and S=3/2 in agreement with the values expected for Co 2+. The voltage vs. current curves showed a slight asymmetry that increase when temperature decrease and lost the linear behaviour at low temperatures. The samples present positive magnetoresistance. This behaviour was previously observed in ZnO films deposited on sapphire.

3 - 9 – Hybrid Spin-Filter / Magnetic Tunnel Junction Heterostructures for Enhanced Spin Transport

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Magnetic thin film heterostructures such as magnetic tunnel junctions (MTJ) and spin filter devices, which involve spin-based tunneling across a nanometer-thick barrier layer, are among the leading architectures for spin-based transport applications. In order to improve these devices, the interfacial magnetism and spin polarization of these thin film materials and heterostructures must be better understood and optimized. Additionally, new device heterostructures should be investigated which may further improve spin-dependent transport. This work investigates how the choice of barrier layer material influences the magnetotransport and magnetic interface properties of highly spin polarized $La_{0.7}Sr_{0.3}MnO_3$ and Fe_3O_4-based devices. Interface effects between these materials are probed directly by multiple synchrotron radiation techniques, and indirectly by incorporating them into magnetic tunnel junctions. Through these studies, we have developed a novel spin-based device, consisting of a ferrimagnetic insulating barrier layer ($NiMn_2O_4$) sandwiched by two highly spin-polarized electrodes ($La_{0.7}Sr_{0.3}MnO_3$ and Fe_3O_4). We find that this structure acts as a hybrid spin-filter / MTJ when the barrier layer is ferrimagnetic, and exhibits junction magnetoresistance values of -30%–among the highest for Fe_3O_4-based devices. Through extensive investigation by X-ray absorption spectrometry, X-ray magnetic circular dichroism, photoemission electron microscopy, and transmission electron microscopy, we find that this hybrid device is made possible by the unique magnetic interactions at the two electrode-barrier interfaces. The isostructural spinel-spinel interface has strong ferromagnetic coupling, which couples the barrier layer to one electrode. However, the non-isostructural perovskite-spinel interface is magnetically decoupled, which allows the two electrodes to switch independently of one another, thus creating two distinct magnetization and resistance states. To optimize the spin transport in these new heterostructures, we are now investigating how a related isostructural spinel barrier layer with more robust magnetism, $NiFe_2O_4$, affects the performance of these hybrid devices.

3 - 10 – Uniform Hartree-Fock ground state of the two-dimensional electron gas with Rashba spin-orbit interaction

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We search for the uniform Hartree-Fock ground state of the two-dimensional electron gas formed in semiconductor heterostructures including the Rashba spin-orbit interaction. We identify two competing quantum phases: a ferromagnetic one with partial spin polarization in the perpendicular direction and a paramagnetic one with in-plane spin. We present a phase diagram in terms of the relative strengths of the Rashba to the Coulomb interaction and the electron density. We compare our theoretical description with existing experimental results obtained in GaAs-AlGaAs heterostructures.