Spintronics, dilute magnetic semiconductors, and semiconducting heterostructures

3 - 1 – Thermoelectric transport properties of a quantum dot, immersed in a quantum wire
Castellanos, R.,¹ Franco, R.,¹ and Silva-Valencia, J.¹
¹Departamento de Física, Universidad Nacional de Colombia - Bogotá.

The thermoelectrical effects in nanostructures 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 devices through the control of the energy transport on a microscopic scale. Recently, it was reported 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 framework 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 temperature 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].


3 - 2 – Electronic and magnetic properties of GaVN compounds as function of the pressure
González Hernández, R.,¹,² López, W.R.,¹ Fajardo, F.,² and Rodríguez, J.A.²
¹Grupo de Física de la Materia Condensada, Departamento de Física, Universidad del Norte. Barranquilla – Colombia
²GEMA - Grupo de Estudio de Materiales. Departamento de Física, Universidad Nacional de Colombia. Bogotá - Colombia

We report an ab-initio study about the pressure effects on the electronic and the magnetic properties of Ga₧V₁₋ₙN 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.

We report an ab-initio study about the pressure effects on the electronic and the magnetic properties of Ga₧V₁₋ₙN 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 μᵦ at P_c≈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_c, the compounds exhibit a metallic behavior.
3 - 3 - Ab initio calculations of the electronic and magnetic properties of Co₂FeSi-Au interface

Makinistian, L.,¹ Albanesi, E.A.,² Nadgorny, B.,³ and Petukhov, A.G.⁴

¹South Dakota School of Mines, Department of Physics, Rapid City, South Dakota 57701-3995, (On live from 2)
²INTEC-CONICET, Güemes 3450, 3000 Santa Fe, Argentina, and Facultad de Ingeniería, Universidad Nacional de Entre Ríos, 3101 Oro Verde (ER), Argentina
³Department of Physics and Astronomy, Wayne State University, Detroit, MI 48201
⁴South Dakota School of Mines, Department of Physics, Rapid City, South Dakota 57701-3995

In this work, we first review the electronic and magnetic properties of the bulk Heusler alloy Co₂FeSi, 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 Co₂FeSi 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 Co₂FeSi-Au structures.

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

Tortarolo, M.,¹ Sirena, M.,¹ Milano, J.,¹ Steren, L.B.,¹ Etgens, V.H.,² and Eddrief, M.²

¹Centro Atómico Bariloche, CNEA, Av. Bustillo 9500 (8400) S. C. de Bariloche, RN, Argentina
²Institut des NanoSciences de Paris, Universités Paris 6 et Paris 7, France.

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 monocrystalline 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

Bilovol, V.,¹ Mudarra Navarro, A.M.,¹ Rodríguez Torres, C.E.,¹ Sánchez, F.H.,¹ and Cabrera, A.F.¹

¹Departamento de Física, Facultad de Ciencias Exactas, UNLP-IFLP-CCT-La Plata-CONICET, C.C 671900, La Plata, Argentina

The study of diluted magnetic semiconductors (DMS), like transition metal doped SnO₂, is of actual interest in magnetism because of their possible use in spintronics technology. In this work we present samples of SnO₂/Fe₂O₃ with 10 at % of Fe prepared by mechanoynthesis. 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 Sn₀.₉Fe₀.₁O₂ 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$_x$O$_2$ (2.5 ≤ x ≤ 15 at.%) nanoparticles**

Mudarra Navarro, A.M.,$^1$ Bilovol, V.,$^1$ Cabrera, A.F.,$^1$ Rodríguez Torres, C.E.,$^1$ and Sánchez, F.H.$^1$

$^1$Dto. Física, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, IFLP-CCT La Plata-CONICET.

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$_x$O$_2$ (x = 2.5, 5, 7, 10, 12.5 and 15 at. %) powders, prepared by mechano-synthesis using TiO$_2$ and Fe$_2$O$_3$ 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**

Helman, C.,$^1$ Ferrari, V.,$^1$ Milano, J.,$^2$ and Llois, A.M.$^1$

$^1$Departamento de Física, Centro Atómico Constituyentes, Comisión Nacional de Energía Atómica, Buenos Aires, Argentina

$^2$Laboratorio de Resonancias, Centro Atómico Bariloche, Comisión Nacional de Energía Atómica, Buenos Aires, Argentina

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**

Golmar, F.,$^1$ Zapata, C.,$^2$ Villafuerte, M.,$^2$ Heluani, S.P.,$^2$ Mudarra Navarro, A.M.,$^3$ and Rodríguez Torres, C.E.$^3$

$^1$Laboratorio de Ablación Láser, Dto. Física, Facultad de Ingeniería, Universidad de Buenos Aires.

$^2$Laboratorio de Física de Sólido, Dto. De Física, Universidad Nacional de Tucumán.

$^3$Dto. Física-IFLP, Facultad de Ciencias Exactas, Universidad Nacional de La Plata.

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$_{0.9}$Co$_{0.1}$O and Zn$_{0.85}$Co$_{0.15}$ 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.
Hybrid Spin-Filter / Magnetic Tunnel Junction Heterostructures for Enhanced Spin Transport


1Dept of Materials Science and Engineering, University of California, Berkeley, CA 94720
2School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853
3Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720

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$_3$O$_4$-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$_2$O$_4$) sandwiched by two highly spin-polarized electrodes (La$_{0.7}$Sr$_{0.3}$MnO$_3$ and Fe$_3$O$_4$). 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$_3$O$_4$-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$_2$O$_4$, affects the performance of these hybrid devices.

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

Juri, L.O. and Tamborenea, P.I.

1Departamento de Fisica, FCEN, Universidad de Buenos Aires

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.