Γενικό Σεμιναρίο Τμηματός Φυσικής

PHYSICS COLLOQUIUM

Thursday 20 Dicember 2007 17:00-18:00

3rd Floor Seminar Room

"Materials and transport phenomena in spintronics studied from first principles calculations"

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Abstract

The developments in nanomagnetism in the past ten years have lead to novel applications in information storage, where the degree of freedom of the electronic spin plays a central role, and to the emergence of the field of magnetoelectronics or spintronics. Calculations from first principles (i.e., without adjustable parameters) are essential for the understanding and prediction of materials and transport phenomena in this field. This presentation will focus on three related subjects:

(i) Spin injection in ferromagnet/semiconductor junctions, where the spin-dependent symmetry of the wavefunctions at the interface can lead to spin-dependent reflectivity and highly polarized spin current.

(ii) Half-metallic ferromagnets, i.e., ferromagnetic alloys which exhibit an energy gap for only one spin direction around the Fermi energy, while the other spin direction shows metallic conduction. While, in principle, they have the property of conducting a 100% spin polarized current, this can be diminished by surface and interface states, spin-orbit coupling, and magnetic excitations at non-zero temperatures.

(iii) Study of ferromagnetic materials at high temperatures and locating the Curie temperature of the ferromagnetic phase transition. Here, a working approach constitutes of using density-functional theory for the calculation of the energy of magnetic excitations, i.e., calculating the exchange constants of a Heisenberg model, and solving this by a Monte Carlo method.