Spin-Density-Functional Theory

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The basic facts of density-functional theory are explained. This is done in a way that allows its application to spin-polarized, i.e. magnetic systems. A brief part is devoted to an overview of the various methods that are commonly used for the actual electronic structure calculations. Examples are given for some representative results covering ferromagnetic, antiferromagnetic and non-collinear order.

Magnetic structure of thin films and finite nanoparticles from first principles

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Thin magnetic films and nanoparticles deposited on different substrates exhibit a rich variety of magnetic structures the knowledge of which is inevitably important for potential technological applications. In many cases, suitable *ab initio* calculations are helpful to explore the underlying physics controlling the formation of such magnetic structures.
Our theoretical approach is based on a fully relativistic implementation of the density functional theory within the local spin-density approximation. The magnetic ground state of the system can be determined either by means of *ab initio* spin-dynamics relying on the so-called constrained
density functional theory or by mapping the first principles total energy onto a Heisenberg like Hamiltonian to be treated via standard methods of statistical physics such as Monte Carlo simulations or real-time spin-dynamics simulations. The relativistic treatment of the electronic structure allows for a full account of the magnetic anisotropy and of the anisotropic exchange interactions and of the Dzyaloshinskii-Moriya (DM) interactions.
I shall give an introduction to the applied methods including very recent developments and present results on magnetic pattern and domain wall formation in thin Mn and Fe films on W(110) and W(001). I shall demonstrate that the chiral degeneracy of the magnon spectrum can be lifted due to DM interactions and present calculations for an Fe monolayer on W(110), with a particular emphasis on the possibility to directly measure the DM interactions in ultrathin films. Finally, I shall focus on finite magnetic nanostructures by showing results on the magnetic configuration and the reorientation transition of Co clusters deposited on Au(111) surface, as well as on the formation of magnetic domain walls through an atomic sized Co nanocontact.

Multi-scale study of IrMn3/Co bilayer as a prototype of Exchange Bias system

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The exchange bias (EB) effect is a unidirectional anisotropy of the system which is characterized by a shift in the hysteresis loops by a amount called exchange bias field (H_E). The EB is related with the coupling between a ferromagnet (FM) and an antiferromagnet (AFM) or ferrimagnet (FI), and its stiffness and stability depends on the exchange coupling through the interface and the stability of the AFM- FI. The exchange bias is used in magnetic devices like giant magneto-resistance (GMR) sensors and magneto resistive spin valves, for magnetic domain stabilization or for pinning the FM layer. Therefore a deeper understanding of the microscopic origin of the exchange bias is necessary, not only to improve the actual knowledge of the physic underlying in this effects also to its applications in magnetic sensor and magnetic media technology.

In this work the magnetic properties of a bilayer of $IrMn_3$/Co are studied using a multiscale modeling, from ab-initio to spin model simulations. The antiferromagnet $IrMn_3$ exhibits a strong second order effetive anisotropy, a non-collinear magnetic ground state within a [111] magnetic easy plane and a high N´eel temperature. When it is capped by a Co layer, sizeable Dzyaloshinskii-Moriya (DM) interactions arise owing to the breaking of symmetry at the interface. These properties make the $IrMn_3$/Co bilayer a promising prototype for a exchange bias (EB) system.

To elucidate the microscopic origin of the exchange bias in the system, we evaluated numerically the hysteresis loops taking into account different relativistic contributions to the exchange interaction. Based on these investigations we conclude that the main origin of the perpendicular exchange bias is the DM interaction at the interface.

Transport in Spin-Orbit Coupled and Inhomogeneous Magnetic System

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Starting from a microscopic Hamiltonian description, one can derive a Boltzmann transport equation that incorporates, within a single framework, effects due to non-trivial band-structure (Spin-Orbit-Interaction, surface Dirac-quasiparticles on the surface of a topological insulator), as well as effects due to an inhomogeneous and/or time-dependent magnetization texture. Another major advantage of the scheme presented is the straightforward inclusion of random impurity scattering. This will be illustrated in the light of transport in ferromagnetic conductors and transport of Dirac-quasiparticles on the surface of a topological insulator with proximity induced (or itinerant) ferromagnetism.