TT 3: Tutorial: Density Functional Theory: A Computational Path to Interesting Spin-Textures and Novel Skyrmions (organized by MA)

Organizer: St. Blügel (FZ Jülich)

Ferromagnetic materials are important constituents of many modern hi-tech devices. In the last years one became however aware that non-collinear spin-textures could revolutionize spintronics. The focus of attention is on the spin-orbit interaction in magnetic solids with lack of inversion symmetry, that give rise to magnetic structures of particular winding sense and can lead to the formation of topological magnetization solitons, so-called magnetic skyrmions. These are then new functional magnetic units with interesting dynamical and novel spin-dependent transport properties. Density functional theory is the most powerful theoretical approach providing microscopic inside into the various magnetic interactions and spin-dependent transport properties, which is an important requisite for the design of materials and the analysis of experiments. While density function theory is practised widely, in this field new concepts and tools are coming into play. These will be introduced with the motivation that experimentalists can follow what we really calculate, what we can do, which assumption are made and how theory papers in this field can be interpreted and theory students might get some insight into this modern methodology, widening their scope or applying them to their own problems. After a brief introduction, the first tutorial focusses on the conceptual foundation of the relativistic, spin-dependent density functional theory, the second on the formation of new magnetic ground states and the third on spin-dependent transport properties.

Time: Sunday 16:00–18:30 Location: H 1012

Introductory Remarks

Tutorial TT 3.1 Sun 16:05 H 1012

Introduction to Spin-Density-Functional Theory — •Nicole Helbig — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

Density functional theory is the most powerful framework for a microscopic analysis of electronic properties of real solids. Spin-density-functional theory (spin-DFT) extends the density functional theory framework to allow for the description of magnetic systems, possibly in the presence of an external magnetic field. In this tutorial we introduce this subject from an elementary point of view and discuss the theoretical background of spin-DFT in both its collinear and non-collinear versions. Approximations for the exchange-correlation energy, which are necessary for practical applications, are also introduced. We give examples for calculations of different magnetic structures within spin-DFT and discuss how the theoretical results compare to experiments.

Tutorial TT 3.2 Sun 16:50 H 1012

Determining chiral magnetism from density functional theory — •Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Spin-orbit interaction in magnetic solids with bulk or structure inversion-asymmetry leads to the Dzyaloshinskii-Moriya interaction [1]. This magnetic interaction is a source of chiral magnetism and can subsequently lead to magnetic skyrmions – topological magnetization solitons – that may open a completely new vista to spintronics. A crucial issue is to find magnetic materials and ultra-thin films that combine the right properties such that these skyrmions can be formed. Density functional theory is a theoretical framework that permits the calculation of magnetic properties of materials from first-principles and is as such a tool for the analysis of experiments, for providing understanding of the magnetic interaction and for the design of the proper materials. In this endeavor your help is requested, many more *ab initio* calculations and experiments are needed. In this tutorial I explain concepts used to find these complex magnetic phases. The tutorial is conceptualized such that experimentalists can follow what we really calculate and what we can do and which assumptions are made, and theory students might get some insight into our methodology [2]. Examples are discussed mostly from the field of thin films [3].

[1] M. Bode *et al.*, Nature **447**, 190 (2007).
[2] see for example `www.juDFT.de`
[3] S. Heinze *et al.*, Nature Physics **7**, 713 (2011).

10 min. break

Tutorial TT 3.3 Sun 17:45 H 1012

Magneto-transport properties in spiralling spin textures — •Yuriy Mokrousov — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Spin-dependent transport properties in chiral magnets are currently of great interest both experimentally and theoretically. In this respect the skyrmion lattices comprised of topologically non-trivial whirls of magnetization which are typically stabilized at small magnetic field in the vicinity of the magnetic transition temperature are particularly intensively studied in B20 compounds. The Hall signal measured in these systems contains two topology-driven contributions due to the topological Hall effect (THE) and the anomalous Hall effect (AHE). It can be shown that the THE and AHE are a consequence of the Berry phases which electrons pick up in real and reciprocal spaces, respectively, while the so-called mixed Berry phases due to coupled dynamics in real and reciprocal space would give rise to a magnetic interaction which favors the chirality of the magnetization and gives rise to the skyrmion lattice - the Dzyaloshinskii-Moriya interaction (DMI). In my talk I will show how first principles methods can be used to justify the validity of the Berry phase concepts, as well as estimate and understand the physics of transport properties and DMI in skyrmion phase of complex materials. Moreover, I will try to convey a point that advanced material-specific modelling is a unique tool, which can be used to explore the emergent field of magneto-transport in nanometer-scale non-collinear textures.