MA 59: Spin Excitations II/ Spin Scattering

Time: Thursday 17:15–19:15 Location: HSZ 04

MA 59.1 Thu 17:15 HSZ 04

Ab initio description of the spin-Hall effect in disordered ferromagnets — •Diemo Ködderitzsch, Stephan Lowitzer, and Hubert Ebert — Ludwig-Maximilians-Universität München, Department Chemie und Biochemie, Physikalische Chemie, Butenandtstraße 11, D-81377 München, Germany

Spin-orbit induced couplings are at the heart of interesting phenomena like the anomalous- and spin-Hall-effects (AHE, SHE), which recently received a lot of attention due to their potential application for spin-separating devices in the field of spintronics. During the last years several theoretical works have dealt with the intrinsic SHE, based on the band structure of pure materials and only a few of them use a parameter free *ab initio* approach.

We present a coherent *ab initio* description of the spin Hall effect that is applicable to pure **and** disordered alloys by treating all sources of the SHE on equal footing. We use an implementation of the Kubo-Středa equation employing the fully relativistic Korringa-Kohn-Rostoker (KKR) Green's function method in conjunction with the Coherent Potential Approximation (CPA) alloy theory.

Whereas former studies concentrate mainly on non-magnetic systems, we apply our recently developed relativistic spin-projection scheme [1] to ferromagnetic transition-metal alloys and give first results.

[1] S. Lowitzer, D. Ködderitzsch and H. Ebert, Phys. Rev. B 82, 140402(R) (2010).

MA 59.2 Thu 17:30 HSZ 04

Anisotropic Spin Hall Effect from First Principles — •Frank Freimuth, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present first-principles calculations [1] of the intrinsic non-dissipative spin Hall conductivity (SHC) for 3*d*, 4*d* and 5*d* transition metals focusing in particular on the anisotropy of the SHC in nonmagnetic hcp metals and in antiferromagnetic bulk Cr. For the metals of this study we generally find large anisotropies. We derive a general relation between the SHC vector and the direction of spin-polarization and discuss the consequences for hcp metals. Especially, it is predicted that for systems, where the SHC changes sign due to the anisotropy, the spin Hall effect may be tuned such that the spin polarization is parallel either to the electric field or to the spin current. Additionally, we describe our computational method [2,3] emphasizing the Wannier interpolation technique and the definition of the conserved spin current. This work is supported by the HGF-YIG grant VH-NG-513.

[1] e-print: http://arxiv.org/abs/1011.2714
[2] F. Freimuth et al. Phys. Rev. B **78**, 035120 (2008)
[3] www.flapw.de

MA 59.3 Thu 17:45 HSZ 04

Unified *ab initio* description of the intrinsic and extrinsic anomalous Hall effect in disordered alloys — Diemo Ködderitzsch, •Kristina Chadova, Stephan Lowitzer, and Hubert Ebert — Ludwig-Maximilians-Universität München, Department Chemie und Biochemie, Physikalische Chemie, Butenandtstraße 11, D-81377 München, Germany

We present a coherent *ab initio*, i.e. parameter free, description of the anomalous Hall effect (AHE) that is applicable to pure as well as disordered alloy systems by treating all sources of the AHE on equal footing. We employ an implementation of the Kubo-Středa equation using the fully relativistic Korringa-Kohn-Rostoker (KKR) Green's function method in conjunction with the Coherent Potential Approximation (CPA) alloy theory. Applications to the pure elemental ferromagnets bcc-Fe, hcp-Co and fcc-Ni lead to results in full accordance to previous *ab initio* studies determining the intrinsic contribution only. However, the power of the approach presented is the ability to explicitly treat also extrinsic contributions to the AHE which is demonstrated by an application to the fcc alloy systems Fe_xPd_{1-x}, Co_xPd_{1-x} and Ni_xPd_{1-x}. We obtain a very satisfying qualitative agreement with experiment over the whole concentration range including the sign reversal of the AH-conductivity. A detailed discussion of skew and side-jump scattering processes exemplifies the capability of the proposed method.

MA 59.4 Thu 18:00 HSZ 04

Side-Jump Scattering Contribution to Anomalous Hall Effect from *ab initio* — •Jürgen Weischenberg[1], Frank Freimuth[1], Jairo Sinova[2], Stefan Blügel[1], and Yuriy Mokrousov[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA

The anomalous Hall conductivity may be decomposed into a scattering-dependent and a scattering-independent term. The extrinsic disorder-driven contribution to the scattering-independent term, the so-called side jump, is usually obtained by extrapolation from calculations with finite disorder. Recently it has been shown [1] that the side jump contribution to the anomalous Hall effect may be calculated directly from the electronic structure of a perfect crystal if a delta-correlated Gaussian disorder model is assumed. We implemented this approach within the full-potential linearized augmented plane-wave method (FLAPW) and computed the side-jump induced transverse conductivity for a variety of ferromagnetic materials such as Fe, Ni, FePt and FePd by means of Wannier interpolation [2]. To interpret our findings we compare them to theoretical and experimental literature values. Financial support by the HGF-YIG Programme VH-NG-513 is gratefully acknowledged.

[1] A. A. Kovalev *et al.*, PRL **105**, 036601 (2010)
[2] F. Freimuth *et al.*, Phys. Rev. B **78**, 035120 (2008)

MA 59.5 Thu 18:15 HSZ 04

First-principles calculation of transport through magnetic impurities in metallic wires with strong spin-orbit coupling — •Björn Hardrat[1], Neng-Ping Wang[2], Frank Freimuth[3], Yuriy Mokrousov[3], and Stefan Heinze[1] — [1]Institut für Theoretische Physik und Astrophysik, CAU Kiel, Germany — [2]Physics Department, Ningbo University, P.R. China — [3]Peter Grünberg Institut and Institute for Advanced Simulation, FZ-Jülich and JARA, Germany

We report the application of our recently developed ballistic transport code for one-dimensional magnetic systems to the spin-dependent transmission through magnetic impurities in metal monowires including spin-orbit coupling (SOC). The electronic structure of the considered systems is obtained with the one-dimensional version of the full-potential linearized augmented plane wave (FLAPW) method as implemented in the FLEUR code. We calculate the transmission and conductance within the Landauer formalism using a Greens function approach. In order to apply the Greens function method we map the electronic structure from our FLAPW calculations to a tight-binding like Hamiltonian via Wannier functions, preserving the accurate description of magnetic systems within the FLAPW method for our transport calculations. We demonstrate the potential of our code by calculating the spin-dependent conductance of ferromagnetic Co monowires with a Pt impurity exhibiting strong SOC and Pt monowires with a Co scatterer. We discuss the energy-dependent transmission in terms of the spin-dependent channels and mixing due to SOC leading to the phenomenon of ballistic anisotropic magnetoresistance (BAMR).

MA 59.6 Thu 18:30 HSZ 04

Magnetic friction in the Heisenberg spin chain — •Martin Magiera, Sebastian Angst, Alfred Hucht, and Dietrich E. Wolf — Faculty of Physics and CeNIDE, University of Duisburg-Essen, D-47048 Duisburg, Germany

Friction forces in purely magnetically interacting systems have been neglected for a long time, although they offer a broad spectrum of phenomena as recent studies show. We present theoretical calculations and simulations of the Heisenberg spin chain, scanned by a magnetic field with a constant velocity, where friction force may appear in a Stokesian way (force proportional to scanning velocity). In the same system additional (higher order) contributions due to spin wave excitations may be present. Finally the system may show non-adiabatic behavior, yielding a Coulomb friction force, which does not depend on velocity. In this talk we focus on the crossover from the Stokes- to the Coulomb-regime. This crossover can also be observed in the Ising model.

MA 59.7 Thu 18:45 HSZ 04

Confinement of kinks in a quantum one-dimensional Ising ferromagnet — •Sergei B. Rutkevich — Universität Duisburg-Essen, Duisburg, Deutchland

Confinement of topological excitations (the kinks) typically takes place in one-dimensional quantum systems having a discrete vacuum degeneracy, if the latter is explicitly broken by an external field. This phenomenon has been recently observed by Coldea et. al. (2010 Science **327** 177) in the Ising spin-chain ferromagnet $CoNb_2O_6$ at low temperatures. A phenomenological model has been proposed by Coldea et. al. to interpret the observed energy spectra of the magnetic excitations - the bound states of two kinks. We solve this model exactly and give explicit formulas for the kink bound state energies and for the related neutron scattering intensities. Possible modifications of the model are discussed as well.

MA 59.8 Thu 19:00 HSZ 04

spin-orbit scattering in molecular transport — •pengxiang xu and daniel wortmann — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

While many molecules considered for molecular transport devices contain only light elements and therefore the spin-orbit interaction generally plays not important role in these junctions, the use of heavier elements in molecules proposed for magnetic transport setups can lead to interesting behavior in spin-polarized transport due to the coupling of the spins to the electric polarization of the molecule.

Applying ab-initio density functional theory in the framework of the linearized-augmented plane-wave method [1] and the Green function formalism for transport, we study some model systems with different magnetization states (collinear/non-collinear) and molecular dipole moment. We report on our investigations of transport through molecules with transition-metal centers and demonstrate the influence of the spin-orbit coupling on the transmission properties of the molecule.

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[1]http://www.flapw.de