MA 30: Electron Theory

Time: Thursday 14:30–18:30 Location: H 1028

MA 30.1 Thu 14:30 H 1028

Predicting the formation of long chains in break junctions — •Alexander Thiess[1,2], Yuriy Mokrousov[1], and Stefan Heinze[1] — [1]Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

We introduce a simple model of chain formation in break junctions by formulating separate criteria for the stability and producibility of suspended monoatomic chains based on total energy arguments. Using the full-potential linearized augmented plane wave method [1] within the density-functional theory, we apply our model to break junctions of 5*d* transition-metals (TMs) and Au including the effect of spin-orbit coupling. Thereby, we can explain the physical reason of the experimentally observed trend of increasing probability for the creation of long suspended chains in break junctions for 5*d*-TMs at the end of the series [2]. Moreover, we predict that the probability of chain elongation can be greatly enhanced by the presence of oxygen in experiments with Au and Ag. Our model also allows us to make predictions on the ballistic transport properties of suspended chains.

[1] Y. Mokrousov *et al.*, Phys. Rev. B **72**, 045402 (2005)
[2] R. H. M. Smit *et al.*, Phys. Rev. Lett. **96**, 266102 (2001)

MA 30.2 Thu 14:45 H 1028

Relativistic optimized potential method for open-shell systems — D Ködderitzsch[1], •H Ebert[1], and E Engel[2] — [1]Ludwig-Maximilians-Universität München, Department Chemie und Biochemie, Physikalische Chemie, Butenandtstraße 11, D-81377 München, Germany — [2]Institut für Theoretische Physik, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, D-60438 Frankfurt/Main, Germany

A formulation of the relativistic optimized potential method (ROPM) within spin-density functional theory is presented.[1] Various forms of the corresponding ROPM equations are given that allow to determine the spin-averaged and spin-dependent exchange correlation potentials. For a implementation numerical of the scheme we use the exact exchange (EXX). Results are presented for a number of free atoms that demonstrate the implication of the fully relativistic approach as well as the impact of making use of the KLI (Krieger-Li-Iafarate) approximation.

[1] D. Ködderitzsch, H. Ebert, E. Engel, Phys. Rev. **B**, accepted

MA 30.3 Thu 15:00 H 1028

An improved s-d model for the dissipative domain wall dynamics — •Lorenzo De Angeli and Manfred Fähnle — Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany

The dissipative dynamics of domain walls induced by an external magnetic field or by spin-polarized transport currents is often described within the framework of the s-d model [1]. Thereby the magnetization is subdivided into a localized part $\mathbf{M}_d(\mathbf{r},t)$ arising from the d electrons and a part $\mathbf{m}(\mathbf{r},t)$ due to the conduction s and p electrons, and the dynamics of $\mathbf{M}_d(\mathbf{r},t)$ is influenced by the torques exerted on the localized magnetization by $\mathbf{m}(\mathbf{r},t)$. A basic assumption of the conventional s-d model is that in a static situation the atomic moments arising from $\mathbf{M}_d$ and $\mathbf{m}$ are collinear. It has been shown that for strongly noncollinear situations (e.g., narrow domain walls, vortex cores, etc.) this assumption is not correct [2]. We have extended the s-d model by taking into account a possible noncollinearity between the d magnetization and the conduction electron magnetization, leading to various new torques. By extending the Walker model for the dynamics of domain walls [3] the influence of such torques on the initial and final velocity of a Neel wall is investigated.

[1] S. Zhang and Z. Li, Phys. Rev. Lett. 93, 127204 (2004).
[2] M. Fähnle, R. Singer and D. Steiauf, Phys. Rev. B 73, 172408 (2006).
[3] N.L. Schryer and L.R. Walker, J. Appl. Phys. 45, 5406 (1974).

MA 30.4 Thu 15:15 H 1028

Ab-initio calculations of adiabatic magnon spectra using the atomic-sphere-approximation for the spin direction — Reinhard Singer, •Frank Dietermann, Daniel Steiauf, and Manfred Fähnle — Max-Planck-Institute für Metallforschung, Heisenbergstrasse 3, D-70569 Stuttgart, Germany

The frozen-magnon calculations of the adiabatic spin-wave spectra, which are often based on the atomic-sphere approximation (spin-ASA), are revisited. There are two complications arising from the spin-ASA: The atomic magnetic moments are not necessarily parallel to the local spin-quantization axes of the spin-ASA, and there may be additional torques acting on the magnetic moments. It is shown that the spin-wave energies obtained from spin-ASA calculations are very similar to those of full-spin calculations if these two complications are taken into account properly.[1]

[1] R.Singer, F.Dietermann, D.Steiauf and M. Fähnle, Phys.Rev.B 76, 052403

MA 30.5 Thu 15:30 H 1028

Wannier-function approach to spin-wave excitations in transition metals — •Ersoy Sasioglu, Arno Schindlmayr, Christoph Friedrich, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

We develop a computational scheme based on many-body perturbation theory to study excitation spectra of magnetic materials from first principles using Wannier functions. The main quantity of interest is the spin-spin correlation function (or dynamical spin susceptibility), from which magnetic excitations, including single-particle spin-flip Stoner excitations and collective spin-wave modes as well as their lifetimes can be obtained. In order to describe collective spin-wave excitations we include appropriate vertex corrections in the form of a multiple-scattering T-matrix, which describes the coupling of electrons and holes with different spin. To reduce the numerical cost for the calculation of the four-point T-matrix we exploit a transformation to maximally localized Wannier functions that takes advantage of the short spatial range of electronic correlation in the partially filled *d* or *f* orbitals of magnetic materials. Our implementation is based on the all-electron full-potential linearized augmented plane-wave (FLAPW) method. As a first step, we calculate the dynamical spin susceptibility of the non-interacting Kohn-Sham electrons and the matrix elements of the Coulomb potential in the Wannier basis. The obtained values for the latter are in good agreement with previous calculations. This work was funded in part by the EU's Sixth Framework Programme through the Nanoquanta Network of Excellence (NMP-4-CT-2004-500198).

MA 30.6 Thu 15:45 H 1028

Modification of the magnetocrystalline anisotropy of transition metal films by external electric fields: density functional calculations — •Hongbin Zhang, Ferenc Tasnadi, Ingo Opahle, and Manuel Richter — IFW Dresden, Dresden, Germany

Recent experiments verified a modification of the Magnetocrystalline anisotropy (MA) of FePt and FePd films by electrochemical charging [1]. We have carried out density functional calculations for such slabs, using the relativistic version of the full-potential local-orbital (FPLO) code. The electric field is simulated by virtual crystal approximation (VCA) applied to the surface atoms. Good agreement between the calculated dependence of the MA on the external field with the experimental data is achieved. It is demonstrated, that the variation of MA is a surface effect. However, correct finite size scaling is important for the quantitative results. We predict that the electric field dependence of MA is even stronger for CoPt films than for FePt films.

[1] M. Weisheit et al., Science 315 (2007) 349.

MA 30.7 Thu 16:00 H 1028

Electronic and magnetic properties of the nitrometalathes $\mathbf{A_3[M^{III}N_3]}$ — •Julia Wildeboer, Joanna Katarzyna Bendyna, Peter Höhn, Walter Schnelle, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Strasse 40, D-01187 Dresden

In solid state physics, geometrically frustated systems enjoy a steadily growing interest. The nitrometalathe compounds $A_3[M^{III}N_3]$ have recently been synthesized. They crystallize in a hexagonal structure containing the planar complex $[M^{III}N_3]^{6-}$ and form a frustated lattice of magnetically active transition metal ions.

We present an comparative experimental and theoretical study of the electronic and magnetic properties of these systems based on thermo-

dynamical measurements; e.g. magnetic susceptibility and electrical resistivity, and density functional theory (DFT) calculations.

The DFT-based results support the experimental data: the compound Sr_3CrN_3 have a non-magnetic ground state whereas all other systems exhibit antiferromagnetic long ranged order.

Similarities and differences with respect to chemical bonding and exchange interaction will be discussed. The influence of strong coulomb repulsion on the transition metal sites will be investigated.

MA 30.8 Thu 16:15 H 1028

Electronic and magnetic properties of Fe_3O_4 in the electronic ground state and in a constrained excited state — •Christos Kostoglou, Reinhard Singer, and Manfred Fähnle — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

Below the Verwey temperature T_V magnetite (Fe_3O_4) exhibits an insulating, ordered phase with a special type of charge, spin and orbital order [1,2] due to an ordered arrangement of two types of atoms Fe(B,1) and Fe(B,2) on the Fe(B) sublattice. For an interpretation of experiments on the electronic conductivity and on the magnetic aftereffect at finite temperatures below T_V it is generally assumed [3] that there are thermally-activated electronic transitions involving pairs of exchanged Fe(B,1) and Fe(B,2) atoms as intermediate configuration. The energy difference between the perfectly ordered state and the state containing such a defect is calculated by the LDA+U method and the augmented spherical wave method.

[1] I. Leonov, A.N. Yaresko, V.N. Antonov, M.A. Korotin, and V.I. Anisimov, Phys. Rev. Lett. 93, 146404 (2004)
[2] Horng-Tay Jeng, G.Y. Guo, and D.J. Huang, Phys. Rev. Lett. 93, 156403 (2004)
[3] F. Walz, J. Phys.: Condens. Matter 14, R285 (2002), M. Fähnle, H. Kronmüller, F. Walz, Physica B 369, 177-180 (2005)

15 Min. Sessoin Break

MA 30.9 Thu 16:45 H 1028

Spin-wave excitations from time-dependent density-functional theory — •Manfred Niesert, Arno Schindlmayr, Christoph Friedrich, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

Spin waves constitute an important class of low-energy excitations in magnetic solids with a characteristic material-specific dispersion and a direct relation to magnetization dynamics. Until now most theoretical studies were based on the Heisenberg model of localized spins or on the frozen-magnon method, but neither is applicable to investigate the dynamics of spin waves in metallic systems with itinerant electrons. As a possible solution, time-dependent density-functional theory gives access to the full frequency-dependent transverse spin susceptibility, from which not only the spin-wave dispersion but also the corresponding excitation lifetimes and other spectral information can be extracted. We have developed a practical scheme to calculate spin-wave spectra from first principles within this framework and illustrate its performance by applications to prototype ferromagnetic transition metals. Our implementation uses the full-potential linearized augmented plane-wave method, and dynamic exchange-correlation effects are in the first instance described by the adiabatic local-density approximation.

MA 30.10 Thu 17:00 H 1028

Towards a linear-scaling algorithm for density-functional calculation for metallic systems — •Rudolf Zeller — Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich

Linear-scaling algorithms for electronic structure calculations are usually based on a truncation of the density matrix, which decays exponentially in band gap systems. For metallic systems, however, it is not yet well understood whether the decay is fast enough or can be made so by introducing finite temperatures. These questions were investigated with the tight-binding (screened) Korringa-Kohn-Rostoker Green-function method. In calculations for large Cu and Pd supercells with fcc geometry, a spatial truncation of the Green function was applied and the dependence of total energy error on the truncation radius was determined. For reasonable electronic temperatures it was found that the error was bounded by about 2 meV per atom if a few thousand atoms are contained in the truncation range. It is shown that a fixed truncation radius leads to a computational effort per atom, which is independent of the number of atoms in the system, if the sparse matrix equations, which arise because of the tight-binding (screening) transformation, are solved iteratively. This linear-scaling feature and a straightforward parallelization strategy over the atoms opens the way to calculate the electronic and magnetic structure of large metallic systems on massively parallel computers.

MA 30.11 Thu 17:15 H 1028

Collapse of strong ferromagnetism in YCo_5 under pressure - a magnetically driven electronic topological transition evidenced by XMCD — •Helge Rosner[1], Angela Trapananti[2], Miriam Schmitt[1], Ulrich Schwarz[1], and Manuel Richter[3] — [1]MPI CPfS Dresden, Nöthnitzer Straße 40, 01187 Dresden — [2]ESRF, BP220, 38043 Grenoble, France — [3]IFW Dresden , PF 270116, 01171 Dresden

Isomorphic lattice collapse under pressure is a rare phenomenon, usually related to a change of chemical valence. The most famous examples are SmS and Ce metal, collapsing isomorphically under pressure with about 15% volume reduction. In SmS the electronic transition is ascribed to a change of valence, in Ce it is connected with altering contributions of the $4f$-electrons to the chemical bonding. In contrast, the investigated YCo5 obviously is a compound with a stable valence. An entirely new type of isomorphic electronic transition under hydrostatic pressure has been reported recently using ab-initio electronic structure calculation and high-pressure x-ray diffraction.[1,2] The volume collapse is characterized as a first-order Lifshitz or electronic topological transition (ETT) and assigned to magnetic exchange interactions. This mechanism is now directly evidenced by a combination of high pressure XMCD measurements and DFT band structure calculations, both revealing a substantial drop of the magnetic moment related to the phase transition.

[1] H. Rosner et al., Nature Physics **2**, 469, (2006).
[2] D. Koudela et al., Phys. Rev. B. (submitted)

MA 30.12 Thu 17:30 H 1028

Temperature dependent magnetic exchange interactions in the paramagnetic state of hcp Gd. — •Khmelevskyi Sergii, Khmelevska Tetyana, Ruban Andrei, and Mohn Peter — Center for Computational Materials Science, Vienna University of Technology, Gumpendorferstrasse 1, Vienna, Austria, A-1060

We use the first-principles magnetic force theorem embodied in the Korringa-Kohn-Rostoker method to calculate pair magnetic exchange interactions in pure hcp Gd metal in the ferromagnetic as well as in the paramagnetic state with disordered local 4f-moments. It is found that the exchange interactions between the localized 4f-moments, in particular also distant ones, depend on the state of magnetic disorder. Such a dependence is a consequence of the electronic structure changes of the conduction band that mediates the interaction between the local moments. The magnetic ordering temperature has been calculated using a Monte-Carlo simulation technique and the results are compared with mean-field based studies. It is also shown that most important interactions between of nearest neighbors Gd 4f moments is essentially non RKKY in character.

MA 30.13 Thu 17:45 H 1028

Electron theory of dissipative spin dynamics — •Jonas Seib, Daniel Steiauf, and Manfred Fähnle — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

Within the breathing Fermi surface model the damping of the magnetization dynamics is related to the change of the Fermi surface with changing magnetic configuration, given by the orientations of the atomic magnetic moments: This change requires a scattering of the electrons among the single-electron states in reciprocal space, and this in turn requires time. The theory yields a Gilbert-type equation of motion for the magnetization with the damping scalar of the original Gilbert equation replaced by a damping matrix. This damping matrix depends on a relaxation time describing the scattering, and on the change of single-electron energies when the directions of the atomic magnetic moments are changing. These derivatives of single-electron energies can be calculated within electron theory. For collinear configurations the breathing of the Fermi surface is caused by spin-orbit coupling, and the derivatives can been calculated with a torque-operator method [1]. For noncollinear situations, also interatomic exchange interaction is the origin of a breathing Fermi surface, and a new Harris-Foulkes approach [2] can be used to calculate the change of single-electron energies. Numerical results for the damping matrix in collinear configurations as obtained by the two methods are compared. A preview on damping in noncollinear situations is given.

[1] D. Steiauf and M. Fähnle, Phys. Rev. B **72**, 064450 (2005).
[2] P. Bruno, Phys. Rev. Lett. **90**, 087205 (2003).

MA 30.14 Thu 18:00 H 1028

Parametrization of the adiabatic magnetic energy on the atomic level: spin-cluster expansion technique vs. Heisenberg modeling — •Reinhard Singer, Frank Dietermann, and Manfred Fähnle — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

A widely adopted analytic representation of the adiabatic magnetic energy on the atomic level is the family of Heisenberg models. There the basic configurational dependence of the adiabatic magnetic energy is assumed to be a sum of pair interactions, $\mathbf{e}_i \cdot \mathbf{e}_j$, with $\mathbf{e}_i$ being the unit vector of the atomic magnetic moment located at site i. The recently introduced spin-cluster expansion (SCE) [1] breaks this limitation and takes account of all possible multi-site spin clusters and of a complete set of site basis functions $Y_{lm}(\mathbf{e}_i)$ which are the spherical harmonics. Under the symmetry restrictions of the Heisenberg model, i.e., time-reversal and rotational invariance, a complete set of SCE basis functions were obtained [2] which contain the Heisenberg interactions as a subset. Practically the interaction parameters of a truncated SCE are obtained by fitting to energies calculated with the ab-initio electron theory for a set of reference configurations. We show how the SCE is constructed and how it offers a more efficient and flexible way of parametrizing the complex adiabatic magnetic energy landscape of fcc-Fe and fcc-Ni. Furthermore we present how the SCE helps to identify new magnetic groundstate candidates in fcc-Fe.

[1] R. Drautz and M. Fähnle, Phys. Rev. B 69, 104404 (2004).
[2] R. Singer and M. Fähnle, J. Math. Phys. 47, 113503 (2006).

MA 30.15 Thu 18:15 H 1028

Spin-mixing in noncollinear ferromagnetic metals as basis of femtosecond magnetization dynamics — •Daniel Steiauf and Manfred Fähnle — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

A simple phenomenological model for the ultrafast demagnetization of a system after laser pulse irradiation is presented. The basic ideas are very similar to those of the Elliott-Yafet mechanism. If the spinor-field wavefunctions of the electrons are mixtures of spin-up and spin-down states depending on the wave vector, the transitions between states with different wave vectors due to scattering at defects or phonons change the spin polarization of the electrons, whereby angular momentum is transferred to the lattice via spin-orbit coupling. In collinear magnetic configurations the spin-mixing arises exclusively from spin-orbit coupling and thus it is very small, requiring very many scattering events for a considerable change of the magnetic moment of the system. In noncollinear magnetic systems there is an additional and much stronger spin-mixing arising from the much larger exchange couplings. For systems like Ni which are ferromagnetic in the ground state a noncollinearity arises at nonzero temperatures due to thermal disordering. The degree of spin-mixing due to spin-orbit coupling on the one hand and due to the noncollinearity on the other hand is calculated quantitatively by the ab-initio density functional electron theory.