MA 30: Electron Theory of Magnetism

Time: Thursday 17:00–18:15 Location: H22

MA 30.1 Thu 17:00 H22

Electronic structure, localization and spin-state transition in Cu-substituted FeSe — •Stanislav Chadov[1], Daniel Schärf[1], Gerhard H. Fecher[1], Claudia Felser[1], Lijun Zhang[2], and David J. Singh[2] — [1]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg Universität, 55099 Mainz — [2]Material Science and Technology Division, Oak Ridge National Laboratory, TN 37831-6114, USA

We report the density functional studies of the $Fe_{1-x}Cu_xSe$ alloy using the coherent potential approximation (CPA) method. Magnetic behaviour was investigated using the disordered local moment (DLM) approach. We find that Cu occurs in a nominal d^{10} configuration and is highly disruptive to the electronic structure of the Fe sheets. This would be consistent with a metal-insulator transition due to Anderson localization. We further find a strong crossover from a weak moment itinerant system to a local moment magnet at $x \approx 0.12$. We associate this with the experimentally observed jump near this concentration. Our results are consistent with the characterization of this concentration-dependent jump as a transition to a spin-glass.

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MA 30.2 Thu 17:15 H22

Theoretical description of spin-spirals using the KKR Green's function method — •Sergiy Mankovsky[1], Gerhard H. Fecher[2], and Hubert Ebert[1] — [1]Dept. Chemie und Biochemie/Phys. Chemie, Universität München, Butenandtstr. 11, D-81377 München, Germany — [2]Universität Mainz, Inst. of Anorg. und Analyt. Chemie, 55099 Mainz , Germany

We present a formalism for the theoretical description of spin-spirals within the KKR (Korringa-Kohn-Rostoker) Green's function formalism. The present technique is applicable to any system, e.g., elemental solids, ordered compounds, as well as it allows also to deal with random alloys using the CPA (Coherent Potential Approximation) alloy theory. As examples, we present results of calculations for pure Fe (bcc and fcc), Ni (fcc), Fe-Pd alloys and Fe-Ni alloys in ordered and disordered phases and compare to available experimental data as well as theoretical results obtained by other authors.

MA 30.3 Thu 17:30 H22

Theoretical study of the stability of AFM order in iron pnictides — •Alexander Yaresko — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

The wave-vector ($\mathbf{q}$) and doping (δ) dependences of the total energy, $E(\mathbf{q})$, in electron ($\delta > 0$) doped $LaFeAsO_{1-x}F_x$ and $M(Fe_{1-x}Co_x)_2As_2$ and hole ($\delta < 0$) doped $M_{1-x}K_xFe_2As_2$ (M=Ba, Sr) are studied by performing self-consistent LSDA calculations for coplanar spin spirals using the LMTO method. For the undoped compounds the minimum of $E(\mathbf{q})$ is found at $\mathbf{q} = (\pi, 0)$ corresponding to stripe AFM order with the Fe magnetic moment of about $1.5\mu_B$. In $LaFeAsO_{1-x}F_x$ the minimum shifts to an incommensurate $\mathbf{q}$ already at δ=0.1 (x=0.1). Similar behavior is also found when FeAs layers in $M(Fe_{1-x}Co_x)_2As_2$ are doped with electrons. In contrast, stripe AFM order in $M_{1-x}K_xFe_2As_2$ remains stable in a wide range of hole doping up to δ=−0.3, which corresponds to the K content x=0.6, although the stabilization energy of the AFM solution rapidly decreases with doping. Spin-spiral calculations for LiFeAs predict a magnetic ground state with $\mathbf{q} = (\pi, 0)$ but with the Fe moment ($0.6\mu_B$) and the stabilization energy which are significantly smaller than in the other two families of Fe pnictides.

According to the calculated q_z dependence of the total energy, the magnetic interactions in LaFeAsO are 2D-like, whereas in MFe_2As_2 compounds FeAs layers are coupled antiferromagnetically, with the coupling in $SrFe_2As_2$ being stronger than in $BaFe_2As_2$.

MA 30.4 Thu 17:45 H22

An ab-initio description of the magnetic shape anisotropy — •Sven Bornemann, Jan Minár, Jürgen Braun, and Hubert Ebert — Department Chemie und Biochemie, LMU München, 81377 München, Germany

For magnetic transition metal systems with reduced dimensionality and low symmetry the shape anisotropy becomes a significant contribution to the magnetic anisotropy. In fact, it can reach the same order of magnitude as the spin-orbit induced anisotropy. So far, the shape anisotropy has always been treated as a classical interaction between magnetic dipoles while the spin-orbit anisotropy has been determined by relativistic band structure calculations. It is uncertain, however, whether such an inconsistent treatment of the two anisotropy contributions is still valid for low-dimensional nano structures such as magnetic thin films, wires or clusters where the magnetic easy axis can depend strongly on the interplay between these two contributions. As an alternative to the classical approach an ab-initio description of the shape anisotropy has been developed. This is achieved by including the Breit interaction, being the natural cause of the shape anisotropy, in the Dirac-equation set up within the framework of spin density functional theory. We have implemented this approach using the fully relativistic KKR band structure scheme. We will present the details of our implementation and show results for the shape anisotropy of thin Fe films on Au(001) as well as for free-standing Fe and Co wires in comparison with the classical treatment.

MA 30.5 Thu 18:00 H22

Ab initio **spin-wave spectra of the bulk magnets Fe, Co, and Ni from many-body perturbation theory** — •Ersoy Sasioglu[1], Christoph Friedrich[1], Arno Schindlmayr[2], and Stefan Blügel[1] — [1]Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department Physik, Universität Paderborn, 33095 Paderborn, Germany

Spin excitations are of fundamental importance in many areas of condensed matter physics. First-principles calculations of spin-wave spectra have so far mostly been carried out within the frozen-magnon approach where the excitation energy is calculated by assuming a static spin-spiral configuration. We study the magnetic excitations of bulk magnets within the framework of many-body perturbation theory (MBPT) as implemented in the full-potential linearized augmented plane-wave (FLAPW) method. Starting from the *GW* approximation we obtain a Bethe-Salpeter equation for the magnetic susceptibility treating single-particle Stoner excitations and magnons on the same footing. We found that the spin-wave dispersion of Fe and Co exhibit gaps close to the middle of the Brillouin zone along the high symmetry directions. For Ni, the theoretical spin-wave dispersion exhibits two branches while those for Fe and Co show only one branch. Furthermore, at high energies the spin waves are heavily damped due to the coupling to single-particle Stoner excitations. In Fe the damping suppresses the spin waves in a large part of the Brillouin zone along the $\Gamma - H - N$ direction. The obtained results are in good agreement with available experimental data as well as previous calculations.