MM 52: Electronic Properties II

Time: Thursday 11:30–13:00 Location: H5

MM 52.1 Thu 11:30 H5

Ab initio **investigation of the Spin Hall Effect for non-magnetic alloys** — •Stephan Lowitzer, Diemo Ködderitzsch, and Hubert Ebert — Department Chemie, Physikalische Chemie, Universität München, Butenandstr. 5-13, 81377 München, Germany

Spin-orbit coupling is responsible for several interesting phenomena like e.g. the anomalous Hall effect (AHE) in magnetic materials. The AHE results from the interaction between spin-orbit coupling and the spin polarization. In comparison to the AHE the spin Hall effect (SHE) needs no spin polarization and is therefore even present in non-magnetic systems. This was shown by several experimental works e.g. [1].

During the last years several publications have appeared which studied the spin Hall effect for pure systems via *ab initio* e.g. [2] or model calculations [3]. However, up to now no publication is available in which the SHE is calculated for alloy systems on an *ab initio* level.

To calculate the SHE we have implemented the Kubo-Středa equation in our fully relativistic SPR-KKR package. The Kubo-Středa equation gives access to the full anti-symmetric conductivity tensor what is necessary for the calculation of the SHE. The disorder is treated via the coherent potential approximation (CPA). We show first results for several non-magnetic $3d$ and $4d$ transition metal alloys.

[1] S. O. Valenzuela and M. Tinkham, Nature **442**, 176 (2006)
[2] Y. Yao and Z. Fang, Phys. Rev. Lett. **95**, 156601 (2005)
[3] T. Tanaka, M. Kontani, M. Naito, T. Naito, D. S. Hirashima, K. Yamada and J. Inoue, Phys. Rev. B **77**, 165117 (2008)

MM 52.2 Thu 11:45 H5

$FeSe_{1-x}$ synthesized under ambient- and high-pressure conditions: a comparative study — •Mariano de Souza, Amir-Abbas Haghighirad, Ulrich Tutsch, Sebastian Köhler, Daniel Hofmann, Michael Lang, and Wolf Assmus — Physikalisches Institut, Goethe-Universität, Max-von-Laue Str. 1, D-60438 Frankfurt (M), Germany

Among the Fe-based superconducting (SC) materials, the binary alloy $FeSe_{1-x}$ with $T_c \simeq 8.5\,K$ [1] has attracted enormous interest. Although a tetragonal-to-orthorhombic transition at high-T takes place, it is not accompanied by long-range magnetic ordering, as it occurs in other Fe-based superconductors. Many questions remain still open, like the right stoichiometry of the SC phase, the symmetry of the SC order parameter and the origin of the high-pressure dependence of T_c [2]. Here, we report resistivity, susceptibility and thermal expansion data on single-crystalline $FeSe_{0.95}$ prepared under ambient- and high-pressure (HP) conditions. We show that SC samples of $FeSe_{1-x}$ can also be obtained well outside the composition range reported in the literature [3]. Our thermal expansion results reveal a tiny feature around $\sim$90 K, most likely related to the structural phase transition, and onset of superconductivity around 8.5 K. For samples synthesized under HP conditions, the saturated magnetic moment of Fe is dramatically reduced and superconductivity is destroyed. [1] F.-C. Hsu *et al.*, Proc. Natl. Acad. Sci. U.S.A. **105**, 1462 (08); [2] S. Medvedev *et al.*, Nat. Mat. **8**, 576 (09); [3] T.M. McQueen *et al.*, Phys. Rev. B **79**, 014522 (08).

MM 52.3 Thu 12:00 H5

Groundstatable fermionic wavefunctions and their associated many-body Hamiltonians — Daniel Charrier[1] and •Claudio Chamon[2] — [1]Max Planck Institut für Physikkomplexer Systeme, Nöthnitzer Straße38, 01187 Dresden, Germany — [2]Physics Department, Boston University, Boston, MA 02215, USA

In the vast majority of many-body problems, it is the kinetic energy part of the Hamiltonian that is best known microscopically, and it is the detailed form of the interactions between the particles, the potential energy term, that is harder to determine from first principles. An example is the case of high temperature superconductors: while a tight-binding model captures the kinetic term, it is not clear that there is superconductivity with only an onsite repulsion and, thus, that the problem is accurately described by the Hubbard model alone. Here we pose the question of whether, once the kinetic energy is fixed, a candidate ground state is groundstatable or not. The easiness to answer this question is strongly related to the presence or the absence of a sign problem in the system. When groundstatability is satisfied, it is simple to obtain the potential energy that will lead to such a ground state. As a concrete case study, we apply these ideas to different fermionic wavefunctions with superconductive or spin-density wave correlations.

MM 52.4 Thu 12:15 H5

Ab initio electron correlation calculations for the structural properties of Cadmium — •Beate Paulus[1], Nicola Gaston[2], Dirk Andrae[1], Ulrich Wedig[3], and Martin Jansen[3] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin — [2]Industrial Research Limited, Gracefield Research Centre, PO Box 31-310, Lower Hutt, New Zealand — [3]Max Planck Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart

Cadmium crystallises in the hcp structure, but with an anomalously large c/a ratio, indicating a strong distortion away from ideal packing. Coupled cluster calculations within the framework of the method of increments with an embedding scheme for metals were performed to explore the potential energy surface of cadmium with respect to the hexagonal lattice parameters [1]. This potential energy surface is compared to density functional theory based surfaces, as calculated with various functionals. The overall behaviour of the method of increments for cadmium is consistent with previous results for zinc [2], emphasising the dominant role of electronic correlation in achieving a sufficiently accurate description of bonding properties for the two elements; however, a detailed analysis shows differences.

(1) N. Gaston, D. Andrae, B. Paulus, U. Wedig, and M. Jansen, Phys. Chem. Chem. Phys., 2010, DOI: 10.1039/b915967c

[2] N. Gaston, B. Paulus, U. Wedig, and M. Jansen, Phys. Rev. Lett. 100, 226404 (2008).

MM 52.5 Thu 12:30 H5

Efficient and accurate method for calculating properties of random alloys with short-range order — •Oleg Peil[1], Andrei Ruban[2], and Börje Johansson[2] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Department of Materials Science, Royal Institute of Technology, Sweden

We present an efficient and accurate method for calculating properties of alloys with short-range order. The method is based on the Green's function approach in the framework of the exact muffin-tin orbital (EMTO) [1] fomralism. An alloy system is represented by a supercell with short-range order parameters controlled up to high coordination sphere numbers (4-10), and the local Green's function of each atom is calculated exactly within the local interaction zone (LIZ). The key ingredients of the method are locality, which makes it linearly-scaling with the number of atoms in the supercell, and self-consistency of the effective medium, which results in fast convergence of the total energy and density of states with respect to the LIZ size.

To test the performance and accuracy of the developed method, we show by several examples that for ordered alloys it correctly reproduces the density of states and total energy for both the single-site limit (LIZ=1) and ordered limit (LIZ$\rightarrow\infty$). The method is then applied to two systems: Fe_2Si and Fe-rich bcc-FeCr that have a strong dependence of the local magnetic moments and interatomic interactions on the local environment.

[1] L. Vitos, Phys. Rev. B **64**, 014107 (2001)

MM 52.6 Thu 12:45 H5

Fermi surface shrinking and interband coupling in iron-based pnictides — •Luciano Ortenzi[1], Emmanuele Cappelluti[2], Lara Benfatto[4,3,2], and Luciano Pietronero[3,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]SMC Research Center, CNR-INFM, c/o ISC-CNR, via dei Taurini 19, 00185 Rome, Italy — [3]Dipart. di Fisica, Università "La Sapienza", P.le A. Moro 2, 00185 Rome, Italy — [4]Centro Studi e Ricerche "Enrico Fermi", v. Panisperna 89/A, 00184, Rome, Italy

Measurements of Fermi surface with de Haas-van Alphen oscillations in LaFePO showed a shrinking of the Fermi pockets with respect to first-principle LDA calculations, suggesting an energy shift of the hole and electrons bands with respect to LDA. In this talk I will show that these shifts are a natural consequence of the strong particle-hole asymmetry of electronic bands in pnictides, and that they provide an

indirect experimental evidence of a dominant interband scattering in these systems. Recent measurement in 122 systems confirm this picture.