TT 36: Superconductivity: Fe-based Superconductors - Fe(Se,Te), LiFeAs, and other Materials

Time: Wednesday 9:30–13:00 Location: H18

TT 36.1 Wed 9:30 H18

Interplay between lattice and spin degrees of freedom in FeSe superconductors — Vladimir Gnezdilov[1], •Peter Lemmens[2], Yurii Pashkevich[3], Tatiana Shevtsova[3], Alexander Gusev[3], Dirk Wulferding[2], Dmitriy Chareev[4], and Alexander Vasiliev[5] — [1]ILTPE, Kharkov, Ukraine — [2]IPKM, TU-BS, Braunschweig — [3]DonFTI, Donetsk, Ukraine — [4]IEM, RAS, Moscow, Russia — [5]Moscow State Univ., Moscow, Russia

Recently grown high quality FeSe single crystals show pronounced anomalies in the temperature dependent Raman spectra. An anomalous hardening of one phonon mode upon decreasing temperature is related to local fluctuations of the Fe orbital occupation, described by the Fe spin state. The enhancement of the low-frequency spectral weight above the structural phase transition temperature T_S and its change below T_S is discussed in connection with the opening of a spin state gap which results in the absence of magnetic order in FeSe. Work supported by DFG, B-IGSM and NTH School for Contacts in Nanosystems.

TT 36.2 Wed 9:45 H18

Phonon driven phase transition in FeSe — •Michael Fechner and Nicola Spaldin — ETH Zurich, Department for Material Theory,CH-8093 Zurich, Switzerland

One of the chemically simplest, but physically complex, iron based superconductors is FeSe. Here we present results from first-principle calculations of its competing magnetic phases. In particular we compare calculated electronic properties of coherent FeSe films under different tensile strains, corresponding to $SrTiO_3$ and MgO substrates, and electron/hole doping with experimental findings. The main result is that for moderate applied strain the spin density wave (SDW) in FeSe is suppressed, whereas there is a sudden strong enhancement for larger strain. Given that superconductivity disappears in highly strained FeSe on MgO, our results thus give an interesting insight in which energy ranges the SDW still compete with superconductivity. The results are finally discussed with respect to the possibility of phonon driven superconductivity in FeSe.

TT 36.3 Wed 10:00 H18

Preparation and characterization of thin films of the superconductor FeSe — Eike Venzmer[1], •Alexander Kronenberg[1], Sebastian ten Haaf[1], Janek Maletz[2], and Martin Jourdan[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, 55128 Mainz, Germany — [2]IFW-Dresden, Institute for Solid State Research, PO Box 270116, D-01171 Dresden, Germany

The recently discovered class of iron pnictide compounds features a presumably unconventional mechanism of superconductivity. We investigate the iron chalcogenide FeSe, which is the structurally simplest representative of this class of materials. Epitaxial thin films are prepared by rf-sputtering from a stoichiometric FeSe target and alternatively by co-sputtering from separate Fe and Se targets. Both methods yield superconducting epitaxial thin films on MgO(100) as well as on $YAlO_3$(010) substrates. The influence of deposition rates and substrate temperature on phase formation, sample homogeneity, morphology and electronic transport properties are discussed. A comparison with the properties of previously prepared by MBE [1] will be presented. The main advantage of the sputter deposited samples is an improved morphology which is promising for the future integration in planar tunneling junctions for spectroscopic investigations.

[1] M. Jourdan, S. ten Haaf, J. Appl. Phys. 108, 023913 (2010)

TT 36.4 Wed 10:15 H18

Terahertz spectroscopy on $Rb_{1-x}Fe_{2-y}Se_2$ — •Zhe Wang, Jonas Fisher, Michael Schmidt, Vladimir Tsurkan, Alois Loidl, and Joachim Deisenhofer — Experimentalphysics V, EKM, Institute of Physics, University of Augsburg, Germany

Single crystals of superconducting and non-superconducting $Rb_{1-x}Fe_{2-y}Se_2$ [1] have been investigated by terahertz time-domain transmission spectroscopy as a function of temperature. In the superconducting samples, we observe the signatures of the superconducting transition [2] and an isosbestic point in the temperature dependence of optical conductivity in the vicinity of 100 K, which could be related to the reported phase separation in these compounds. In the non-superconducting samples, the optical conductivity exhibits features which can be interpreted in terms of spin wave excitations in agreement with neutron experiments [3].

[1] V. Tsurkan et al. Phys. Rev. B 84, 144520 (2011)
[2] A. Charnukha et al. Phys. Rev. B 85, 100504 (2012)
[3] M. Wang et al. Nature Communications 2, 580 (2011)

TT 36.5 Wed 10:30 H18

Terahertz spectroscopy of superconducting Fe(Se,Te) — •G. Chanda[1], A. V. Pronin[1], J. Wosnitza[1], S. Molatta[2], R. Hühne[2], B. Holzapfel[2], and K. Iida[2] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]IFW Dresden, Institute of Metallic Materials , 01171 Dresden, Germany

Among the iron-based superconductors, Fe(Se,Te) has received special attention due to its simple crystal structure, which is formed by Fe(Se,Te) layers only. Studies of the optical conductivity at terahertz and far-infrared frequencies may bring information about the superconducting energy gap size and symmetry. Here, we present a terahertz investigation of superconducting Fe(Se,Te) thin films at temperatures from 2 to 300 K. The measurements have been performed with a backward-wave-oscillator spectrometer, which allows phase-sensitive measurements of transmission at terahertz frequencies. Thus, both components of the complex dynamical conductivity can be directly obtained from these measurements. In this talk, we will discuss the frequency and temperature dependence of complex conductivity in Fe(Se,Te).

TT 36.6 Wed 10:45 H18

Incommensurate magnetism and structural phase transition in $Fe_{1+y}Te$ — •Oliver Stockert[1], Sahana Rössler[1], Enrico Faulhaber[2], Astrid Schneidewind[2], Cevriye Koz[1], Dona Cherian[3], Suja Elizabeth[3], Ulrich Schwarz[1], and Steffen Wirth[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany — [2]Gemeinsame Forschergruppe, Helmholtz-Zentrum Berlin - TU Dresden, Lichtenbergstraße 1, 85474 Garching — [3]Department of Physics, Indian Institute of Science, Bangalore 560012, India

The superconductivity with transiton temperature $T_c = 8$ K found in $Fe_{1.01}Se$ ignited interest due to its simple crystal structure. The bulk $Fe_{1+y}Te$ is non-superconducting, but exhibits an antiferromagnetic order that is not driven by the Fermi suface nesting and relatively large ordered moment on the Fe-sublattices. $Fe_{1+y}Te$ also undergoes a structural distortion at low temperatures, and both magnetic and structral transitions can be strongly influenced by tunig parameters such as excess Fe (y) or external pressure [1, 2]. The themodynamic measurements revealed a single first-order transition for $Fe_{1.11}Te$, whereas two distinct phase transitions have been found for $Fe_{1.13}Te$. Here we present the results of neutron diffraction experiments on single crystalline $Fe_{1.11}Te$ and $Fe_{1.13}Te$ samples and show that $Fe_{1+y}Te$ display unique interplay of incommensurate magnetism and structural phase transition in comparison to the other parent Fe-superconductors.

[1] S. Rößler et al., Phys. Rev. B 84, 174506 (2011)
[2] C. Koz et al., Phys. Rev. B 86, 094505 (2012)

15 min. break

TT 36.7 Wed 11:15 H18

Structural phase transitions in the vicinity of putative tricritical point in $Fe_{1+y}Te$ — Cevriye Koz, •Sahana Rössler, Alexander A. Tsirlin, Steffen Wirth, and Ulrich Schwarz — Max Planck Institute for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany

$Fe_{1+y}Te$, the parent compound to the chalcogenide superconductors displays a complex phase diagram with several structural and magnetic phase transitions within the homogeneity range $0.06 \leq y \leq 0.15$. The control parameters such as external pressure and excess Fe content (y) have similar influence on the phase transitions [1, 2]. Upon increasing y, the first-order transition temperature systematically decreases from 70 K to 58 K. For y $\geq$ 0.12, two transitions occur: first a continuous magnetic transition followed by a first-order structural

transition at a lower temperature. This behavior suggests the presence of a tricritical point close to this composition. We present low-temperature synchrotron powder x-ray diffraction studies on $Fe_{1+y}Te$ in the vicinity of this putative tricritical point. From a careful analysis of the powder diffraction patterns and the temperature dependence of the peak-width, we conclude that for y $\geq$ 0.12 the phase transitions are sluggish due to a strong competition between different phases. We present a revised temperature-composition phase diagram for $Fe_{1+y}Te$ based on the temperature dependence of the crystal structure, specific heat, and magnetization measurements.

[1] Rößler *et al*. Phys. Rev. B, 84, 174506 (2011)
[2] Koz *et al*. Phys. Rev. B, 86, 094505 (2012)

TT 36.8 Wed 11:30 H18

Mössbauer and muon spin rotation investigations of magnetic and structural phase transitions in $Fe_{1+y}Te$ — •Philipp Materne[1], Til Goltz[1], Sirko Bubel[1], Rajib Sarkar[1], Mathias Doerr[1], Cevriye Koz[2], Sahana Rössler[2], Steffen Wirth[2], Ulrich Schwarz[2], Ulrich K. Rössler[3], Hubertus Luetkens[4], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, TU Dresden, 01062 Dresden, Germany — [2]MPI for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany — [3]IFW Dresden, 01171 Dresden, Germany — [4]PSI, 5232 Villigen, Switzerland

$Fe_{1+y}Te$, the antiferromagnetic parent compound of the Fe-chalcogenide superconductors displays separated magnetic (T_N) and structural (T_s) transitions with $T_N > T_s$ for $y > 0.12$ [1]. Such behavior is uncommon for the parent systems of pnictide superconductors. We performed Mössbauer spectroscopy and muon-spin relaxation experiments on two representative levels of iron excess: i) $Fe_{1.06}Te$ with $T_N = T_s = 69$ K and ii) $Fe_{1.13}Te$ with well separated transitions at $T_N = 57$ K followed by $T_s = 46$ K. Both Mössbauer and muon-spin relaxation results clearly display a precursor magnetic state which is only present in $Fe_{1.13}Te$. Further, in $Fe_{1.13}Te$ a complex magnetic phase has been observed in the temperature range 40 K $\lesssim T \lesssim$ 75 K. We discuss our experimental results in the context of recently published thermodynamic and neutron scattering data on $Fe_{1+y}Te$[1], [2].

[1] S. Rößler et al., Phys. Rev. B **84** (2011) 174506
[2] E. E. Rodriguez et al., Phys. Rev. B. **84** (2011) 064403

TT 36.9 Wed 11:45 H18

Iron Chalcogenides: Correlated Materials far from Mott — •Markus Aichhorn[1], Gianluca Giovannetti[2], Massimo Capone[2], and Christoph Heil[1] — [1]Institut für theoretische Physik - Computational Physics, TU Graz, Austria — [2]SISSA, Trieste, Italy

Combining density-functional theory and dynamical mean-field theory we investigate the ground-state of iron-chalcogenide materials, focusing on the materials KFe_2Se_2 and $K_2Fe_4Se_5$. We show that, although having large substantial mass enhancements and scattering rates, these materials are not close to a Mott Metal-To-Insulator transition. However, increasing interaction parameters in a physically reasonable range does lead to enhanced orbital differentiation. From RPA susceptibility calculations we get further evidence that also superconducting pairing is mediated by local spin-fluctuations, and not by Fermi-nesting mechanisms.

TT 36.10 Wed 12:00 H18

Resolving the quasiparticle scattering paradox in superconducting LiFeAs — •Christian Hess[1], Steffen Sykora[1], Torben Hänke[1], Ronny Schlegel[1], Danny Baumann[1], Volodymyr Zabolotnyy[1], Luminita Harnagea[1], Sabine Wurmehl[1], Jeroen van den Brink[1,2], and Bernd Büchner[1,2] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Department of Physics, TU Dresden, D-01069 Dresden, Germany

Several angle resolved photoemission spectroscopy (ARPES) studies reveal a poorly nested Fermi surface of LiFeAs, far away from a spin density wave instability, and clear-cut superconducting gap anisotropies. On the other hand a very different, more nested Fermi surface and dissimilar gap anisotropies have been obtained from quasiparticle interference (QPI) data, which were interpreted as arising from intraband scattering within hole-like bands. Here we show that this ARPES-QPI paradox is completely resolved by interband scattering between the hole-like bands. The resolution follows from an excellent agreement between experimental quasiparticle scattering data and T-matrix QPI calculations (based on experimental band structure data), which allows disentangling interband and intraband scattering processes.

TT 36.11 Wed 12:15 H18

The electronic phase diagram for $Na_{1-\delta}FeAs$ with partial substitution of Co, Rh, Ni, Ru, Pd, Cr and Mn — •Robert Beck[1], Maria Roslova[2], Igor Morozov[2], Saicharan Aswartham[1], Christian G. F. Blum[1], Mahmoud Abdel-Hafiez[1], Dirk Bombor[1], Frank Steckel[1], Jürgen Eckert[1], Anja U. B. Wolter-Giraud[1], Christian Hess[1], Sabine Wurmehl[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, D-01171 Dresden, Germany — [2]Moscow State University, Moscow, 119991 Russia

Single-crystals of $Na_{1-\delta}FeAs$ with partial substitution of Fe by Co, Rh, Ni, Ru, Pd, Cr and Mn were grown by a self-flux technique. A systematic investigation of the structure by powder X-ray diffraction, temperature dependence of magnetic susceptibility, electronic transport and specific heat were carried out. We map out the corresponding electronic phase diagram for the Co substituted $Na_{1-\delta}FeAs$, compared with Literature [1, 2] and map out the corresponding electronic phase diagram for the Rh substituted $Na_{1-\delta}FeAs$.

[1] Parker, D. R. et al., Chem. Commun. 16, 2189 (2009)
[2] Wang, A.F. et al., Phys. Rev. B 85, 224521 (2012)

TT 36.12 Wed 12:30 H18

Superconducting thin films of As-free pnictide $LaPd_{1-x}Sb_2$ grown by reactive molecular beam epitaxy — •Reiner Retzlaff, Alexander Buckow, Jose Kurian, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

We use reactive molecular beam epitaxy as synthesis technique for the search of arsenic free pnictide superconductors. Epitaxial thin films of $LaPd_{1-x}Sb_2$ were grown on (100) MgO substrates from elemental sources by simultaneous evaporation of high purity La, Pd and Sb metals by e-gun. $LaPd_{1-x}Sb_2$ belongs to a *novel class* of pnictide superconductors with a peculiar *pnictide square net layer* [1]. Previously, we have reported epitaxial growth of isostructural Bi based compounds [2]. The substitution of Bi by Sb leads to thin films with metallic behavior and room temperature resistivity of about 85 $\mu\Omega$cm. The highest observed transition temperature T_c in$LaPd_{1-x}Sb_2$ is 3.1 K and does not depend on x. We discuss strategies to increase T_c in this pnictide subfamily.

[1] H. Mizoguchi *et al.*, Phys. Rev. Lett. **106**, 057002 (2011)
[2] A. Buckow *et al.*, Appl. Phys. Lett. **101**, 162602 (2012).

TT 36.13 Wed 12:45 H18

Local Mn character and P-derived ligand-hole states in LaMnPO — •Nils Hollmann[1], Anna Efimenko[1], Zhiwei Hu[1], Maurits Haverkort[2], Jack Simonson[3], Hong-Ji Lin[4], Chien-Te Chen[4], Zhiping Yin[5], Meigan Aronson[3], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada — [3]Department of Physics and Astronomy, Stony Brook University, Stony Brook, USA — [4]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [5]Department of Physics and Astronomy, Rutgers, USA

We have investigated the electronic structure of LaMnPO by means of x-ray absorption and photoelectron spectroscopy, as well as LDA+U bandstructure calculations. From the spectroscopy, we found that the Mn ions have local moments and we also observed the strong presence of P-derived ligand hole states. Using LDA+U, we investigate how pressure can first make the system metallic while retaining local moments before entering a metallic state with weak delocalized moments. We also investigate theoretically how electron doping can quench the magnetism as to perhaps facilitate superconductivity like it is present in the Fe compounds.