TT 23: Superconductivity: Fe-based Superconductors - Fe(Se/Te)

Time: Wednesday 9:30–11:15

TT 23.1 Wed 9:30 H 2053

Separation of iron spin states in chalcogenide superconductors — VLADIMIR GNEZDILOV¹, •PETER LEMMENS², YURII PASHKEVICH³, ALEXANDER GUSEV³, TATIANA SHEVTSOVA³, KARINA LAMONOVA³, DIRK WULFERDING², EKATERINA POMJAKUSHINA⁴, and KAZIMIERZ CONDER⁴ — ¹ILTPE NAS, Ukraine — ²IPKM, TU-BS, Braunschweig, Germany — ³DonFTI, Donetsk, Ukraine — ⁴PSI, Villigen, Switzerland

We present a Raman study of superconducting single crystals $M_{1-x}Fe_{2-y}Se_2$ (M = Rb, Cs). Our data together with ab-initio spinpolarized band structure and phonon calculations show the presence of two phases: an insulating vacancy ordered Rb₂Fe₄Se₅ phase and a metallic phase with iron in a low spin state. At high frequencies we observe electronic d-d interband transitions, indicating the insulating state. Our results show that iron is in close proximity to a spin state instability. Work supported by DFG and Rus-Ukr.

TT 23.2 Wed 9:45 H 2053

Phase separation in superconducting and antiferromagnetic $Rb_{0.8}Fe_{1.6}Se_{2.0}$ probed by Mössbauer spectroscopy — •VADIM KSENOFONTOV¹, GERHARD WORTMANN², SERGEY A. MEDVEDEV^{1,3}, VLADIMIR TSURKAN^{4,5}, JOACHIM DEISENHOFER⁴, ALOIS LOIDL⁴, and CLAUDIA FELSER¹ — ¹Institut für Anorganische und Analytische Chemie, Johannes Gutenberg-Universität, D-55099 Mainz, Germany — ²Department Physik, Universität Paderborn, D-33095 Paderborn, Germany — ³Max-Planck Institute for Chemistry, D-55128 Mainz, Germany — ⁴Experimental Physics V, University of Augsburg, D-86159 Augsburg, Germany — ⁵Institute of Applied Physics, Academy of Sciences, MD-2028, Chisinau, Republic of Moldova

⁵⁷Fe Mössbauer studies of superconducting Rb_{0.8}Fe_{1.6}Se_{2.0} with $T_c =$ 32.4 K were performed on single-crystalline and polycrystalline samples in the temperature range 4.2 K to 295 K. They reveal the presence of 88% magnetic and 12% non-magnetic Fe²⁺ species with the same polarization dependence of their hyperfine spectra. The magnetic species are attributed to the 16i sites of the $\sqrt{5} \times \sqrt{5} \times 1$ superstructure and the non-magnetic Fe species to a nano-sized phase observed in recent structural studies of superconducting $K_x Fe_{2-y}Se_2$ systems. The ⁵⁷Fe spectrum of a single-crystalline sample in an external field of 50 kOe applied parallel to the crystallographic c-axis confirms the antiferromagnetic order between the fourfold ferromagnetic Fe(16i) supermoments and the absence of a magnetic moment at the Fe sites in the minority phase. Our study provides convincing evidence about the nano-scale phase separation in Rb_{0.8}Fe_{1.6}Se_{2.0}.

TT 23.3 Wed 10:00 H 2053

Itinerant magnetic excitation in $Rb_{0.8}Fe_{1.6}Se_2 - \bullet G$. FRIEMEL¹, J.T. PARK¹, Y. LI¹, V. TSURKAN², J. DEISENHOFER², H.-A. KRUG VON NIDDA², A. LOIDL², A. INVANOV³, B. KEIMER¹, and D. S. INOSOV¹ - ¹Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany - ²Experimentalphysik V, Center for Electronic Correlations and Magnetism, Institute for Physics, Augsburg Univ., 86135 Augsburg, Germany - ³Institut Laue-Langevin, 6 rue Jules Horowitz, F-38042 Grenoble Cedex 9, France

The recently discovered superconductors $A_x Fe_{2-y}Se_2$ (A=K, Rb, Cs) concurrently exhibit strong magnetism (T $_{\rm N}$ =534 K) and superconductivity (SC) with $T_c = 32$ K. Recent reports relate the magnetic ordering to an insulating phase with a $\sqrt{5} \times \sqrt{5}$ iron vacancy superstructure. Superconductivity, however, seems to originate from a separate phase, which possesses large electron pockets at the M point and no hole pocket at the Γ point, according to ARPES. We present investigations of the magnetic response of this phase by inelastic neutron scattering experiments. We found resonant enhancement of magnetic excitations near $Q = (\pi, 0.5\pi)$ and E = 14 meV and mapped out its Q-dependence in the (HK0)-plane and out of the plane. Our results agree well with published RPA-calculations of the normal state and SC state [1], which peak at the nesting vectors of the Fermi surface seen by ARPES and which suggest a sign changing d-wave SC order parameter for this new family of superconductors. Maier et al., Phys. Rev. B, 83, 100515, (2011).

Location: H 2053

Magneto-structural investigations on $\operatorname{Fe}_{1+x}(\operatorname{Te}_{1-y}\operatorname{Se}_y)$ single crystals — •MATHIAS DOERR¹, WOLFRAM LORENZ¹, DONA CHERIAN², SAHANA RÖSSLER³, STEFFEN WIRTH³, PHILIPP MATERNE¹, and MICHAEL LOEWENHAUPT¹ — ¹Technische Universität Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany — ²Dept. of Physics, Indian Inst. of Science, Bangalore-560012, India. — ³Max-Planck-Institut für Chemische Physik fester Stoffe, D-01187 Dresden, Germany

The class of $\operatorname{Fe}_{1+x}(\operatorname{Te}_{1-y}\operatorname{Se}_y)$ compounds is the counterpart of Fepnictides, special effects as magnetic order or superconductivity are found. A special topic is the interplay of magnetic and lattice properties which is crucial for a number of correlation phenomena. Thermal expansion and isothermal magnetostriction was measured on Fe_{1+x} Te (x = 0, 0.06, 0.13) and compared to other experiments and model concepts. As one fact, it is shown that magnetic order exists independently of lattice distortions, already at higher temperatures than the latter ones. Moreover, strong thermal hysteresis effects occur. This behaviour differs from that of the Fe-pnictides and therefore, microscopic mechanisms (as for example magnetic fluctuations) should stay a matter of particular interest.

TT 23.5 Wed 10:30 H 2053 Superconductivity of $Fe_{1.07}Se_{0.5}Te_{0.5}$ studied by Spectroscopic-Imaging Scanning Tunneling Microscopy — •UDAI RAJ SINGH¹, SETH WHITE¹, STEFAN SCHMAUS¹, JOACHIM DEISENHOFER², VLADIMIR TSURKAN², ALOIS LOIDL², and PETER WAHL¹ — ¹Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — ²Lehrstuhl für Experimentalphysik V, Universität Augsburg, Augsburg, Germany

The unconventional superconductivity in the recently discovered ironbased superconductors has become an active field of research [1]. We study the electronic structure of $Fe_{1.07}Se_{0.5}Te_{0.5}$ ($T_c \sim 15$ K) by spectroscopic-imaging scanning tunneling microscopy (SI-STM). SI-STM has been shown to be an important tool to investigate the electronic inhomogeneities and electronic structure in high temperature superconductors [2]. The iron chalcogenide superconductor $Fe_{1.07}Se_{0.5}Te_{0.5}$ provides a well defined cleavage plane, making it an ideal candidate for STM investigation. We find the superconducting gap consistent with earlier studies [3]. We show in our study the temperature dependence of the superconducting gap. We observe significant nanoscale inhomogeneity of the superconducting gap.

Y. Kamihara, et al., J. Am. Chem. Soc. 128, 10012 (2006) and Y. Kamihara, et al., J. Am. Chem. Soc. 130, 3296 (2008).

[2] J. E. Hoffman, et al., Science 297, 1148 (2002); K. McElroy, et al., Nature 422, 592 (2003).

[3] T. Hanaguri, et al., Science 328, 474 (2010).

TT 23.6 Wed 10:45 H 2053 Lattice dynamics of FeTe: a combined DFT and inelastic neutron scattering study — •ROLF HEID, KLAUS-PETER BOHNEN, SVEN KRANNICH, LOTHAR PINTSCHOVIUS, and FRANK WEBER — Karlsruher Institut für Technologie, Institut für Festkörperphysik

For all pnictide families DFT calculations of lattice dynamical properties predict a high sensitivity on structural and magnetic degrees of freedom. Comparison with experiment thus can provide valuable information about the appropriate theoretical model. For the 1111 and 122 families, however, DFT significantly overestimates the size of the ordered magnetic moment which potentially hampers such a comparison. In contrast, the Fe chalcogenide family represents a much better test case, as both theory and experiment agree on the existence of large ordered moments.

Here we present results of a combined DFT and inelastic neutron scattering study of the phonon dispersion of FeTe. Large parts of the dispersion curves were mapped out at low temperature and compared with DFT results for nonmagnetic and antiferromagnetic phases using various lattice structures. A satisfactory description of the data is obtained only when the Fe-Te distance of the magnetic calculation is used. The spin-polarization itself, however, is found to be of minor importance.

 $TT~23.7 \quad Wed~11:00 \quad H~2053 \\ \textbf{Paramagnons in FeSe close to Magnetic Phase Transition}$

TT 23.4 Wed 10:15 H 2053

— •Leonid Sandratskii, Frank Essenberger, Pawel Buczek, Arthur Ernst, and Eberhard Gross — Max-Planck-Institut für Mikrostrukturphysik, Halle

The magnetic excitations in FeSe are studied from first principles applying linear response density functional theory. The position of the selenide layer is varied to model the transition between paramagnetic and antiferromagnetic phases. In the paramagnetic phase, close to the point of magnetic instability we find a branch of long lived collective spin excitations, paramagnons. The phase transition to the AFM phase changes the character of the spin excitations drastically.