TT 39: SC: Iron-Based Superconductors - 1111

Time: Friday 10:15–12:45 Location: H19

TT 39.1 Fri 10:15 H19

Insight, puzzles, and problems into the physics of Fe-pnictides from optics — •S.-L. Drechsler[1], H. Rosner[2], R. Schuster[1], F. Roth[1], M. Grobosch[1], M. Rotter[3], K. Koepernik[1], D. Singh[4], L. Zhang[4], D. Jorendt[3], N. Wizent[2], G. Behr[1], J. van den Brink[1], N.L. Wang[5], B. Buechner[1], and M. Knupfer[1] — [1]Inst. f. Festkörper- & Werkstoffforsch., Dresden — [2]Max-Planck-Inst. f. Chem. Physik fester Stoffe, Dresden — [3]Department Chemie & Biochemie, Ludwig-Maximillians Universität München, München — [4]Oak Ridge Nat. Lab., Oak Ridge, Tennessee, USA — [5]Beijing Nat. Lab., f. Cond. Mat. Phys. Inst. of Phys., Chin. Acad. of Sci., Beijing, China

We report Drude plasma frequencies (PF) for 12 Fe-pnictides from density functional theory (DFT) based calculations and compare them with experimental PF from reflectivity. The observed renormalization points to moderate many-body effects beyond the DFT like in ordinary transition metals. From large empirical background dielectric constants $\varepsilon_\infty \sim 10$, we estimate strong As and P polarizabilities which significantly reduce the Hubbard U_d from about 4 eV as suggested by significantly correlated [1] "bad metal" scenarios to below 2 eV pointing to rather strong polaronic effects [2]. We compare the dielectric and loss functions calculated within the RPA employing the DFT band structure for the parent compounds LaOFeAs and LaOFeP with single crystal derived data [1] and determine the frequency region with the strongest many-body effects beyond the RPA.

[1] M.M. Qazilbash *et al. Nature Phys.* **5**, (2009) 647.
[2] G. Sawatzky *et al. Europhys. Lett.* **86** (2009) 17006.

TT 39.2 Fri 10:30 H19

Nature of Magnetism in Iron Pnictides: an *ab initio* study — •Yu-Zhong Zhang, Ingo Opahle, Harald Jeschke, and Roser Valenti — Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

While it is commonly believed that magnetic-mediate pairing is the source of superconductivity in the iron-based superconductors, the nature of magnetism is still under debate. We apply *ab initio* molecular dynamics to investigate physical properties of LaOFePn, $BaFe_2Pn_2$ and LiFePn (Pn = As, Sb), so-called 1111, 122 and 111 compounds, respectively. We find that, with substitution of As by Sb, the stripe-type antiferromagnetic orderings are always enhanced. By calculating Pauli susceptibility, we attribute the enhancement of magnetization to the increase of instability at (π, π) when As is substituted by Sb. Furthermore, we study the magnetic and lattice properties of LaOFePn (Pn=P, As, Sb, Bi) as well as ScOFeP, ScOFeAs and YOFeP and argue that LaOFeSb would be a candidate for a superconductor with highest transition temperature among the investigated compounds. We further suggest that the absence of antiferromagnetic phase in LaOFeP and the presence in LaOFeAs are due to the competition of instability in Pauli susceptibility between (π, π) and $(0, 0)$ and therefore argue that superconductivity can only occur through doping in LaOFeSb.

TT 39.3 Fri 10:45 H19

Effect of doping and pressure on the high-T_c superconductor YOFeAs – comparison with LaOFeAs — •Ingo Opahle[1], Yu-Zhong Zhang[1], Hem C. Kandpal[2], Harald O. Jeschke[1], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Universität Frankfurt, 60438 Frankfurt/Main, Germany — [2]IFW Dresden, P.O.B. 270016, D-01171 Dresden, Germany

The electronic structure of the high-T_c superconductor YOFeAs is calculated in the framework of density functional theory. Undoped YOFeAs is found to show the same spin density wave (SDW) instability as previously reported for LaOFeAs. The calculated Fe moment at ambient pressure is slightly smaller in YOFeAs than in LaOFeAs, but remains nonzero up to higher pressures compared to LaOFeAs. The Fermi surface shows similar strong nesting features like the one of LaOFeAs, stabilizing the spin density wave state. The effect of doping on the SDW state and implications for the superconductivity will be discussed.

TT 39.4 Fri 11:00 H19

High field ESR spectroscopy on (Gd,La)OFeAs superconductors — •A. Alfonsov[1], F. Murányi[2], V. Kataev[1], N. Leps[1], R. Klingeler[1], A. Kondrat[1], C. Hess[1], S. Wurmehl[1], J. Werner[1], G. Behr[1], and B. Büchner[1] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Universität Zürich, CH-8057 Zürich, Schweiz

In the present work we have studied polycrystalline samples of the $(Gd,La)O_{1-x}F_xFeAs$ superconductor with different levels of fluorine and gadolinium doping by means of high field/high frequency electron spin resonance (HF-ESR) spectroscopy. The Gd ESR signal is found to be sensitive to the magnetic phase transition from the paramagnetic to the spin density wave (SDW) state occurring in the parent (Gd,La)OFeAs compounds at temperatures $T_{SDW} \sim 130 - 150$K. In addition, in case of $LaO_{1-x}F_xFeAs$ with 5% Gd doping there is a clear indication of the suppression of the magnetic order in the samples with the superconducting ground state. The GdOFeAs samples reveal an antiferromagnetic coupling between Gd and Fe planes which reflects in the splitting and shift of Gd ESR line below $T_{SDW} \sim 130$K. Surprisingly, the 15% and 17% fluorine doped GdOFeAs samples, with T_c=20K and T_c=45K respectively, show the low-T ESR response similar to the undoped sample which indicates that the SDW is not completely suppressed in the SC samples. We compare HF-ESR data with results of transport measurements on these samples and discuss a possible contribution of magnetic rare-earths to the interplay between magnetism of the FeAs planes and superconductivity which evolves upon the fluorine doping.

15 min. break

TT 39.5 Fri 11:30 H19

Structural transition and magnetic ordering in $(Sm,Ce)FeAsO_{(1-x)}F_x$ — •Jorge E. Hamann-Borrero[1], Agnieszka Kondrat[1], Hemke Maeter[2], Ralf Feyerherm[3], Hans-Henning Klauss[2], Ruediger Klingeler[1], Christian Hess[1], Guenther Behr[1], Dimitri Argyriou[3], and Bernd Buechner[1] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany — [2]Institut fuer Festkoerperphysik, TU Dresden, D-01069 Dresden, Germany — [3]Helmholtz Zentrum Berlin. Albert Einstein Str.15 12489 Berlin

The tetragonal to orthorhombic transition of the layered compounds $(Sm, Ce)FeAsO_{(1-x)}F_x$ is studied by means of synchrotron x-ray diffraction, μSR and resistivity. We particularly focus on the onset of the SDW and superconducting states by monitoring the structural transition temperature T_s the magnetic ordering temperature T_N and the critical temperature T_c. In the case of $SmFeAsO_{(1-x)}F_x$ the SDW state is only gradually suppressed upon doping until it is entirely suppressed in favour of the superconducting state. This is in contrast to $CeFeAsO_{(1-x)}F_x$ where the SDW state is suppressed much more efficiently and where superconductivity coexists with magnetism. Moreover, in further contrast to the findings by Zhao et al [1], we do not observe any orthorhombic distortion in superconducting samples.

[1] Zhao et al. Nature Materials, 2008, 7, 953-959.

TT 39.6 Fri 11:45 H19

Interplay of rare earth and FeAs magnetism in the iron pnictides GdOFeAs and CeOFeAs studied by muon spin relaxation and ^{57}Fe moessbauer spectroscopy — •N. Yèche[1], H.-H. Klauss[1], T. Dellmann[1], H. Luetkens[2], R. Khasanov[2], A. Amato[2], R. Klingeler[3], B. Büchner[3], and G. Behr[3] — [1]Institut für Festkörperphysik, TU Dresden — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden

*R*OFeAs with *R* = La, Ce, Pr, Sm, Gd are the magnetic mother compounds of the iron pnictide superconductors. We have investigated the magnetic properties and the interplay of iron and rare earth magnetic order in GdOFeAs by means of muon spin relaxation (μ^+SR) and ^{57}Fe moessbauer spectroscopy and compare these to other undoped *R*OFeAs. We find that the Gd mother compound shows magnetic interaction between the rare earth and the FeAs layers similar to the Ce compound as allready reported in [1]. This results indicate that the rare-earth-FeAs electronic interaction is not crutial for the enhanced T_C in these systems.

[1] H. Maeter et al., Phys.Rev.B 80, 094524 (2009)

TT 39.7 Fri 12:00 H19

Anomalous Nernst Effect and spin fluctuations in

$LaFeAsO_{1-x}F_x$ — •Christian Hess, Agnieszka Kondrat, Günter Behr, Rüdiger Klingeler, and Bernd Büchner — Institute for Solid State Research, IFW Dresden, Helmoltzstrasse 20, 01069 Dresden

We present Nernst-effect investigations on $LaFeAsO_{1-x}F_x$. In the parent compound the formation of a SDW state leads to a huge enhancement of the Nernst coefficient at $T < T_N$. Despite the absence of SDW order at underdoped superconducting doping levels, a similar anomalous behavior is also observed (with smaller magnitude), which is suggestive of a spin-fluctuation enhanced Nernst-effect. Interestingly, at optimal doping level the Nernst coefficient is only weakly temperature dependent and appears more conventional.

TT 39.8 Fri 12:15 H19

Unusual disorder effects in $LaFeAs_{1-\delta}O_{0.9}F_{0.1}$ as revealed by NMR spectroscopy — •Franziska Hammerath[1], Stefan-Ludwig Drechsler[1], Hans-Joachim Grafe[1], Guillaume Lang[1], Günter Fuchs[1], Günter Behr[1], Ilya Eremin[2], Maxim Korshunov[2,3], and Bernd Büchner[1] — [1]Leibniz-Institut für Festkörper- & Werkstoffforschung, Dresden, Germany — [2]MPI für Physik komplexer Systeme, Dresden — [3]L.V. Kirensky Inst. of Physics, Sib. Branch of Russ. Acad. Scs., Krasnoyarsk, Russia

We report ^{75}As NMR measurements of the spin-lattice relaxation in the superconducting state of $LaFeAsO_{0.9}F_{0.1}$ and As-deficient samples, $LaFeAs_{1-\delta}O_{0.9}F_{0.1}$ with a drastic change of the $1/T_1$ temperature dependence below T_c from a T^3-law for $LaFeAsO_{0.9}F_{0.1}$ to a T^β-law ($\beta = 5-6$) for $LaFeAs_{1-\delta}O_{0.9}F_{0.1}$. T_c and the slope of the upper critical field near T_c increase unexpectedly in the As-deficient samples. Our results are discussed in terms of non-universal SC gaps in Fe-pnictides and the effect of As deficiency as an exotic case when non-magnetic 'smart' impurities even stabilize an $s_\pm$−wave superconductor as well as within a scenario of a disorder driven change to conventional s_{++} superconductivity.

[1] H.-J. Grafe *et al.*, Phys. Rev. Lett. **101**, 047003 (2008).

TT 39.9 Fri 12:30 H19

Superconductivity and Ferromagnetism in $CeFeAs_{1-x}P_xO$ — •Anton Jesche, Cornelius Krellner, and Christoph Geibel — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The emergence of superconductivity in RFeAsO (R = rare earth) is connected with the suppression of the antiferromagnetic (AFM) ordering of Fe which can be achieved by the substitution of e.g. La by Sr, Fe by Co, As by P, and O by F. A special case here is $CeFeAs_{1-x}P_xO$, which shows AFM ordering of Fe at $T_N^{Fe} = 145\,K$ and AFM ordering of Ce at $T_N^{Ce} = 3.7\,K$ for pure CeFeAsO, whereas pure CeFePO is a paramagnetic heavy fermion metal. The substitution of As by P results in a decrease of T_N^{Fe} similar to F doping. An extrapolation suggests a complete suppression of the Fe ordering for $x \simeq 0.35$. However, instead of the 'expected' superconducitivity, the Ce ordering changes from AFM to FM at the disappearance of T_N^{Fe} and superconductivity emerges only in a small concentration range around $x = 0.3$. We report on measurements of electrical resistivity, specific heat, and magnetic susceptibility on single- and polycrystalline samples. Our results are supported by NMR, ESR, and μSR measurements and reveal a competition of superconductivity and ferromagnetic ordering of Ce.