TT 79: Superconductivity: Fe-based Superconductors - 122

Time: Thursday 15:30–18:30 Location: H21

TT 79.1 Thu 15:30 H21

Magnetic Excitations in Na-doped $BaFe_2As_2$ — •Florian Wasser[1], Sabine Wurmehl[2], Saicharan Aswarthem[2], Yvan Sidis[3], Astrid Schneidewind[4,5], Jitae Park[5], Bernd Büchner[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zuKöln, Zülpicher Strasse 77, D-50937 Köln, Germany — [2]Institute for Solid State Research, IFW Dresden,D-01171 Dresden, Germany — [3]Laboratoire LéonBrillouin, CEA-CNRS, CEA Saclay, 91191 Gif-sr-Yvette Cedex,France — [4]Jülich Centre for Neutron Science-JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ,D-85747, Garching, Germany — [5]Forschungsneutronenquelle Heinz Maier-Leibnitz(FRM-II), TU München, D-85747 Garching, Germany

Our neutron scattering study of magnetic excitations in $Ba_{1-x}Na_xFe_2As_2$ show that the presence of static antiferromagnetic (AFM) order dominates the low-energy part of the spectrum even in the superconducting (SC) state. In the coexistence regime i.e. at 35% and 39% Na-doping an additional sharp and intense low-energy resonance mode, centred at ∼4meV, develops below T_c. This low-energy resonance excitation is predominantly polarized along the *c*-direction, which corresponds to a longitudinal alignment due to the spin-reorientation in this material. In the SC phase the elastic AFM signal becomes strongly reduced suggesting that the corresponding spectral weight is shifted to higher energies and in particular to the development of the 4meV-mode. In contrast, at 40% Na-doping static AFM order is absent and the 4meV-mode is fully suppressed.

TT 79.2 Thu 15:45 H21

A light scattering study of detwinned $BaFe_2As_2$ — •Andreas Baum[1,2], Milan Tomić[3], Daniel Jost[1,2], Ali Özkü[1,2], Bernhard Muschler[1], Florian Kretzschmar[1,2], Thomas Böhm[1,2], Nitin Chelwani[1,2], Jiun-Haw Chu[4,5], Ian R. Fisher[4,5], Roser Valentí[3], and Rudi Hackl[1] — [1]Walther-Meissner-Institut, 85748 Garching, Germany — [2]Fakultät für Physik E23, Technische Universität München, 85748 Garching, Germany — [3]Institut für Theoretische Physik, Goethe-Universität Frankfurt — [4]SIMES, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — [5]GLAM and Department of Applied Physics, Stanford, University, Stanford, CA 94305, USA

The magneto-structural phase transition of $BaFe_2As_2$ is studied by Raman spectroscopy with a focus on lattice dynamics. Using uniaxial pressure to detwin the sample allows us to resolve anisotropic features. The As A_{1g} phonon shows a resonance at high energies with distinct differences between the antiferromagnetically and the ferromagnetically ordered direction. The splitting of the E_g phonon at $130\,cm^{-1}$ into two modes having B_{2g} and B_{3g} symmetry can be attributed to the transition into the magnetically ordered state rather than the structural transition. Both effects can be attributed to the emergence of magnetic order by DFT calculations.

TT 79.3 Thu 16:00 H21

Electronic correlations in the hole-doped superconductor $RbFe_2As_2$ probed via ^{75}As NMR — •S. Molatta[1,2,3], Z. Zhang[1], D. Dmytriieva[1], S. Khim[4], S. Wurmehl[2,3,4], H.-J. Grafe[4], B. Büchner[2,3,4], H. Kühne[1], and J. Wosnitza[1,2,3] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]TU Dresden, Germany — [3]DFG GRK-1621 — [4]IFW Dresden, Germany

We will present latest ^{75}As NMR data in the normal state of the stoichiometric superconductor $RbFe_2As_2$. This will be put into context to known results for the heavily hole-doped compound KFe_2As_2. The static and dynamic magnetic correlations were probed via measurements of the Knight shift and nuclear spin-lattice relaxation rate in a wide temperature range from 0.3 to 300 K. Although neither a magnetic nor a structural transition were observed down to lowest temperatures, the very close proximity of the ground state to a magnetic instability is indicated by a pronounced Curie-Weiss-like behavior of spin fluctuations. At around 100 K, we find a maximum of the Knight shift and a changing exponent of the temperature-dependent relaxation rate. This is phenomenologically similar to the case of KFe_2As_2 and was proposed to stem from a incoherence-coherence crossover mechanism of electronic correlations.

TT 79.4 Thu 16:15 H21

Coexistence of superconductivity and magnetism in $Ca_{1-x}Na_xFe_2As_2$: Universal suppression of the magnetic order parameter in 122 iron pnictides — •Philipp Materne[1], Sirko Kamusella[1], Rajib Sarkar[1], Luminita Harnagea[2], Sabine Wurmehl[1,2], Bernd Büchner[1,2], Hubertus Luetkens[3], Carsten Timm[4], and Hans-Henning Klauss[1] — [1]IFP, TU Dresden, 01062 Dresden, Germany — [2]IFW Dresden, Postfach 270016, 01171 Dresden, Germany — [3]PSI, 5232 Villigen, Switzerland — [4]ITP, TU Dresden, 01062 Dresden, Germany

We examined $Ca_{1-x}Na_xFe_2As_2$ single crystals with $x = 0.00$, 0.35, 0.50, and 0.67 by means of muon spin relaxation and Mössbauer spectroscopy to investigate the electronic and structural properties of these compounds. $CaFe_2As_2$ is a semimetal, which shows spin density wave order below 167 K. By hole doping via Ca→Na substitution, the magnetic order is suppressed and superconductivity emerges with $T_c \approx 34$ K at optimal doping including a substitution level region where both phases coexist. We have studied the interplay of order parameters in this coexistence region and found nanoscopic coexistence of both order parameters. This is proven by a reduction of the magnetic order parameter by 7 % below the superconducting transition temperature. We present a systematic correlation between the reduction of the magnetic order parameter and the ratio of the transition temperatures, T_c/T_N, for the 122 family of the iron-based superconductors [1].

[1] Ph. Materne *et al.*, PRB **92**, 134511 (2015)

TT 79.5 Thu 16:30 H21

Reversible tuning of the collapsed tetragonal phase transition in $CaFe_2As_2$ by separate control of chemical pressure and electron doping — •kan zhao and philipp gegenwart — Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Single crystals of $Ca(Fe_{1-x}Ru_x)_2As_2$ ($0 \leq x \leq 0.065$) and $Ca_{1-y}La_y(Fe_{0.973}Ru_{0.027})_2As_2$ ($0 \leq y \leq 0.2$) have been synthesized and studied with respect to their structural, electronic and magnetic properties. The partial substitution of Fe by Ru induces a decrease of the c-axis constant leading for $x \sim 0.023$ to the suppression of the coupled magnetic and structural (tetragonal to orthorhombic) transitions. At $x_{cr} = 0.023$ a first order transition to a collapsed tetragonal (CT) phase is found, which behaves like a Fermi liquid and which is stabilized by further increase of x. The absence of superconductivity near xcr is consistent with truly hydrostatic pressure experiments on undoped $CaFe_2As_2$. Starting in the CT regime at x=0.027 we investigate the additional effect of electron doping by partial replacement of Ca by La. Most remarkably, with increasing y the CT phase transition is destabilized and the system is tuned back into a tetragonal ground state at $y \sim 0.08$. This effect is ascribed to a weakening of interlayer As-As bonds by electron doping. Upon further electron doping filamentary superconductivity with T_c of 41 K at y=0.2 is observed.

TT 79.6 Thu 16:45 H21

Charge dynamics of $BaFe_2(As_{1-x}P_x)_2$: infrared spectroscopy study under pressure — •Ece Uykur[1], Tatsuya Kobayashi[2], Wataru Hirata[2], Shigeki Miyasaka[2], Setsuko Tajima[2], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, D-86195 Augsburg, Germany — [2]Department of Physics, Graduate School of Science, Osaka University, Osaka 560-0043, Japan

Temperature-dependent reflectivity measurements under pressure (up to 5 GPa) have been performed on $BaFe_2(As_{1-x}P_x)_2$ single crystals with $x = 0$ and 0.20 between ∼ 85 - 7000 cm^{-1} down to 6 K. Normal state charge dynamics as well as the low temperature dynamics (magnetically ordered (SDW) state and superconducting (SC) state) under pressure have been investigated. At temperatures above the magnetic phase transition, the metallicity of the system is increasing with pressure. At lower temperatures, with increasing pressure the partial suppression of the SDW state and the appearance of the SC state (at around 3.6 GPa) is observed for the parent compound with $x = 0$. The coexisting of these two states has been clearly demonstrated. The results of this study indicate a possible competing order scenario for these two orders. On the other hand, for the compound with $x = 0.20$, the SDW state has been completely suppressed above 2.5 GPa. The

normal state and the superconducting state in this compound will be discussed in comparison to the parent compound.

15 min. break

TT 79.7 Thu 17:15 H21

Shifted Van Hove singularities (VHS) vs. vicinity to a selective Mott transition in K(Rb,Cs)Fe_2As_2: How strong is the el.-el. interaction? — •Stefan-Ludwig Drechsler[1], Sergey Borisenko[1], Sabine Wurmehl[1], Seunghyun Khim[1], Bernd Buechner[1], Steffen Backes[2], Harald Jeschke[2], Roser Valenti[3], and Helge Rosner[3] — [1]ITF at the Leibniz Institute IFW-Dresden, 01171 Dresden, Germany — [2]Inst. f. Theor. Phys., University of Frankfurt, Germany — [3]MPI-CPfS, Dreden, Germany

We report high precision scalar and full relativistic DFT calculations for the title compounds to get a trustable starting point for the discussion of many-body effects which become visible in the mass enhancement and shifted position of various VHS as observed by ARPES and STM [1]. For KFe_2As_2 we observe a Fe $3d_{xz}$-$3d_{yz}$ VHS shift from $\sim$ 65 meV below the Fermi energy ε_F in the DFT to $\sim$ -14 meV in our ARPES data and a squezing by a factor of 2 pointing to a moderate mass enhancement for this subgroup of electrons. For the $3d_{xy}$ derived band a shift from -300 meV to -50 meV has been detected. The shifted VHS contributes to an enlarged DOS at ε_F explaning in part the large Sommerfeld coefficient γ seen in el. specific heat data. In recent DMFT calculations [2] the VHS related DOS-maxima are even closer to ε_F for an Hubbard interaction $U_d = 4$ eV and Hund's rule coupling. We suggest that the systems under consideration are less strongly correlated as compared to sophisticated selective Mott and Kondo-like scenarios.

[1] D. Fang, *et al.*, PRB **92**, 144513 (2015)
[2] S. Backes, H. Jeschke, and R. Valenti, PRB **92**, 195128 (2015)

TT 79.8 Thu 17:30 H21

Charge doping versus impurity scattering in substitutionally disordered Ba-122 — •Alexander Herbig[1], Rolf Heid[1], and Jörg Schmalian[2,1] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie — [2]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie

The iron-based superconductors are a prominent example how chemical substitution can be used as a tuning parameter for the electronic properties and the superconductivity of a complex material. Until now, first principle calculations addressing disorder effects on the electronic structure via methods beyond supercells are rare. Also the role of doping and the impact of chemical substitution on superconductivity is not fully understood. Based on ealier work [1], we recently implemented Blackman, Esterling and Berk's [2] extension of the coherent potential approximation within a pseudopotential framework using a linear combination of atomic orbitals basis. We present electronic structure calculations for the Ba-122 compound using this method with various species substitutions at different sites and arbitrary impurity concentrations. We focus on disorder effects on electron and hole bands near the Fermi level. We observe non-rigid level shifts and band selective broadenings due to impurity scattering which strongly depend on the substituent species [3]. Our finding of an enhanced intraband compared to interband scattering is in accordance with an s^{+-} paring state.

[1] K. Koepernik et al., PRB **55**, 5729 (1997)
[2] J. A. Blackman et al., PRB **4**, 2412 (1971)
[3] A. Herbig et al., arXiv:1510.06941v1 (2015)

TT 79.9 Thu 17:45 H21

Angle-resolved photoemission spectroscopy calculations on antiferromagnetic $BaFe_2As_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$ based on the one-step model — •Gerald Derondeau[1], Jürgen Braun[1], Ján Minár[1,2], and Hubert Ebert[1] — [1]Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany — [2]NewTechnologies-Research Center, University of West Bohemia, Pilsen, Czech Republic

The Korringa-Kohn-Rostoker-Green function (KKR-GF) method provides a very suitable platform to describe the electronic structure of iron pnictide superconducting compounds with substitutional disorder. [1] Having direct access to the Green function allows in a rather straightforward manner to perform calculations on angle-resolved photoemission spectroscopy (ARPES). This can be done on the basis of the one-step model of photoemission leading to results that can be directly compared to experimental ARPES data, unveiling significantly more information than pure band structure calculations. Corresponding ARPES calculations have been done with a focus on the strong in-plane anisotropy in antiferromagnetic $BaFe_2As_2$ and its evolution under Co substitution in $Ba(Fe_{1-x}Co_x)_2As_2$. The resulting ARPES spectra are discussed in comparison with experimental ARPES data measured on detwinned crystals. [2] In particular it is demonstrated that the variation of the electronic structure with Co substitution as monitored by ARPES is well reproduced by theory.

[1] G. Derondeau *et al.*, Phys. Rev. B **90**, 184509 (2014).
[2] M. Yi *et al.*, PNAS **108**, 6878 (2011).

TT 79.10 Thu 18:00 H21

High field properties of superconducting $BaFe_{2-x}Ni_xAs_2$ thin films — •Stefan Richter[1,2], Fritz Kurth[1], Kazumasa Iida[3], Vadim Grinenko[1], Kirill Pervakov[4], Chiara Tarantini[5], Jan Jaroszynski[5], Aurimas Pukenas[2], Werner Skrotzki[2], Kornelius Nielsch[1], and Ruben Hühne[1] — [1]Institute for Metallic Materials IFW Dresden — [2]Technical University Dresden — [3]Nagoya University, Japan — [4]Russian Academy of Sciences, Russia — [5]National High Magnetic Field Laboratory, USA

Fe based superconductors combine the advantages of cuprates (high upper critical field) with the small Hc_2 anisotropy of classic low temperature superconductors, which makes them suitable candidates for high field applications. The study of Fe-based superconducting thin films is one crucial step to explore this potential in more detail.

We present results for epitaxial $BaFe_{2-x}Ni_xAs_2$ thin films, which have been successfully grown for the first time using pulsed laser deposition. Superconducting transition temperatures of up to 19 K have been realized in slightly overdoped films, which is in good agreement with results obtained for single crystals. The behavior of the upper critical field and critical current density has been measured in high magnetic fields up to 35 T. The results will be correlated to the observed microstructure and compared to high field data for single crystals with similar composition.

Funding of this work by DFG GRK 1621 is gratefully acknowledged.

TT 79.11 Thu 18:15 H21

Electrical transport properties of the unconventional superconductor YFe_2Ge_2 — •Konstantin Semeniuk[1], Jiasheng Chen[1], Zhuo Feng[2], Philip Brown[1], Yang Zou[1], Giulio Lampronti[3], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge UK — [2]London Centre of Nanotechnology, University College London, London UK — [3]Dept. of Earth Sciences, University of Cambridge, Cambridge UK

YFe_2Ge_2 is a paramagnetic d-electron system which stands out due to its high Sommerfeld ratio of its specific heat capacity of 100 mJ/(mol K^2) and non Fermi-liquid $T^{3/2}$ power law temperature dependence of the electrical resistivity. The material was found to be superconducting below about 1.8 K [1].

Advances in YFe_2Ge_2 crystal growth allowed us to obtain high quality samples with residual resistivity ratios of the order of 200. Recent measurements of magnetisation and heat capacity provide further evidence for superconductivity, and the correlation between the transition temperature and the sample quality, the enhanced Sommerfeld coefficient and the anomalous T-dependence of the resistivity indicate that superconductivity in YFe_2Ge_2 is unconventional [2]. We report the results of detailed electrical resistivity measurements on YFe_2Ge_2 as a function of temperature, magnetic field and hydrostatic pressure, which provide further insight into the nature of superconducting and normal states of the material.

[1] Y. Zou et al., Physica Status Solidi (RRL) **8**, 928 (2014).
[2] J. Chen et al., arXiv:1507.01436v2.