Location: HSZ 304

# TT 36: SC: Fe-based Superconductors - 122 - Properties, Electronic Structure, Mechanisms

Time: Wednesday 14:00–18:30

TT 36.1 Wed 14:00 HSZ 304

High-resolution thermal expansion of  $Ba(Fe_{1-x}Co_x)_2As_2$ : evidence for quantum criticality — •CHRISTOPH MEINGAST<sup>1</sup>, FREDERIC HARDY<sup>1</sup>, PHILIPP BURGER<sup>1,2</sup>, DEVANG JOSHI<sup>1</sup>, PE-TER ADELMANN<sup>1</sup>, DORIS ERNST<sup>1</sup>, RAINER FROMKNECHT<sup>1</sup>, PETER SCHWEISS<sup>1</sup>, ROLF HEID<sup>1</sup>, and THOMAS WOLF<sup>1</sup> — <sup>1</sup>Karlsruhe Institute of Technology, Institute for Solid State Physics, 76021 Karlsruhe, Germany — <sup>2</sup>Karlsruhe Institute of Technology, Fakultät für Physik, 76128 Karlsruhe, Germany

Unconventional superconductivity is often found in the vicinity of a doping- or pressure-induced magnetic instability, or quantum phase transition (QPT). For a pressure-induced QPT, the Grüneisen parameter is expected to diverge as temperature approaches zero and is thus a very sensitive parameter for detecting a QPT. Experimentally, the Grüneisen parameter can be determined by the ratio of the thermal expansivity to the specific heat. Here we report on high-resolution thermal expansion and specific heat measurements of  $Ba(Fe_{1-x}Co_x)_2As_2$  single crystals as a function of doping. We show that the electronic Grüneisen parameter exhibits all the features expected at a QPT: 1) non-Fermi-liquid behavior, 2) sign change of the Grüneisen parameters at the beginning and end points of the superconducting dome.

TT 36.2 Wed 14:15 HSZ 304 Thermodynamic investigations of the doping and pressure dependences of the electronic density of states and the superconducting gaps in the electron-doped iron pnictide  $Ba(Fe_{1-x}Co_x)_2As_2 - \bullet Frédéric Hardy^1$ , Philipp Burger<sup>1</sup>, THOMAS WOLF<sup>1</sup>, PETER SCHWEISS<sup>1</sup>, PETER ADELMANN<sup>1</sup>, DORIS ERNST<sup>1</sup>, ROBERT A. FISHER<sup>2</sup>, ROBERT EDER<sup>1</sup>, ROLF HEID<sup>1</sup>, HILBERT V. LÖHNEYSEN<sup>1</sup>, and CHRISTOPH MEINGAST<sup>1</sup> - <sup>1</sup>Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany - <sup>2</sup>Lawrence Berkeley National Laboratory, Berkeley CA 94720. USA

Using specific-heat and high-resolution thermal-expansion measurements, we present an extensive study of the normal- and superconducting state properties of high-quality single crystals of the electrondoped iron pnictide  $Ba(Fe_{1-x}Co_x)_2As_2$ . We determine the evolution of the electronic density of states and superconducting gaps with Codoping and pressure. Our measurements illustrate the competition between magnetism and superconductivity to monopolize the Fermi surface and also reveal the existence of large gapless contributions in strongly under- and over-doped conditions. These observations are discussed in terms of pair-breaking and changes of the electronic band structure, in line with recent theories.

## TT 36.3 Wed 14:30 HSZ 304

Simulation of pressure effects in the 122 family of iron pnictides — •MILAN TOMIĆ, ROSER VALENTI, and HARALD O. JESCHKE — Institut für Theoretische Physik, Johan Wolfgang Goethe Universität, Frankfurt am Main, Germany

In this talk we will present first principles structural relaxations for the Family of 122 iron pnictide materials under hydrostatic and uniaxial pressure. We discuss the properties of the structures predicted at different pressure values and compare to experiment. We determine the critical pressures for the phase transitions in CaFe<sub>2</sub>As<sub>2</sub> and BaFe<sub>2</sub>As<sub>2</sub>.

TT 36.4 Wed 14:45 HSZ 304 **Doping dependent electronic anisotropies in Ba** $(Fe_{1-x}Co_x)_2As_2$ — •F. KRETZSCHMAR<sup>1</sup>, B. MUSCHLER<sup>1</sup>, R. HACKL<sup>1</sup>, J.-H. CHU<sup>2,3</sup>, J. G. ANALYTIS<sup>2,3</sup>, and I. R. FISHER<sup>2,3</sup> — <sup>1</sup>Walther Meissner Institute, 85748 Garching — <sup>2</sup>SIMES, SLAC, Menlo Park, CA 94025, USA — <sup>3</sup>GLAM, Stanford University, CA 94305, USA

Superconductivity in the iron pnictides with  $T_c$  up to 56 K does probably not originate from electron-phonon coupling. The compounds have well nested hole and electron pockets with similar cross sections encircling the  $(\pi, 0)$  points and the center of the (1 Fe) unit cell which can essentially be probed independently by electronic Raman scattering (ERS) in  $A_{1g}$  and  $B_{1g}$  symmetry, respectively. We present results of ERS experiments on Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub> measured as a function of temperature,  $T > T_c$ , and doping x. The data of five samples with x = 0.045, 0.051, 0.055, 0.061, and 0.085 with  $T_c^{\max} = 24$  K at x = 0.061 were analyzed applying an extended Drude model. The resulting dynamical relaxation rates  $\Gamma_{\mu}(\omega, T)$  are distinctly different in the two symmetries  $\mu$ . In particular, the zero-energy extrapolation values  $\Gamma_{\mu}(\omega \to 0, T)$  vary strongly for  $B_{1g}$  and weakly for  $A_{1g}$  symmetry indicating a band dependence of the electronic relaxation. Surprisingly,  $(\Gamma_{A1g} + \Gamma_{B1g})/2$  compares well with the temperature dependence of the DC resistivity. The anisotropy resembles that in cuprates. However, in the cuprates the electronic relaxation depends on the location on a single Fermi surface rather than on the individual sheet. We conclude, that in either case only the coupling of the electrons to spin and/or charge excitations can explain these anisotropies.

TT 36.5 Wed 15:00 HSZ 304 Chemical Pressure and Physical Pressure in Phosphorous doped BaFe<sub>2</sub>As<sub>2</sub> — •LINA KLINTBERG — University of Cambridge Measurements of the superconducting transition temperature, T<sub>c</sub>, under pressure via bulk AC susceptibility were carried out on several concentrations of phosphorous substitution in BaFe<sub>2</sub>As<sub>2</sub>. The pressure dependence of unsubstituted BaFe<sub>2</sub>As<sub>2</sub>, phosphorous concentration dependence of substituted BaFe<sub>2</sub>As<sub>2</sub>, as well as the pressure dependence of phosphorous substituted BaFe<sub>2</sub>As<sub>2</sub> all point towards an identical maximum T<sub>c</sub> of 31 K. This indicates that phosphorous substitution and physical pressure are similar in terms of superconductivity in this compound, and that phosphorous substitution does not induce substantial impurity scattering.

TT 36.6 Wed 15:15 HSZ 304 Tetragonal lattice collapse in  $SrFe_2As_2$  - a combined experimental and theoretical study — •MIRIAM SCHMITT<sup>1</sup>, DEEPA KASINATHAN<sup>1</sup>, ALIM OMERCI<sup>1</sup>, KATRIN MEIER<sup>1</sup>, ULRICH SCHWARZ<sup>1</sup>, MICHAEL HANFLAND<sup>2</sup>, KLAUS KOEPERNIK<sup>3</sup>, YURI GRIN<sup>1</sup>, ANDREAS LEITHE-JASPER<sup>1</sup>, and HELGE ROSNER<sup>1</sup> — <sup>1</sup>MPI CPfS, Dresden, Germany — <sup>2</sup>ESRF, Grenoble, France — <sup>3</sup>IFW, Dresden, Germany

In a joint experimental and theoretical study we investigate the crystal structure of the Fe pnictide compounds  $SrFe_2As_2$  under applied hydrostatic pressure. Applying high pressure X-ray diffraction, for a critical pressure of about 10 GPa we observe a sudden collapse of the tetragonal *c* axis, accompanied by a small expansion of the basal plane. This results in a drastic reduction of the c/a ratio and a significant decrease of the unit cell volume. This tetragonal collapse is well described by DFT band structure calculations and can be assigned to the formation of an additional As-As bond along the tetragonal *c* axis.

#### 15 min. break

TT 36.7 Wed 15:45 HSZ 304 High Pressure investigation of pressure-induced superconductivity in CaFe<sub>2</sub>As<sub>2</sub> — •PATRICK REUVEKAMP<sup>1</sup>, REINHARD KREMER<sup>1</sup>, RENATO GONNELLI<sup>2</sup>, and JANUSZ KARPINSKI<sup>3</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — <sup>2</sup>Dipartimento di Fisica and CNISM, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino (TO), Italy — <sup>3</sup>ETH Zurich, Rämistrasse 101, 8092 Zurich, Switzerland

Since the discovery of superconductivity in iron pnictides, many compounds in this family have been heavily studied due the easily induced superconductivity using chemical doping. In the case of CaFe<sub>2</sub>As<sub>2</sub>, high pressure can be used to establish and tune superconductivity instead. In this investigation, the phase diagram and the pressure induced onset/disappearance of superconductivity were studied using ac-resistive measurements in magnetic fields up to 11 T.

TT 36.8 Wed 16:00 HSZ 304 Interplay of antiferromagnetism, ferromagnetism and superconductivity in EuFe<sub>2</sub>( $As_{1-x}P_x$ )<sub>2</sub> single crystals — •HIRALE S. JEEVAN, JANNIS MAIWALD, and PHILIP GEGENWART — I. Physikalisches Institut, Georg-August-Universitaet Goettingen, Friedrich Hund Platz 1, 37077 Goettingen, Germany

We present a systematic study on the influence of antiferromagnetic and ferromagnetic phases of  $Eu^{2+}$  moments on the superconducting phase upon doping the As site by isovalent P, which acts as chemical pressure on  $EuFe_2As_2$ . In this contribution, we shall report the

#### TT 36.9 Wed 16:15 HSZ 304

Bridging angle-resolved photoemission spectroscopy (ARPES) with other experiments in case of iron arsenides — •DANIIL EVTUSHINSKY, VOLODYMYR ZABOLOTNYY, ALEXANDER KORDYUK, TIMUR KIM, BERND BÜCHNER, and SERGEY BORISENKO — IFW Dresden

The single crystals of (Ba,K)Fe<sub>2</sub>As<sub>2</sub> and LiFeAs were measured with angle-resolved photoemission spectroscopy (ARPES). After clarification of the Fermi surface topology, we address the issue of the superconducting gap in these compounds, which was determined via fitting the distribution of the quasiparticle density to a model, incorporating finite lifetime and experimental resolution effects. Low energy electronic structure defines many macroscopic properties of a solid, which allowed us to perform the calculation of the London penetration depth and Hall coefficient purely on the basis of ARPES data. The agreement with different measurements of the superfluid density and with magnetotransport experiments was observed. Overview of the available experimental results suggests two-gap superconductivity for most of the studied iron arsenides.

## TT 36.10 Wed 16:30 HSZ 304

Electronic structure studies of parent  $Ba(Eu)Fe_2As_2$  and their superconducting derivatives using angle-resolved photoemission spectroscopy (ARPES) — •S. THIRUPATHAIAH<sup>1</sup>, E.D.L. RIENKS<sup>1</sup>, E. VAN HEUMEN<sup>2</sup>, H.S. JEEVAN<sup>3</sup>, P. GEGENWART<sup>3</sup>, M.S. GOLDEN<sup>2</sup>, and J. FINK<sup>1,4</sup> — <sup>1</sup>HZB, Berlin — <sup>2</sup>Uni. Amsterdam, The Netherlands — <sup>3</sup>Georg-August- universität-Göttingen, Germany — <sup>4</sup>IFW, Dresden

The advent of  $LaO_{1-x}F_x$ FeAs with  $T_c=26$  K has brought enormous interest to the high-Tc superconductor community. It is most important to study the electronic structure of these new superconductors, i.e., Fermi surfaces and band dispersions near the Fermi level at high symmetry points in order to obtain microscopic understanding of superconductivity. We have studied the electronic structure of Fe based 122 type parent compounds and their superconducting derivatives to reveal the important information on the Fermi surface nesting conditions (between hole pockets at the Brillouin zone center and electron pockets at zone corner) as a function of electron, hole doping, and isovalent substitution of P at As site in Ba(Eu)Fe<sub>2</sub>As<sub>2</sub>. Our findings show that electron doping into parent BaFe<sub>2</sub>As<sub>2</sub> destroy the nesting conditions and superconductivity emerges, accompanied by increase in the dimensionality of electronic structure. We observe that charge carrier doping into parent compounds show a rigid-band-like behavior of electronic structure where as isovalent substitution show a non rigid-band-type nature.

### TT 36.11 Wed 16:45 HSZ 304

Electronic dispersion anomalies in iron-pnictide superconductors — •ANDREAS HEIMES<sup>1</sup>, ROLAND GREIN<sup>2</sup>, and MATTHIAS ESCHRIG<sup>1</sup> — <sup>1</sup>Department of Physics, Royal Holloway, University of London — <sup>2</sup>Institut für Theoretische Festkörperphysik, Karlsruhe Institut of Technology

Recently, experimental studies of the spin excitation spectrum revealed a strong temperature dependence in the normal state and a resonance feature in the superconducting state of several Fe-based superconductors. Based on these findings, we develop a model of electrons interacting with a temperature dependent magnetic excitation spectrum and apply it to angle resolved photoemission in  $Ba_{1-x} K_x$  Fe<sub>2</sub> As<sub>2</sub>. We reproduce in quantitative agreement with experiment a renormalization of the quasiparticle dispersion both in the normal and the superconducting state, and the dependence of the quasiparticle linewidth on binding energy. We estimate the strength of the coupling between electronic and spin excitations. Our findings support a dominantly magnetic pairing mechanism.

TT 36.12 Wed 17:00 HSZ 304

Electronic structure of TM doped Ba122 Iron Arsenide superconductors — •ANNA BULING<sup>1</sup>, ERNST KURMAEV<sup>2</sup>, JOHN MCLEOD<sup>3</sup>, NIKOLAI A. SKORIKOV<sup>2</sup>, MANFRED NEUMANN<sup>1</sup>, ALEXAN-DER MOEWES<sup>3</sup>, YURI A. IZYUMOV<sup>2</sup>, LARISA D. FINKELSTEIN<sup>2</sup>, NI NI<sup>4</sup>, SERGEY L. BUD'KO<sup>4</sup>, and PAUL C. CANFIELD<sup>4</sup> — <sup>1</sup>Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — <sup>2</sup>Institute of Metal Physics, Russian Academy of Sciences-Ural Division, 620219 Yekaterinburg, Russia — <sup>3</sup>Department of Physics and Engineering Physics, University of Saskatchewan, 116 Science Place, Saskatoon, Saskatchewan S7N 5E2, Canada — <sup>4</sup>Ames Laboratory U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

We report on a detailed investigation of the electronic structure of undoped and 3d-metal doped Ba122 superconductors by means of x-ray spectroscopy.

Suprisingly it is found that in spite of the localized magnetic moments a substitution of Fe sites in  $BaFe_2As_2$  with Ni and Co results in superconductivity. The characteristic changes in the electronic structure of Ba122 induced by doping are determined by XPS and RIXS measurements. DFT calculations are added to underline the influence of the doping.

The main goal of this work is to illuminate the superconductivity mechanism in this compound.

### 15 min. break

TT 36.13 Wed 17:30 HSZ 304 Unconventional Raman scattering in the line node superconductor  $BaFe_2(As_{1-x}P_x)_2 - \bullet$ Peter Lemmens<sup>1</sup>, VLADIMIR GNEZDILOV<sup>1,2</sup>, YURII PASHKEVICH<sup>3</sup>, SERGEI GNATCHENKO<sup>2</sup>, SHIREGU KASAHARA<sup>4</sup>, and YUJI MATSUDA<sup>4</sup> - <sup>1</sup>IPKM, TU-BS, Braunschweig, Germany - <sup>2</sup>ILTPE NAS, Ukraine - <sup>3</sup>DonFTI NAS, Ukraine -<sup>4</sup>Dep. of Phys., Kyoto University, Japan

The phase diagram of the system  $BaFe_2(As_{1-x}P_x)_2$  is probed using Raman scattering. We observe a breakdown of selection rules and a pronounced effect of the folding back of the energy versus wave vector of dispersion curves in the non-Fermi liquid regime. This behavior contrasts with the observation of quantum oscillations in magneto transport. Possible mechanisms of such unexpected behavior are discussed. Work supported by DFG.

TT 36.14 Wed 17:45 HSZ 304 Optical Investigations of the Superconducting State in 122 Iron-Pnictides — •Dan Wu<sup>1</sup>, Martin Dressel<sup>1</sup>, Guanghan Cao<sup>2</sup>, Philipp Gegenwart<sup>3</sup>, Bernhard Holzapfel<sup>4</sup>, Jules Carbotte<sup>5</sup>, and Ewald Schachinger<sup>6</sup> — <sup>1</sup>1.Physikalisches Institut, Unversitat Stuttgart — <sup>2</sup>Zhejiang University, China — <sup>3</sup>Universitat Gottingen — <sup>4</sup>IFW, Dresden — <sup>5</sup>McMaster University,Canada — <sup>6</sup>Graz University of Technology, Austria

The new high-Tc iron pnictide superconductors have a pronounced multiband character, which complicates the electronic properties and allows for a variety of possible superconducting ground states. We have used the infrared spectroscopy-one of the most powerful tools to investigate the low-energy electrodynamic properties of superconductors-to study several pnictide families. We made a comparison between them with the aim to answer the following questions: (1) Is it possible to have more than one superconducting gap in iron pnictide? (2) Can their order parameters be distinct from each other? (3) How does the coupling between different bands influence the gap? (4) Do the gaps have a three-dimensional character? (5) Is the gap scenario universal for all the iron pnictides? We could show that the pairing condition depends sensitively on the similarity of geometry and dimension between hole and electron Fermi-surfaces.

TT 36.15 Wed 18:00 HSZ 304 Highly anisotropic energy gap in superconducting  $Ba(Fe_{0.9}Co_{0.1})_2As_2$  from optical conductivity measurements — •A. V. PRONIN<sup>1</sup>, T. FISCHER<sup>1</sup>, J. WOSNITZA<sup>1</sup>, K. IIDA<sup>2</sup>, F. KURTH<sup>2</sup>, S. HAINDL<sup>2</sup>, L. SCHULTZ<sup>2</sup>, B. HOLZAPFEL<sup>2</sup>, and E. SCHACHINGER<sup>3</sup> — <sup>1</sup>Dresden High Magnetic Field Laboratory (HLD), FZ Dresden-Rossendorf, 01314 Dresden, Germany — <sup>2</sup>IFW Dresden, Institute for Metallic Materials, 01171 Dresden, Germany — <sup>3</sup>Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

We have measured the complex dynamical conductivity,  $\sigma = \sigma_1 + i\sigma_2$ , of superconducting Ba(Fe<sub>0.9</sub>Co<sub>0.1</sub>)<sub>2</sub>As<sub>2</sub> ( $T_c = 22$  K) in the terahertz and infrared ranges. The temperature dependence of  $\sigma_1$  demonstrates a pronounced coherence peak at frequencies below 15 cm<sup>-1</sup> (1.8 meV). The temperature dependence of the penetration depth, calculated from  $\sigma_2$ , shows power-law behavior at the lowest temperatures. Analysis of the conductivity data with a two-gap model, gives the smaller isotropic *s*-wave gap of  $\Delta_A = 3$  meV, while the larger gap is highly anisotropic with possible nodes and its rms amplitude is  $\Delta_0 = 8$  meV. Overall, our results are consistent with a two-band superconductor with an  $s_{\pm}$ gap symmetry.

TT 36.16 Wed 18:15 HSZ 304 Pseudogap-like phase in  $Ca(Fe_{1-x}Co_x)_2As_2$  revealed by <sup>75</sup>As NQR — •SEUNG-HO BAEK, HANS-JOACHIM GRAFE, GUILLAUME Lang, Lumanita Harnagea, S. Singh, Sabine Wurmehl, and Bernd Buechner — IFW-Dresden, Institute for Solid State Research, PF 270116, 01171 Dresden, Germany

We report <sup>75</sup>As nuclear quadrupole resonance (NQR) measurements on single crystalline Ca(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub> (0 < x < 0.09). The nuclear spin-lattice relaxation rate  $T_1^{-1}$  as a function of temperature T and Co dopant concentration x reveals a normal-state pseudogap-like phase below a crossover temperature  $T^*$  in the under- and optimally-doped region. The resulting x-T phase diagram shows that, after suppression of the spin-density-wave order,  $T^*$  intersects  $T_c$  falling to zero rapidly near the optimal doping regime. Possible origins of the pseudogap are discussed.