# **TT 40:** Superconductivity: Ferropnictides 1

Time: Thursday 14:00-19:00

TT 40.1 Thu 14:00 HSZ 03

Antiferromagnetic correlations in the normal state of LaFeAsO<sub>1-x</sub> $F_x$  with  $0 \le x \le 0.125$  — •Rüdiger Klingeler, Norman Leps, Liran Wang, Christian Hess, Günter Behr, Vladislav Kataev, and Bernd Büchner — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

We have studied the interplay of magnetism and superconductivity in  $LaFeAsO_{1-x}F_x$  with  $0 \le x \le 0.125$ . For low doping with  $x \le 0.04$ , our data confirm a moderate suppression of both the structural transition and the antiferromagnetic spin density wave formation. For  $x \ge 0.05$ , both anomalies are completely suppressed and superconductivity is observed. Remarkably, the temperature dependence of the normal state susceptibility well above  $T_C$  is almost independent of doping, i.e. both the absolute value and the slope are nearly unchanged compared to the undoped case [1]. This implies at least local antiferromagnetic interactions which barely depend on hole doping although the ground state changes entirely from an orthorhombic antiferromagnetic poor metal ( $x \le 0.04$ ) to a tetragonal superconductor ( $x \ge 0.05$ ). These surprising results are discussed in terms of (i) - pseudogap formation, (ii) - antiferromagnetic correlations, and (iii) - preformed bipolarons which might be relevant to the pairing mechanism.

[1] R. Klingeler et al., Preprint at http://arxiv.org/abs/0808.0708

TT 40.2 Thu 14:15 HSZ 03

Electronic phase diagram of the  $LaO_{1-x}F_xFeAs$  superconductor: A muon spin relaxation study — •H. LUETKENS<sup>1</sup>, H.-H. KLAUSS<sup>2</sup>, F.J. LITTERST<sup>3</sup>, T. DELLMANN<sup>3</sup>, R. KLINGELER<sup>4</sup>, C. HESS<sup>4</sup>, R. KHASANOV<sup>1</sup>, A. AMATO<sup>1</sup>, C. BAINES<sup>1</sup>, M. KOSMALA<sup>5</sup>, O.J. SCHUMANN<sup>5</sup>, M. BRADEN<sup>5</sup>, J. HAMANN-BORRERO<sup>4</sup>, N. LEPS<sup>4</sup>, A. KONDRAT<sup>4</sup>, G. BEHR<sup>4</sup>, J. WERNER<sup>4</sup>, M. KRAKEN<sup>3</sup>, and B. BÜCHNER<sup>4</sup> — <sup>1</sup>Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, Villigen, Switzerland — <sup>2</sup>Institut für Festkörperphysik, TU Dresden — <sup>3</sup>Institut für Physik der Kondensierten Materie, TU Braunschweig — <sup>4</sup>Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden — <sup>5</sup>II. Physikalisches Institut, U Köln

The structural and electronic phase diagram of  $LaO_{1-x}F_xFeAs$  and, in particular, the exact nature of the change from the magnetically ordered to the superconducting state that was determined by means of x-ray scattering, muSR and Mössbauer spectroscopy will be presented [1-3]. A discontinuous first-order-like change of the Néel temperature, the superconducting transition temperature, the sublattice magnetisation and the superfluid density is found between x=0.04 and x=0.05. While these results strongly question the relevance of quantum critical behaviour in iron pnictides they prove an important role of the structural orthorhombic distortion disappearing exactly at the SDW magnetism and superconductivity phase boundary.

- [1] H. Luetkens et al., Phys. Rev. Lett. 101, 097009 (2008).
- [2] H.-H. Klauss et al., Phys. Rev. Lett. 101, 077005 (2008).
- [3] H. Luetkens et al., arXiv:0806.3533 (2008).

### TT 40.3 Thu 14:30 HSZ 03

#### **Functional renormalization group study of the iron pnictides** — •CHRISTIAN PLATT, CARSTEN HONERKAMP, and WERNER HANKE

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Recently, a new class of superconductors (sc) - Fe-based sc - was discovered. These sc iron pnictides are most likely less correlated than the high- $T_c$  cuprates but present again a challenging case of competing magnetic and superconducting orders at low temperatures. Therefore, perturbative functional renormalization group (fRG) methods appear adequate for the theoretical modelling of the phase diagram. Here, we apply the fRG to a four-band (Fe-d-orbital) model including intraand interband couplings as well as interband pair hoppings. We compute the leading instabilities, i.e. spin-ordered phase in the "under-doped" situation and the leading pairing instability as a function of the electron density and interaction parameters.

TT 40.4 Thu 14:45 HSZ 03 **Thermodynamic study of the Co-doped Ba-122 iron pnic tide** — •Frédéric Hardy<sup>1</sup>, Christoph Meingast<sup>1</sup>, Thomas Wolf<sup>1</sup>, Rolf Heid<sup>1</sup>, Peter Adelmann<sup>1</sup>, Peter Schweiss<sup>1</sup>, Doris Ernst<sup>1</sup>, and Hilbert v. Löhneysen<sup>1,2</sup> — <sup>1</sup>Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany<br/> —  $^2\rm Physikalisches Institut, Universität Karlsruhe, 76128$ Karlsruhe, Germany

Since the discovery of the new high-T<sub>c</sub> iron pnictides, many scenarios were put forward to describe the symmetry of the order parameter including d-wave and unconventional s-wave. Early heat capacity measurements suggested that the electron-doped 1111 compounds show a nodal gap, while K-hole-doped 122 materials are fully gapped. Here we present a critical analysis of our own specific-heat data on Co-doped 122 single crystals, in which we pay particular attention to the details of the phonon background subtraction as well as to the contribution of impurity phases. We also discuss an interesting field-dependence of the thermal expansivity below  $T_c(H)$ .

TT 40.5 Thu 15:00 HSZ 03 **Strong coupling of superconductivity to c/a in Ba(Fe,Co)**<sub>2</sub>**As**<sub>2</sub> — •CHRISTOPH MEINGAST<sup>1</sup>, FREDERIC HARDY<sup>1</sup>, PETER ADELMANN<sup>1</sup>, PETER SCHWEISS<sup>1</sup>, DORIS ERNST<sup>1</sup>, HILBERT V. LÖHNEYSEN<sup>1,2</sup>, and THOMAS WOLF<sup>1</sup> — <sup>1</sup>Forschungszentrum Karlsruhe, Institut für Festkörperphysik, — <sup>2</sup>Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany.

Just as in the cuprates, magnetism and superconductivity occur in close proximity to each other in the newly discovered FeAs-based materials. Here, using high-resolution thermal expansion and specific heat measurements, we study the thermodynamic response of the lattice parameters to superconducting and magnetic order in Ba(Fe,Co)<sub>2</sub>As<sub>2</sub> single crystals. We show that there is a strong coupling of the c/a ratio to both the superconducting and magnetic/structural phase transitions. According to the Ehrenfest relationship, the ordering temperatures of both ordered states are expected to increase with increasing c/a. This suggests that the occurrence of superconductivity is strongly linked to the magnetic/structural transition.

TT 40.6 Thu 15:15 HSZ 03 Electronic phase separation in the slightly underdoped iron pnictide superconductor  $Ba_{1-x}K_xFe_2As_2 - \bullet JI$  TAE PARK<sup>1</sup>, D. S. INOSOV<sup>1</sup>, CH. NIEDERMAYER<sup>2</sup>, G. L. SUN<sup>1</sup>, D. HAUG<sup>1</sup>, N. B. CHRISTENSEN<sup>2</sup>, R DINNEBIER<sup>1</sup>, A. V. BORIS<sup>1</sup>, A. J. DREW<sup>3</sup>, L. SCHULZ<sup>3</sup>, T. SHAPOVAL<sup>4</sup>, U. WOLFF<sup>4</sup>, V. NEU<sup>4</sup>, X. YANG<sup>1</sup>, C. T. LIN<sup>1</sup>, B. KEIMER<sup>1</sup>, and V. HINKOV<sup>1</sup> - <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, Stuttgart, Germany - <sup>2</sup>ETHZ & PSI, Villigen PSI, Switzerland - <sup>3</sup>Department of Physics, University of Fribourg, Chemin du Musée 3, Fribourg, Switzerland - <sup>4</sup>IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

We performed a combined study of the slightly underdoped novel iron pnictide superconductor  $\operatorname{Ba}_{1-x} K_x \operatorname{Fe}_2 \operatorname{As}_2$  by means of X-ray powder diffraction, neutron scattering, muon spin rotation ( $\mu$ SR), and magnetic force microscopy (MFM). Commensurate static magnetic order sets in below  $T_m \sim 70$  K as inferred from the emergence of the magnetic (1 0 3) reflection in the neutron scattering data and from the observation of damped oscillations in the zero-field- $\mu$ SR asymmetry. Transverse-field  $\mu$ SR below  $T_c$  shows a coexistence of magnetically ordered and non-magnetic states, which is also confirmed by MFM imaging. This coexistence could be explained by electronic phase separation into antiferromagnetic and superconducting/normal state regions on a scale of several tens of nanometers indicating that such mesoscopic phase separation can be considered an intrinsic property of some iron pnictide superconductors.

### 15 min. break

TT 40.7 Thu 15:45 HSZ 03 The intrinsic electronic phase diagram of iron-pnictide superconductors — •C. HESS, A. KONDRAT, A. NARDUZZO, J. E. HAMANN-BORRERO, R. KLINGELER, H. GRAFE, G. LANG, F. HAM-MERATH, D. PAAR, A. ALFONSOV, V. KATAEV, J. WERNER, G. BEHR, and B. BÜCHNER — Leibniz-Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany

We present a detailed study of the intrinsic electronic phase diagram of the oxypnic tide superconductors in the normal state based on the analysis of the electrical resistivity  $\rho$  of both LaO<sub>1-x</sub>F<sub>x</sub>FeAs and  $\rm SmO_{1-x}F_xFeAs$  for a wide range of doping. Our data give clear-cut evidence for unusual normal state properties in these new materials. As a function of doping  $\rho$  of  $\rm LaO_{1-x}F_xFeAs$  shows a clear transition from pseudogap to Fermi liquid-like behavior, mimicking the phase diagram of the cuprates. Moreover, our data reveal a correlation between the strength of the pseudogap signatures and the stability of the superconducting phase. The pseudogap signatures, which are clearly connected with the structural and magnetic transitions of the parent material, become stronger in  $\rm SmO_{1-x}F_xFeAs$  where superconductivity is enhanced and vanish when superconductivity is reduced in the doping region with Fermi liquid-like behavior [1]. We further present evidence for the connection between the pseudogap signatures in electrical transport and the slowing-down of spin fluctuation.

[1] C. Hess et al., Preprint at http://arxiv.org/abs/0811.1601

TT 40.8 Thu 16:00 HSZ 03 **Magnetic properties of LaO\_{1-x}F\_xFeAs** — •SANGEETA SHARMA<sup>1,2</sup>, JOHN KAY DEWHURST<sup>1,2</sup>, SAM SHALLCROSS<sup>3</sup>, CHRISTOPHE BERSIER<sup>1,2</sup>, FRANCESCO CRICCHIO<sup>4</sup>, ANTONIO SANNA<sup>2,5</sup>, SANDRO MASSIDDA<sup>5</sup>, E. K. U GROSS<sup>2</sup>, and LARS NORDSTROEM<sup>4</sup> — <sup>1</sup>Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, D-14195 Berlin, Germany — <sup>2</sup>Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — <sup>3</sup>Lehrstuhl für Theoretische Festkörperphysik, Staudstr. 7-B2, 91058 Erlangen, Germany. — <sup>4</sup>Department of Physics, Uppsala University, Box 530, SE-75121 Uppsala, Sweden. — <sup>5</sup>Dipartimento di Fisica, Universita' di Cagliari, Cittadella Universitaria, I-09042 Monserrato(CA), Italy

Using state-of-the-art first-principles calculations we have elucidated the complex magnetic and structural dependence of LaOFeAs upon doping. Our key findings are that (i) doping results in an orthorhombic ground state and (ii) there is a commensurate to incommensurate transition in the magnetic structure between x = 0.025 and x = 0.04. Our calculations further imply that in this system magnetic order persists up to the onset of superconductivity at the critical doping of x = 0.05. Finally, our investigations of the undoped parent compound reveal a small itinerant moment and orthorhombic structure with both moment and distortion angle in excellent agreement with experiments.

## TT 40.9 Thu 16:15 $\,$ HSZ 03 $\,$

Doping dependence of the charge distribution of iron pnictides — •GUILLAUME LANG<sup>1</sup>, HANS-JOACHIM GRAFE<sup>1</sup>, KATARINA MANTHEY<sup>1</sup>, FRANZISKA HAMMERATH<sup>1</sup>, DALIBOR PAAR<sup>1,2</sup>, KATRIN KOCH<sup>3</sup>, HELGE ROSNER<sup>3</sup>, GÜNTHER BEHR<sup>1</sup>, JOCHEN WERNER<sup>1</sup>, and BERND BÜCHNER<sup>1</sup> — <sup>1</sup>IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — <sup>2</sup>Dept. of Physics, Fac. of Science, Univ. of Zagreb, P. O. Box 331, HR-10002 Zagreb, Croatia — <sup>3</sup>Max Planck Inst. for Chem. Phys. of Solids, Nöthnitzer Str. 40, D-01187 Dresden, Germany

We have investigated the evolution, on doping, of the charge distribution in the new  $LaO_{1-x}F_x$ FeAs superconductor. This is done using <sup>75</sup>As Nuclear Quadrupole Resonance (NQR), which is a sensitive local probe of the electric field gradient generated by the charge distribution. A significant increase of the quadrupole frequency is observed when going from the undoped situation to the superconducting region of the phase diagram, reflecting the change in density or spatial distribution of the electrons ([1], and subsequent measurements to be published). This increase cannot be properly accounted for by LDA calculations, even though there is good agreement between theory and experience for the undoped case. We discuss this discrepancy as well as the relation to the superconductivity, i.e., the link to the doping-dependence of the critical temperature.

[1] H.-J. Grafe, G. Lang et al., arXiv:0811.4508, submitted to New Journal of Physics (invited paper, special issue on iron pnictides superconductors)

#### TT 40.10 Thu 16:30 HSZ 03

Observation of the many body satellite in  $Ba_{1-x}K_xFe_2As_2$ single crystals by resonant x-ray photoemission spectroscopy — ANDREAS KOITZSCH<sup>1</sup>, THOMAS KROLL<sup>1</sup>, ROBERTO KRAUS<sup>1</sup>, MAR-TIN KNUPFER<sup>1</sup>, BERND BÜCHNER<sup>1</sup>, DAVID BATCHELOR<sup>2</sup>, GUOLI SUN<sup>3</sup>, DUNLU SUN<sup>3</sup>, and •CHENGTIAN LIN<sup>3</sup> — <sup>1</sup>IFW Dresden, Postfach 270116, 01171 Dresden — <sup>2</sup>Forschungszentrum Karlsruhe, Hermannvon-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen — <sup>3</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

Valence band and core level measurements of  $Ba_{1-x}K_xFe_2As_2$  single crystals with photon energies across the Fe L<sub>3</sub> absorption edge are re-

ported. Within the resonance regime of the photon energy profile an intensity enhancement centered at  ${\rm E}=3.6~{\rm eV}$  is observed which can be identified as the many body satellite. The energy position of the satellite matches the expectations based on previously extracted parameters from Fe L x-ray absorption spectroscopy and Fe 2p x-ray photoemission spectroscopy. The results show, that the Hubbard repulsion U, although smaller than the bandwidth, preserves a clear physical meaning giving rise to local electron phenomena in an otherwise itinerant environment.

TT 40.11 Thu 16:45 HSZ 03 Momentum dependence of the superconducting gap in  $Ba_{1-x}K_xFe_2As_2 - \bullet D.$  V. EVTUSHINSKY<sup>1</sup>, D. S. INOSOV<sup>1,2</sup>, V. B. ZABOLOTNYY<sup>1</sup>, A. KOITZSCH<sup>1</sup>, M. KNUPFER<sup>1</sup>, B. BÜCHNER<sup>1</sup>, G. L. SUN<sup>2</sup>, V. HINKOV<sup>2</sup>, A. V. BORIS<sup>2</sup>, C. T. LIN<sup>2</sup>, B. KEIMER<sup>2</sup>, A. VARYKHALOV<sup>3</sup>, A. A. KORDYUK<sup>1,4</sup>, and S. V. BORISENKO<sup>1</sup> - <sup>1</sup>Institute for Solid State Research, IFW Dresden, P. O. Box 270116, D-01171 Dresden, Germany - <sup>2</sup>Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany - <sup>3</sup>BESSY GmbH, Albert-Einstein-Strasse 15, 12489 Berlin, Germany - <sup>4</sup>Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine

The precise momentum dependence of the superconducting gap in the iron-arsenide superconductor with  $T_c=32\,\mathrm{K}$  (BKFA) was determined from angle-resolved photoemission spectroscopy (ARPES) via fitting the distribution of the quasiparticle density to a model. The model incorporates finite lifetime and experimental resolution effects, as well as accounts for peculiarities of BKFA electronic structure. We have found that the value of the superconducting gap is practically the same for the inner  $\Gamma$ -barrel, X-pocket, and "blade"-pocket, and equals 9 meV, while the gap on the outer  $\Gamma$ -barrel is estimated to be less than 4 meV, resulting in  $2\Delta/k_{\mathrm{B}}T_{\mathrm{c}}=6.8$  for the large gap, and  $2\Delta/k_{\mathrm{B}}T_{\mathrm{c}}<3$  for the small gap. We also observe that below  $T_{\mathrm{c}}$  photoemission signal contains large non-superconducting part.

TT 40.12 Thu 17:00 HSZ 03 Correlations in Ferrophictides — •Klaus Koepernik and Hel-MUT Eschrig — IFW Dresden, Germany

The strenght of correlations in the ferropnic tide superconductors is still under debate. While arguments for an electron-electron interaction U of 5eV have been made, some experimental results support a U of merely 1eV. Density functional theory in the local spin density approximation (LSDA) seems to describe several aspects of the electronic structure quite reasonably, which would also support a smaller U. However, the unusually large error of the calculated lattice structure remains a puzzle. We discuss the influence of correlations on the electronic structure and the properties of the ferropnic tides in the framework of LSDA+U calculations.

#### 15 min. break

TT 40.13 Thu 17:30 HSZ 03 Theory for magnetic excitations in Fe-pnictide superconductors — •MAXIM KORSHUNOV<sup>1,2</sup> and ILYA EREMIN<sup>1,3</sup> — <sup>1</sup>Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany — <sup>2</sup>L.V. Kirensky Institute of Physics, Siberian Branch of RA, 660036 Krasnoyarsk, Russia — <sup>3</sup>Institute für Mathematische und Theoretische Physik, TU Braunschweig, D-38106 Braunschweig, Germany

We analyze the spin response in the normal and superconducting states of the Fe-pnictide High-T<sub>c</sub> superconductors. While the normal state spin excitations are dominated by the continuum of the interorbital antiferromagnetic (AFM) spin density wave fluctuations (SDW) and the incommensurate intraband SDW fluctuations, the unconventional superconductivity yields different feedback: the resonance peak in form of the well-defined spin exciton occurs only for the interband scattering at the AFM momentum  $Q_{AFM}$  for the extended s-wave  $(s_{\pm})$  superconducting order parameter and it is extremely weak for the d-wave order parameter due to the specific Fermi surface (FS) topology. We discuss this essential difference in the context of neutron scattering experiments used for determination of the superconducting wave function symmetry.

For the non-superconducting state, we show that the commensurate AFM SDW transition disappears already at the doping concentration  $x \sim 0.04$  reflecting the evolution of the FS. Correspondingly, with further increase of the doping the AFM fluctuations are suppressed for x > 0.1 and the  $\text{Im}\chi(Q_{AFM},\omega)/\omega$  becomes nearly temperature

independent, in agreement with recent NMR experiments.

TT 40.14 Thu 17:45 HSZ 03 Interplay between crystal structure and magnetism in the superconducting  $AFe_2As_2$  (A = Ca, Sr, Ba and Eu) Systems: A First-principles Study — •ALIM ORMECI, DEEPA KASINATHAN, KATRIN KOCH, MIRIAM SCHMITT, and HELGE ROSNER — MPI CPFS, Dresden

Although the recently discovered FeAs-based superconducting compounds crystallize in different structures, they have the same Fe-As substructure and display very similar electronic properties including similar patterns of structural and magnetic transitions. However, experimentally important differences are also found between the REOFeAs (RE = rare-earth) and the  $AFe_2As_2$  families. Because sample composition and quality are easier to control in the latter family, we focus on the AFe<sub>2</sub>As<sub>2</sub> systems. Using all-electron full-potential calculations, we study the relation between the onset of spin-density wave (SDW) and the tetragonal-to-orthorhombic transition. We find that the SDW pattern is necessary for the structural transition to take place. We also explore how electronic structure and magnetic behavior change when all free structural parameters, As-z, c/a and a/b, are optimized at different unit cell volumes (pressures). All four systems are compared with each other based on the calculation results. Most calculated properties agree well with the measured properties, but several of them are rather sensitive to the As z position. For a microscopic understanding of the electronic structure of this new family of superconductors this structural feature is crucial, but its correct ab initio treatment still remains an open question.

TT 40.15 Thu 18:00 HSZ 03 Renormalized in-plane plasma frequencies and insight into the superconductivity of iron pnictides from optical studies and low-temperature  $\mu$ SR data — •STEFAN-LUDWIG DRECHSLER<sup>1</sup>, HELGE ROSNER<sup>2</sup>, KLAUS KOEPERNIK<sup>1</sup>, MANDY GROBOSCH<sup>1</sup>, GUENTER BEHR<sup>1</sup>, ROMAN SCHUSTER<sup>1</sup>, FRIEDRICH ROTH<sup>1</sup>, SAAD ELGAZZAR<sup>3</sup>, BERND BUECHNER<sup>1</sup>, and MARTIN KNUPFER<sup>1</sup> — <sup>1</sup>IFW-Dresden, D-01171 Dresden, Germany — <sup>2</sup>MPI-CPfS Dresden, Germany — <sup>3</sup>Menoufia Univ., Shebin El-kom, Egypt & Uppsala Univ., Sweden

Theoretical values for the unscreened plasma frequencies of several Fe pnictides from DFT-LDA based calculations are compared with experimental plasma frequencies obtained from reflectivity measurements on both polycrystalline samples [1] and single crystals. The sizable renormalization observed for all considered compounds points to the presence of significant many-body effects beyond the LDA. From the measured large empirical background polarizabilities  $\varepsilon_{\infty} \stackrel{>}{\sim} 10\text{-}15$  we discard a sizable value of the Coulomb repulsion  $U \sim 4 \text{ eV}$  on Fe sites as proposed in the literature. From the extrapolated  $\mu$ SR (muon spin rotation) penetration depth data at very low-temperature and the experimental unscreened plasma frequency the total coupling constant  $\lambda_{tot}$  for the electron-boson interaction is estimated within the framework of the Eliashberg-theory within an effective single band approximation. For  $LaFeAsO_{0.9}F_{0.1}$  a weak to intermediately strong coupling regime is found whereas in the pronounced multiband case a constraint for various intraband coupling constants is obtained.

[1] S.-L. Drechsler, M. Grobosch et al., PRL 101 in press (2008).

### TT 40.16 Thu 18:15 HSZ 03 $\,$

**Pressure-induced structural and magnetic transitions in the 122 iron arsenide compounds** — •YUZHONG ZHANG, HEM KAND-PAL, INGO OPAHLE, HARALD JESCHKE, CLAUDIUS GROS, and ROSER VALENTI — Institut für Theoretische Physik, Goethe Universität Frankfurt, Germany

The parent compounds of the new superconductor family (Ca, Sr, Ba)Fe<sub>2</sub>As<sub>2</sub> under hydrostatic pressure at low temperature are investigated within the framework of ab initio molecular dynamics. Structural phase transitions from orthorhombic to tetragonal phase are de-

tected in all these materials. These transitions are simultaneously accompanied by magnetic phase transitions from a stripe-type antiferromagnetic state to a paramagnetic state. While the obtained first-order phase transition in CaFe<sub>2</sub>As<sub>2</sub> is consistent with the experimental results, we predict from our calculations that the phase transitions in SrFe<sub>2</sub>As<sub>2</sub> and BaFe<sub>2</sub>As<sub>2</sub> are of weak first order and continuous order, respectively. Analysis of Fermi surfaces, partial density of state as well as bandstructures as a function of chemical and hydrostatic pressure reveals the differences among these compounds. Finally we discuss, out of our calculations, the possible mechanism of the superconducting states.

We present an investigation of superconductivity and magnetism in EuFe<sub>2</sub>As<sub>2</sub> by doping of K, Ni,Co and P. The recent discovery of superconductivity in FeAs and related systems has a great impact in the field of superconductivity research. Superconductivity is found close to a magnetic and non-magnetic phase transition suggesting an unconventional pairing mechanism. We have synthesized single crystals and powder samples of both doped and undoped samples of EuFe<sub>2</sub>As<sub>2</sub> and investigated their physical properties. We found rather unique behavior due to the additional ordering of  $Eu^{2+}$ , which is absent in other systems like  $BaFe_2As_2$ ,  $SrFe_2As_2$  etc. The heat capacity, resistivity and magnetization measurements carried out at ambient pressure on the parent compound show an antiferromagnetic spin-density-wave  $(T_{SDW})$  at  $\approx 190$ K related to the Fe<sub>2</sub>As<sub>2</sub> layers and magnetic ordering of Eu<sup>2+</sup> (T<sub>N</sub>) moments at  $\approx$  20K. Upon doping Eu with K >30%,  $T_{SDW}$  gets suppressed and superconductivity appears at  $\approx 32$ K and also  $\operatorname{Eu}^{2+}$  ordering suppressed to the low temperature. On the other hand, doping of Co and Ni to the Fe site suppresses the SDW transition but no SC is found, possibly due to Eu ordering which appears unchanged at  $\approx$  19K. We will also discuss the effect of P doping to the As site.

Collaboration with: C.Geibel, Z.Hossain, Deepa Kasinathan, C. F. Miclea, M. Nicklas and H. Rosner

TT 40.18 Thu 18:45 HSZ 03 **ESR spectroscopy on (Gd,La)O\_{1-x}F\_xFeAs superconductors** — •A. Alfonsov, F. Murányi, V. Kataev, N. Leps, R. Klingeler, A. Kondrat, C. Hess, A. Köhler, J. Werner, G. Behr, and B. Büchner — IFW Dresden, Institute for Solid State Research, D-01171 Dresden, Germany

We present results on electron spin resonance (ESR) spectroscopy of polycrystalline samples of the  $(Gd,La)O_{1-x}F_xFeAs$  superconductor with different levels of fluorine and gadolinium doping. The ESR signal of a small amount of Gd spins doped to the parent compound LaOFeAs is sensitive to the structural and in particular to the magnetic phase transition occurring in this material at temperatures  $\sim 130 - 150 \,\mathrm{K}$ . Fluorine doping suppresses both transitions and leads to superconductivity. Correspondingly, the Gd ESR response shows no signatures of the magnetic order in the FeAs planes of samples with a superconducting ground state. In the concentrated compound GdOFeAs the Gd ESR response is sensitive to the magnetism of the FeAs planes, too. Doping of this material with  $\sim 15\%$  of fluorine yields superconductivity with  $T_c \approx 21$  K. Surprisingly, Gd ESR gives clear indications of the enhancement of (quasi)-static magnetic correlations in the superconducting samples which set in below  $\sim\,80\,\mathrm{K}$  and continue to develop even in the superconducting state. We compare ESR data with results of thermodynamic and transport measurements on these samples and discuss a possible role of magnetic rare-earths for the magnetism of the FeAs-planes in which the superconductivity evolves upon the fluorine doping.