TT 15: Superconductivity: Fe-based Superconductors - Other Materials and Theory

Time: Monday 15:00–19:00 Location: H23

TT 15.1 Mon 15:00 H23

Specific heat of $RbEuFe_4As_4$ - a magnetic superconductor — •Kristin Willa[1,2], Matthew Smiley[2], Roland Willa[2,3], Alex Koshelev[2], Jin-Ke Bao[2], Mercoury Kanatzidis[2], Ulrich Welp[2], and Wai-Kwong Kwok[2] — [1]Institute for Solid-State Physics, Karlsruhe Institute of Technology, Germany — [2]Materials Science Division, Argonne National Laboratory, USA — [3]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, Germany

We report detailed nanocalorimetric measurements on the newly discovered magnetic superconductor $RbEuFe_4As_4$. We investigated the superconducting transition at T_c=37K and extracted the phase boundary for in and out of plane magnetic fields obtaining an anisotropy ratio of 1.8. Large superconducting fluctuations are observed as well as a vortex lattice melting transition identified as a step of 4-5% of the zero field jump in specific heat. The melting line is considerably below the upper-critical-field line which is in quantitative agreement with theoretical predictions. In small fields near the magnetic transition $T_m = 14.9$K, we resolved a cusp-like behavior of the specific heat curve that shifts to lower temperatures for fields along the *c*-axis and a broad shoulder that shifts to higher temperatures for in-plane fields. We can reproduce our measured calorimetry data quantitatively by Monte-Carlo simulations of an anisotropic easy-plane 2D Heisenberg model that suggests that the cusp in specific heat is due to a BKT transition and the high temperature hump at higher fields marks a crossover from a paramagnetically disordered to an ordered state.

TT 15.2 Mon 15:15 H23

Magnetic order and superconductivity in $RbEuFe_4As_4$ — •Noah Winterhalter-Stocker[1], Stefan Gorol[1], Stevan Arsenijevic[2], Yurii Skourski[2], Hans-Albrecht Krug von Nidda[3], Mamoun Hemmida[3], Anton Jesche[1], Veronika Fritsch[1], and Philipp Gegenwart[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

$RbEuFe_4As_4$ is an ordered member of the class of iron based superconductors with a structure similar to half doped 122 iron based superconductors like $Ca_{0.5}Na_{0.5}Fe_2As_2$. In contrast to the latter $RbEuFe_4As_4$ shows a superstructure with distinct Eu and Rb positions. The material shows a superconducting transition at T_c=36.8 K and an onset of magnetic order of the paramagnetic Eu 4f moments at T_m=15 K [1]. This leads to a unique interplay between magnetic order and superconductivity which we study by magnetization, magnetotransport and ESR measurements. Our analysis reveals the temperature dependence of the lower and upper critical fields which we compare to appropriate theoretical models.

[1] M. P. Smylie *et al.*, Phys. Rev. B **98**, 104503 (2018)

TT 15.3 Mon 15:30 H23

Disentangling magnetism and superconductivity in LaOFeAs: A NQR study — •Piotr Lepucki[1], Igor Morozov[1,2], Ilya Silkin[2], Rhea Kappenberger[1], Sabine Wurmehl[1], Saicharan Aswartham[1], Markus Witschel[1], Bernd Büchner[1], and Hans-Joachim Grafe[1] — [1]IFW Dresden, Helmholtzstraße 20, 01069 Dresden — [2]Moscow State University, Moscow, Russia

The nature of the coexistence of magnetism and superconductivity in iron-based superconductors is still not well understood. The main discussion is whether there is a microscopic phase coexistence or phase separation (e.g. [1, 2]). We performed 75As nuclear quadrupole resonance (NQR) measurements on P- and Co-doped LaOFeAs powders in search of different behavior in magnetic and superconducting samples, and compare our results to F doped samples [3]. Our measurements show that independent of the dopant (isovalent P doping, in plane Co doping, or out of plane F doping), the electronic structure is changed only locally, leading to regions with different charge environments of the As, and therefore well separated NQR peaks. The relative weight of these regions is equal to the relative spectral weight of the corresponding NQR peaks and is a measure of the doping level [3]. Below the magnetic or superconducting transitions, these NQR peaks change differently, indicating that those regions which are largely unaffected by the doping are driving the magnetism, whereas the doped regions harbor superconductivity. These results suggest a microscopic phase separation in LaOFeAs irrespective of the dopant type.

[1] PRB 97, 224508
[2] PRB 80, 024508
[3] PRB 94, 014514

TT 15.4 Mon 15:45 H23

Tracking nematic fluctuations using the Nernst effect in Co-doped LaFeAsO — •Christoph Wuttke[1], Federico Caglieris[1], Steffen Sykora[1], Frank Steckel[1], Xiaochen Hong[1], Seunghyun Kim[1], Rhea Kappenberger[1], Saicharan Aswartham[1], Sabine Wurmehl[1], Sheng Ran[2], Paul C. Canfield[2], Bernd Büchner[1,3,4], and Christian Hess[1,4] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — [3]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany — [4]Center for Transport and Devices, Technische Universität Dresden, 01069 Dresden, Germany

We use the Nernst coefficient to track the nematic fluctuations through the Co-doped phase diagram of LaFeAsO. Similarly to our previous measurements in an 122-iron based superconductor system, we obtain a significant enhancement of the signal in the nematic fluctuation regime. The doping dependence of the Nernst coefficient exhibits a non-monotonic behavior featuring a local maximum in the vicinity of optimal doping. This peculiar doping dependence is also in agreement with our theoretical prediction and hence demonstrates the universality of the sensitivity of the Nernst effect on nematic fluctuations in iron based superconductors.

TT 15.5 Mon 16:00 H23

Strain-derivative of thermoelectric coefficients: a sensitive probe for nematic fluctuations — •Federico Caglieris[1], Christoph Wuttke[1], Xiaochen Hong[1], Steffen Sykora[1], Rhea Kappenberger[1], Saicharan Aswartham[1], Sabine Wurmehl[1], Bernd Büchner[1,2,3], and Christian Hess[1,2] — [1]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, 01069 Dresden — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

The role of nematic fluctuations in iron-based superconductors is still a strongly debated topic with many open questions concerning their origin and their relationship with the emerging superconductivity. In this work we tackle this issue with a new experimental technique, which combines the high sensitivity of the thermoelectric transport properties with the gentle strain offered by a piezoelectric device. The idea is to use the strain derivative of the Seebeck and the Nernst coefficients as a new tool to investigate the nematicity in the 1111 family of iron based superconductors, so far almost unexplored due to the lack of sizable single crystals. The main outcomes of our study are: i) nematic fluctuations are peaked at the structural transition temperature TS and not at the magnetic one; ii) not all the bands contribute to the measured anisotropy; iii) the Curie-Weiss scaling, previously found for the resistivity anisotropy for T>TS, also exists in the Seebeck and Nernst anisotropy, suggesting the existence of a common mechanism. Our results point towards an orbital origin of nematicity.

TT 15.6 Mon 16:15 H23

Nematicity in $BaFe_2As_2$ and LaFeAsO single crystals studied by elastoresistance and shear modulus measurements — •Sven Sauerland[1], Xiaochen Hong[2], Liran Wang[1], Francesco Scaravaggi[2,3], Anja U.B. Wolter[2], Rhea Kappenberger[2,3], Saicharan Aswartham[2], Sabine Wurmehl[2], Steffen Sykora[2], Federico Caglieris[2], Christian Hess[2], Bernd Büchner[2,3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Leibniz Institute for Solid State and Materials Research, IFW Dresden, Dresden, Germany — [3]Institute for Solid State Physics, TU Dresden, Germany

We report shear modulus and elastoresistivity measurements on LaFeAsO single crystals[1] and study the critical nematic response. The results are compared with corresponding data on $BaFe_2As_2$. In both materials, softening of the shear modulus towards the structural phase transition is observed by means of the three-point-bending technique and similar Curie-Weiss-like divergence of the nematic susceptibilities deduced from both the shear modulus and the elastoresistivity are found. The data are analysed by means of a Landau approach. Comparison of the bare and the renormalized nematic susceptibilities provides the characteristic energy of the coupling between the lattice and the electronic degrees of freedom. Nematic susceptibilities obtained from shear modulus and elastoresistivity data are compared for LaFeAsO and $BaFe_2As_2$.

[1] R. Kappenberger et al., J. Cryst. Growth 483, 9 (2018)

TT 15.7 Mon 16:30 H23

Checkerboard electronic structure in $Na_{0.96}Li_{0.04}FeAs$ — •Jose M. Guevara[1], Zhixiang Sun[1], Steffen Sykora[1], Chanhee Kim[2], Aga Shahee[2], Dilipkumar Bhoi[2], Kee Hoon Kim[2], Bernd Büchner[1], and Christian Hess[1] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]CeNSCMR, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, South Korea

Electronic order recently emerged as a general ingredient of unconventional superconductivity. A prominent example is the checkerboard electronic order, present in the pseudo-gap regime of the cuprates.

Lately, a new type of electronic order, lacking magnetic order has been reported in Li doped NaFeAs. We performed spectroscopic imaging scanning tunneling microscopy to reveal this new electronic order in real space and to clarify its relation with the nematic and superconducting phases. We present here evidence of electronic order that strikingly resembles the checkerboard order in the cuprates. Our finding thus constitutes the first example of this type of order in the iron-based superconductor (IBS). We characterize the associated q-vector equal to $\sim 0.18\frac{2\pi}{a_{Fe}}$ and discuss it in the context of further evidence of electronic order in the IBS.

TT 15.8 Mon 16:45 H23

Bandwidth controlled insulator-metal transition in $BaFe_2S_3$: A Mössbauer study under pressure — •Philipp Materne[1], Wenli Bi[2,1], Jiyong Zhao[1], Michael Yu Hu[1], Maria Lourdes Amigó[3], Silvia Seiro[3], Saicharan Aswartham[3], Bernd Büchner[3,4], and Esen Ercan Alp[1] — [1]Argonne National Laboratory, Lemont, IL 60439, USA — [2]Department of Geology, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA — [3]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, D-01069, Germany — [4]Institute of Solid State and Materials Physics, TU Dresden, D-01069 Dresden, Germany

$BaFe_2S_3$ is a quasi one-dimensional Mott insulator that orders antiferromagnetically below 117(5) K. The application of pressure induces a transition to a metallic state, and superconductivity emerges. The evolution of the magnetic behavior on increasing pressure has up to now been either studied indirectly by means of transport measurements, or by using local magnetic probes only in the low pressure region. Here, we investigate the magnetic properties of $BaFe_2S_3$ up to 9.9 GPa by means of synchrotron ^{57}Fe Mössbauer spectroscopy experiments, providing the first local magnetic phase diagram. The magnetic ordering temperature increases up to 185(5) K at 7.5 GPa, and is fully suppressed at 9.9 GPa. The low-temperature magnetic hyperfine field is continuously reduced from 12.9 to 10.3 T between 1.4 and 9.1 GPa, followed by a sudden drop to zero at 9.9 GPa indicating a first-order phase transition.

TT 15.9 Mon 17:00 H23

Finite electronic correlations and two-dome superconductivity across a clean nematic quantum phase transition — •Pascal Reiss[1], David Graf[2], Amir A Haghighirad[1,3], William Knafo[4], Loïc Drigo[4,5], Matt Bristow[1], Andrew J Schofield[6], and Amalia I Coldea[1] — [1]Clarendon Laboratory, University of Oxford, UK — [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, USA — [3]Institut fur Festkörperphysik, Karlsruhe Institute of Technology, Germany — [4]Laboratoire National des Champs Magnétiques Intenses (LNCMI-EMFL), Toulouse, France — [5]Géosciences Environnement Toulouse (CNRS), Toulouse, France — [6]School of Physics and Astronomy, University of Birmingham, UK

In the proximity of a nematic quantum critical point, electronic nematic fluctuations have been identified as a candidate for enhancing superconductivity in various unconventional superconductors. However, the coexistence of long-range magnetic order has hindered detailed studies of nematic criticality. To address this challenge, we combine chemical pressure in $FeSe_{1-x}S_x$ to suppress long-range magnetic order, and physical pressure to study the uncovered, clean nematic quantum phase transition. Using magneto-transport and quantum oscillations measurements, we trace the strength of electronic correlations and their role played in promoting superconductivity. We demonstrate that electronic correlations remain finite, the Fermi surface suffers a Lifshitz transition, and superconductivity is weakened across the nematic quantum phase transition. We interpret these results in light of recent theoretical and experimental advances, and sample quality.

15 min. break.

Invited Talk TT 15.10 Mon 17:30 H23

Theory of superconducting pairing in iron-based superconductors — •Andreas Kreisel — Universität Leipzig, Germany

Theoretical studies of high temperature superconductivity seem to struggle with the question whether the electronic states should be treated in an itinerant approach or using a picture where electrons are almost localized. In the case of iron-based materials, both approaches can explain a number of physical effects and the appearance of various phases. Guided by recent experimental results in the superconducting phase, we use a spin-fluctuation pairing theory that also contains low-energy aspects of strong correlations. A main ingredient of this itinerant approach is to incorporate reduced coherence of quasiparticles occupying specific orbital states into the description of the Fermi liquid. It is demonstrated that this paradigm yields remarkably good agreement with the experimentally observed anisotropic gap structure in 3 different materials: Bulk and monolayer FeSe, as well as LiFeAs. The first system has created a lot of interest recently, because it shows a strong anisotropy in its nematic state. For a deeper understanding of the connection to the Fermi liquid picture, we study the magnetic excitation spectrum [1] and consequences for the vortex formation in the superconducting state and discuss these in view of recent inelastic neutron scattering data and magnetic penetration depth measurements[2].

[1] A. Kreisel, Brian M. Andersen, P. J. Hirschfeld, arXiv:1807.09482
[2] P. Biswas, et al., Phys. Rev. B 98, 180501(R) (2018)

TT 15.11 Mon 18:00 H23

Symmetry-resolved strain tuning of composite nematic order — •Roland Willa, Max Fritz, and Jörg Schmalian — Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Electronic nematicity in iron pnictide superconductors and charge order in the high-T_c cuprates are two phenomena that are associated with the appearance of composite order. The response of these systems to external strain has proven to be a powerful tool to study their symmetry properties [1,2]. We deploy a long-wavelength field theory to investigate the nematic transition temperature and excitation spectrum of a low-dimensional system under strain. In certain symmetry channels, strain lifts the degeneracy of the nematic order—similar to magnetic field lifting the degeneracy of Ising spins—and a crossover replaces the phase transition. In degeneracy-preserving strain channels, we find a quadratic dependence of the transition temperature with respect to strain. The magnitude of this effect as the system approaches the 2d limit reveals a logarithmic divergence for specific symmetry channels (B_{ng} sector), while evaluating to order unity in others (A_{ng} sector). This finding is in good agreement with the strong effects observed in the B_{1g}-channel of $Ba(Fe_{0.975}Co_{0.025})_2As_2$, as reported in Ref. [2], and underlines the importance of anisotropy in this system.

[1] H.-H. Kim *et al.*, Science (accepted)
[2] M. Ikeda *et al.*, arXiv:1803.09273 (2018)

TT 15.12 Mon 18:15 H23

Quasiparticle Interference and Symmetry of Superconducting Order Parameter in Strongly Electron-Doped Iron-based Superconductors — •Jakob Böker[1], Pavel Volkov[2], Peter Hirschfeld[3], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey, 08854, USA — [3]Department of Physics, University of Florida, Gainesville, Florida32611, USA

Motivated by recent experimental reports of significant spin-orbit coupling (SOC) and a sign-changing order-parameter in the $Li_{1-x}Fe_x(OHFe)_{1-y}Zn_ySe$ superconductor with only electron Fermi surface present, we study the possible Cooper-pairing symmetries and their quasiparticle interference (QPI) signatures. We find that each of the resulting states - s-wave, d-wave and helical p-wave - can have a fully gapped density of states (DOS) consistent with angle-resolved photoemission experiments (ARPES) experiments and, due to spin-orbit coupling, are a mixture of spin singlet and triplet components leading to intra- and inter-band features in the QPI signal. Analyzing predicted QPI patterns we find that only the s- and d-wave pairing states with a dominant even parity triplet component can fit the experimental data with two dominant peaks in the DOS at energies roughly corresponding to the gap sizes at each pocket. Moreover, we show that pairing states with dominant triplet component may exist and can be identified using spin-resolved STM.

TT 15.13 Mon 18:30 H23

Enhanced Friedel oscillations by nematic fluctuations in an iron-based superconductor — •Steffen Sykora[1], Zhixiang Sun[1], Jose M. Guevara[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

Nematic fluctuations are known to provide an additional superconducting pairing channel which is considered as a possible explanation for the large critical temperatures in iron-based superconductors. We study its influence on the impurity scattering using a minimal microscopic model of nematic fluctuations in an effective two-band system of conduction electrons. Applying a projective renormalization method to integrate out the nematic interaction we find that the impurity scattering potential can be strongly renormalized at small scattering momentum through virtual particle-hole excitations in the d_{xz}/d_{yz} orbital channel. For the particular material LiFeAs we explicitly calculate the Fourier-transformed local density of states and find excellent agreement with recent scanning tunneling experiments* where resonantly enhanced Friedel oscillations have been attributed to the first spectroscopic evidence of nematic fluctuations in an iron-based superconductor.

[1] arXiv:1811.03489

TT 15.14 Mon 18:45 H23

Nematic fluctuations close to quantum criticality: a new method for comparing simulations and experiments — •Daniel Jost[1,2], Samuel Lederer[3], Thomas Böhm[1,2], Yoni Schattner[4,5], Erez Berg[6], Steven Kivelson[4], and Rudi Hackl[1,2] — [1]Walther-Meissner-Institute, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Cornell University, 14850 Ithaca, USA — [4]Department of Physics, Stanford University, 94305 Stanford, USA — [5]Stanford Institute of Material and Energy Science, 94025 Menlo Park, USA — [6]Department of Physics, University of Chicago, 60637 Chicago, USA

The comparison of numerical simulations and spectroscopic results is notoriously difficult due to the analytic continuation in the complex energy plane. Additionally, life times and mass enhancement factors must be extracted from the experimental spectra using, e.g., the Kramers-Kronig transformation with the well-known problems resulting from the extrapolations to low and high energies. One way out of this dilemma is a transformation of the experimental results from real to imaginary frequencies which provides us with an imaginary-time-ordered correlation function $\Lambda(\tau)$. From this transformation, one can extract the quantity $\beta\Lambda(\beta/2)$ with $\beta = 1/k_{\mathrm{B}}T$. In this contribution we derive this quantitiy from the electronic Raman spectra of the iron pnictide $\mathrm{Ba(Fe_{1-x}Co_x)_2As_2}$ as a function of doping and temperature. Additionally, we highlight the perspectives of this method with view on quantum criticality and the comparison of experiment and theory.