TT 54: Fe-based Superconductors

Time: Thursday 9:30–13:15 Location: HSZ 201

TT 54.1 Thu 9:30 HSZ 201

Many-body interaction in iron-based superconductors — •Jörg Fink[1,2,3], Emile Rienks[4], Jörn Bannies[2], Sabine Wurmehl[1], Saicharan Aswartham[1], Igor Morozov[1], Luis Craco[1], Helge Rosner[2], Claudia Felser[2], and Bernd Büchenr[1,3] — [1]IFW Dresden — [2]MPI Chemical Physics of Solids, Dresden — [3]TU Dresden — [4]HZB Berlin

In this talk we will report on the determination of the energy and momentum dependence of scattering rates in iron-based superconductors using angle-resolved photoemission spectroscopy. We receive information on the location of hot spots on the Fermi surface determining antiferromagnetism and superconductivity as well as on cold spots determining the normal state transport and optical properties. For the hole doped compounds, we obtain scattering rates well above the Planckian limit, indicating a highly incoherent normal state electronic structure. In this way we obtain a microscopic understanding of the electronic structure of these systems in the normal and in the superconducting state. The experimental results on ferropnictides are compared with DFT+DMFT calculations describing Hunds metal behavior. There are remarkable differences between theory and experiment. The reason for this is possibly that DFT+DMFT uses only local correlation effects and does not include non-local spin fluctuation excitations.

TT 54.2 Thu 9:45 HSZ 201

DMFT study of Hund's metals: the charge response of Fe-based superconductors — •Alexander Kowalski — Institut für Theoretische Physik und Astrophysik, Universität Würzburg

We investigate various multi-orbital Hubbard models for iron-based superconductors, from a five-orbital Wannier-based Hamiltonian of $BaFe_2As_2$ down to simpler three- and two-orbital descriptions. These systems have previously been analyzed using techniques such as slave-spin mean field [1], which have shown the existence of a Hund-driven strongly-correlated phase close in doping to the half-filled Mott transition. Our DMFT calculations using a continuous-time quantum Monte Carlo solver for one- and two-particle quantities [2] reveal the presence of regions of phase separation with diverging charge compressibility.

[1] L. de' Medici, Phys. Rev. Lett **118**, 167003 (2017)
[2] M. Wallerberger, A. Hausoel, P. Gunacker, A. Kowalski, N. Parragh, F. Goth, K. Held, G. Sangiovanni, Comput. Phys. Commun. **235**, 388 (2019)

TT 54.3 Thu 10:00 HSZ 201

Impurity-induced bound states in Fe-based superconductors with spin-orbit coupling — •Peayush Choubey and Ilya Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany

We investigate the effects of residual spin-orbit coupling (SOC), inherently present in Fe-based superconductors (FeSCs), and consequent admixture of singlet and triplet Cooper-pairing in the even parity channel in the superconducting state, on the in-gap bound states induced by point-like, magnetic and non-magnetic impurities. Using low-energy models, which capture all the symmetries of FeSCs and treat the atomic SOC consistently, we solve the impurity scattering problem in the T-matrix framework. We find that if $s_{\pm}$ pairing state has a significant triplet contribution at the electron pockets around $M = (\pi, \pi)$-point, the impurity-induced bound states are robust against the out-of-plane Zeeman field. The heavily suppressed Zeeman splitting of impurity states is a consequence of reduction in effective Landé g-factor caused by atomic SOC.

TT 54.4 Thu 10:15 HSZ 201

Tracking nematic fluctuations using the Nernst effect in iron based superconductors — •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

The role of nematic fluctuations, shown to be present across the phase diagram of iron based superconductors, especially their correlation with possible quantum critical points and high temperature superconductivity, has been under constant debate. Here we show that the Nernst coefficient is sensitive to the nematic fluctuations in iron based superconductors. We detect a similar behavior of the Nernst effect and elastoresistivity measurements in Co doped LaFeAsO while a difference of these probes can be obtained in Rh doped $BaFe_2As_2$. In both materials the Nernst effect is tracking the superconducting dome upon doping, providing evidence for superconductivity supported by nematic fluctuations.

TT 54.5 Thu 10:30 HSZ 201

Elasto-Nernst effect: a sensitive probe for nematicity — •Federico Caglieris[1], Xiaochen Hong[1], Michael Wissmann[1], Christoph Wuttke[1], Steffen Sykora[1], Rhea Kappenberger[1], Saicharan Aswartham[1], Sabine Wurmehl[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [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 discovery of a divergent elasto-resistivity in iron-based superconductors promoted the nematicity to the class of the electronic orders together with superconductivity and density-waves, supporting the intriguing idea of an intimate link among all electronic instabilities. In this work we investigate the nematic phenomenology in different families of iron-based superconductors using a novel technique, which combines a state-of-art setup for Nernst effect measurements with a piezoelectric device for the application of uniaxial strain. By studying the temperature-dependence of the strain-derivative of the Nernst coefficient, we discovered that a Curie-Weiss-like fashion governs also the elasto-Nernst effect, as a fingerprint of strong nematic fluctuations. However, despite the universal diverging behavior, we show that elasto-Nernst and elasto-resistivity are not equivalently representative of the nematic susceptibility, offering a new insight into the nematic puzzle. Moreover, the emerging scenario provides an evidence of a band-dependent nematicity.

TT 54.6 Thu 10:45 HSZ 201

^{75}As NMR under uniaxial pressure in $BaFe_2As_2$ — •Adam P. Dioguardi[1], Tobias Schorr[1], Clifford W. Hicks[2], Saicharan Aswartham[1], Sabine Wurmehl[1], Bernd Büchner[1,3], and Hans-Joachim Grafe[1] — [1]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Institut für Festkörperphysik, TU Dresden, 01062 Dresden, Germany

We have conducted systematic ^{75}As nuclear magnetic resonance (NMR) experiments in $BaFe_2As_2$ under controlled conditions of uniaxial pressure. We find that the electric field gradient (EFG), spin-lattice relaxation rate T_1^{-1}, spin-spin relaxation rate T_2^{-1} and Knight shift K at the As site are sensitive to applied uniaxial pressure. We find that uniaxial pressure increases, broadens, and separates the Néel temperature T_N and the tetragonal-to-orthorhombic structural transition T_S. Our spectral measurements in the magnetic state exhibit no evidence of a predicted spin reorientation for both positive and negative applied uniaxial pressure up to the point of sample failure.

TT 54.7 Thu 11:00 HSZ 201

Unconventional superconductivity and electronic structure of ultra-pure single crystal YFe_2Ge_2 — •Jiasheng Chen[1], Jordan Baglo[1,2], Keiron Murphy[1], Devashibhai Adroja[3], Pabitra Biswas[3], Jacintha Banda[4], Manuel Brando[4], and Malte Grosche[1] — [1]Cavendish Laboratory, Cambridge, UK — [2]Université de Sherbrooke, Canada — [3]ISIS Neutron and Muon Source Science, RAL, UK — [4]MPI CPfS, Dresden, Germany

The layered iron-based superconductor YFe_2Ge_2 exhibits an unusually high Sommerfeld coefficient of ~ 100 mJ/molK^2 and a $T^{3/2}$ temperature dependence of electrical resistivity at low temperature [1-3], indicating strong electronic correlations. While superconductivity in YFe_2Ge_2 is widely observed below $T_c \sim 1.9$ K in electric transport measurements, it is strongly suppressed by lattice disorder [1-3], hinting at an unconventional pairing mechanism.

Our new generation of single crystals reach residual resistivity ratios (RRR) in excess of 650. These crystals display a sharp superconducting heat capacity anomaly just below 1.2 K. For the first time, they enable detailed thermodynamic and spectroscopic studies of the normal and superconducting states of YFe_2Ge_2. These include low temperature heat capacity measurements, the resolution of key aspects of the electronic structure of YFe_2Ge_2 by quantum oscillation techniques and the determination of the penetration depth by muon spin rotation measurements.

[1] Y. Zou et al., PSS-RRL **8**, 928 (2014)
[2] J. Chen et al., PRL, **116**, 127001 (2016)
[3] J. Chen et al., PRB, **99**, 020501(R) (2019)

15 min. break.

TT 54.8 Thu 11:30 HSZ 201

Oxygen vacancies modulated superconductivity in monolayer FeSe on SrTiO3-δ — •Lili Wang — Tsinghua University, Beijing, China

The monolayer FeSe on SrTiO3-δ exhibits a twofold enlarged pairing gap compared with other electron-doped FeSe, which is postulated to originate from cooperative effects of interface charge transfer and electron-boson interaction that relate closely to surface oxygen vacancies in SrTiO3. We create gradient oxygen vacancies on the surface of SrTiO3-δ substrates by using direct current heating. Combining spatially resolved spectroscopy characterizations, we disclose gradient pairing gaps but negligible doping variation in monolayer FeSe on such substrates. As oxygen vacancy concentration gradually increases from anode to cathode region, the pairing gap increases from 12 to 17 meV, right beyond the values of electron-doped FeSe. This modulation provides a platform for spatially resolved investigations to unveil the interplay between electronic correlation and electron-phonon interaction and their cooperation to drive superconductivity.

TT 54.9 Thu 11:45 HSZ 201

Field-dependent Elastoresistance in FeSe — •Michael Wissmann[1], Federico Caglieris[1], Steffen Sykora[1], Saicharan Aswartham[1], Sabine Wurmehl[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]IFW Dresden — [2]Institute for Solid State Physics, TU Dresden — [3]Center for Transport and Devices, TU Dresden

In iron-based superconductors, nematicity has been proposed to be closely related to the emergence of superconductivity. The introduction of uniaxial strain as a tuning parameter has been established as an important tool to probe nematic fluctuations at temperatures higher than the structural transition temperature T_S. This type of elastoresistance measurement has opened an exciting new route to understanding the interplay of nematicity, superconductivity and magnetism. However, the physical meaning of elastoresistance data for temperatures below T_S is rarely discussed. Here, we investigate the elastoresistance-behaviour in low temperatures under application of external magnetic fields inside the nematic phase of iron selenide (FeSe). FeSe is, under many aspects, an exceptional representative of the iron-based-superconductor-class. We observe a strong field-dependence as well as a second divergence towards the superconducting phase. Various scenarios for the origin of this novel observations will be discussed.

TT 54.10 Thu 12:00 HSZ 201

One-Electron-Pocket Model of FeSe: Quasiparticle Interference — •Matthias Eschrig[1,2], Luke C. Rhodes[2,3,4], Matthew D. Watson[4], and Timur K. Kim[4] — [1]Universität Greifswald, Germany — [2]Royal Holloway, University of London, UK — [3]University of St. Andrews, UK — [4]Diamond Light Source, Harwell Campus, UK

The one-electron-pocket model of FeSe was introduced to account for experimental observations in angle-resoved photoemission (ARPES) experiments. Quasiparticle interference (QPI) measurements of FeSe, obtained via scanning tunneling microscopy, have previously been interpreted as being consistent with a theoretical model where the Fermi surface consists of one hole pocket and two electron pockets and exhibits a large difference in the quasiparticle weight of the d_{xz} and d_{xy} orbitals. On the contrary, orbital sensitive measurements from ARPES have been interpreted as being consistent with a model with roughly equivalent quasiparticle weights for the d_{xz} and d_{yz} orbitals, but with only one hole pocket and one electron pocket at the Fermi surface present. Here, we show that the second, one-electron-pocket, model also explains QPI experiments. We find, that it is important to apply a selection rule for QPI, that only electronic states with vanishing component of the Fermi velocity perpendicular to the scanning surface contribute to the interference pattern. By using a three-dimensional tight-binding model of FeSe, fit to ARPES measurements, we directly reproduce the experimental QPI results, within a T-matrix formalism. This unifying result for QPI and ARPES on FeSe also highlights the importance of selection rules for QPI experiments via STM.

TT 54.11 Thu 12:15 HSZ 201

***Ab initio* investigation of dipole-dipole interactions in response to lattice distortions in FeSe** — •Felix Lochner[1], Ilya Eremin[2], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, 44801 Bochum, Deutschland

The electronic structure in unconventional superconductors holds a key to understand the momentum-dependent pairing interactions and the resulting superconducting gap function. In superconducting Fe-based chalcogenides, there have been controversial results regarding the importance of the k_z dependence of the electronic dispersion, including non-trivial topology and the gap structure and the pairing mechanisms of iron-based superconductivity. Here, we present a detailed investigation of the dipole-dipole response in FeSe, known as van-der-Waals (vdW) interaction, and its interplay with magnetic disorder and real space structural properties. Using density functional theory we show that they need to be taken into account upon investigation of the 3-dimensional effects, including non-trivial topology, of $FeSe_{1-x}Te_x$ and $FeSe_{1-x}S_x$ systems. In addition, the impact of paramagnetic disorder is considered within the spin-space average approach. Our calculations show, that the PM relaxed structure supports the picture of different competing ordered magnetic states in the nematic regime, yielding magnetic frustration.

TT 54.12 Thu 12:30 HSZ 201

MBE preparation and in-situ characterization of FeTe thin films — •Vanda M. Pereira[1], Chi-Nan Wu[1,2], Cheng-En Liu[1,3], Sheng-Chieh Liao[1], Chun-Fu Chang[1], Chang-Yang Kuo[1,4], Cevriye Koz[1], Ulrich Schwarz[1], Hong-Ji Lin[4], Chien-Te Chen[4], Liu Hao Tjeng[1], and Simone G. Altendorf[1] — [1]MPI-CPfS, Dresden, Germany — [2]Dept. of Physics, NTHU, Hsinchu, Taiwan — [3]Dept. of Electrophysics, NCTU, Hsinchu, Taiwan — [4]NSRRC, Hsinchu, Taiwan

Within the family of Fe based superconductors, Fe chalcogenides have received particular attention due to their simple crystal structure. $Fe_{1+y}Te$, which is not superconducting, has been studied extensively in bulk form and, more recently, some efforts have been made regarding the synthesis of thin films, resorting to pulsed laser deposition and molecular beam epitaxy (MBE). Here we report the results of $Fe_{1+y}Te$ thin films grown by MBE under Te-limited growth conditions. We found that epitaxial layer-by-layer growth is possible for a wide range of excess Fe values, wider than expected from studies on the bulk material. Using XMCD at the Fe $L_{2,3}$ and Te $M_{4,5}$ edges, we observed that films with high excess Fe contain ferromagnetic clusters while films with lower excess Fe remain nonmagnetic. Moreover, x-ray absorption spectroscopy showed that it is possible to obtain films with very similar electronic structure as that of a high-quality bulk single crystal $Fe_{1.14}Te$. Our results suggest that MBE with Te-limited growth may provide an opportunity to synthesize FeTe films with smaller amounts of excess Fe as to come closer to a possible superconducting phase.

TT 54.13 Thu 12:45 HSZ 201

X-ray absorption spectroscopy measurements of $Fe_{1+x}Te$ — •Jan Fikáček[1], Jonas Warmuth[2], Fabian Arnold[3], Sunil Wilfred[4], Cinthia Piamonteze[5], Martin Bremholm[3], Ján Minár[4], Ján Lančok[1], Philip Hofmann[3], Jens Wiebe[2], and Jan Honolka[1] — [1]Institute of Physics of CAS, Prague, Czech Republic — [2]Hamburg University, Hamburg, Germany — [3]Aarhus University, Aarhus, Denmark — [4]University of West Bohemia, Plzeň, Czech Republic — [5]Paul Scherrer Institut, Villigen, Switzerland

Iron based chalcogenides (IBC) have a quasi two-dimensional crystal structure, which is the simplest one among Fe-based superconductors and makes IBC good candidates for both experimental and theoretical studies. FeSe is superconducting below T_c = 8 K [1] going above 100 K when an FeSe monolayer is grown on $SrTiO_3$ [2]. In contrast, the analog non-superconducting $Fe_{1+x}Te$ has an antiferromagnetic (AFM) ground state varying with the excess Fe concentration x.

Here, we report on results of X-ray absorption spectroscopy measurements of $Fe_{1+x}Te$ with x = 0.094 ordering antiferromagnetically below $T_N = 62$ K. X-ray magnetic circular dichroism up to 7 T scales linearly with the bulk magnetization. Both drop when $Fe_{1.094}Te$ enters the AFM state. In contrary, X-ray magnetic linear dichroism (XMLD) increases monotonically below T_N down to lowest temperatures. XMLD data are compared with results of our density functional theory calculations taking into account Fe excess up to x = 1.1.

[1] F. C. Hsu et al., PNAS 105, 14262 (2008).
[2] S. L. He et al, Nat. Mater. 12, 605 (2013).

TT 54.14 Thu 13:00 HSZ 201

Scanning tunneling microscopy and spectroscopy on $Fe_{1+y}Te$ (y=0.11, 0.12) — •Sahana Roessler, Cevriye Koz, Ulrich Schwarz, and Steffen Wirth — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany

The antiferromagnetic compound $Fe_{1+y}Te$ with tetragonal structure at room temperature displays a complex phase diagram with several structural and magnetic phase transitions within the homogeneity range $0.06 \leq y \leq 0.15$ [1]. While $Fe_{1.11}Te$ undergoes a single-phase transition from a paramagnetic tetragonal to an antiferromagnetic monoclinic phase, $Fe_{1.12}Te$ exhibits a two-phase mixture of orthorhombic and monoclinic phases at temperatures below about 46 K. We compare the low-temperature microstructure [2] of these two compositions using scanning tunneling microscopy. The tunneling spectra on $Fe_{1.11}Te$ displayed a shoulder at a bias voltage of 7 mV, likely related to the energy scale of the antiferromagnetic spin-density-wave order. In contrast, in $Fe_{1.12}Te$, we occasionally observed a zero-bias conductance peak in the tunneling spectra, induced by magnetic impurity scattering originating from the segregated excess interstitial Fe on the surface.

[1] C. Koz et al., Phys. Rev. B, **88**, 094509 (2013)
[2] S. Rößler et al., Proc. Natl. Acad. Sci. **116**, 16697 (2019).