TT 5: Superconductivity: Fe-based Superconductors - FeSe and 122

Time: Monday 9:30–13:00 Location: H23

TT 5.1 Mon 9:30 H23

Elastoresistance and resistivity anisotropy in FeSe under uniaxial strain — •Alexander Steppke[1], Jack Bartlett[1,2], Suguru Hosoi[3], Takasada Shibauchi[3], Andrew Mackenzie[1,2], and Clifford Hicks[1] — [1]Max-Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, Dresden, 01187, Germany — [2]University of St Andrews, School of Physics and Astronomy, St Andrews KY16 9SS, United Kingdom — [3]University of Tokyo, Department of Advanced Materials Science, Kashiwa, Chiba 277-8561, Japan

The phase diagram of iron-based superconductors features breaking of rotational symmetry, the electronic nematic order. Its microscopic origin and consequences for the transport and magnetic properties are under intense debate. We set out to tune the crystal structure of FeSe using uniaxial strain. Without magnetic order at ambient pressure this material undergoes a tetragonal-to-orthorombic transition around 90 K. Whereas this transition only leads to small changes in the lattice constants, the electrical transport, i.e., the resistivity can exhibit anisotropies of several percent. With the development of a sample-on-platform technique we were able to apply uniaxial strains up to 0.6% in a wide temperature range for this very ductile material. This enables continuous tuning of FeSe from the twinned to fully detwinned state and beyond. We report on the non-monotonic elastoresistance, the resistance anisotropy and characterize the contribution of domains to the resistivity within the nematic phase.

TT 5.2 Mon 9:45 H23

Thermal expansion study on $Fe_{1+y}Te_{1-x}Se_x$ — •Liran Wang[1,2], Anna Böhmer[2], Frédéric Hardy[2], Thomas Wolf[2], Peter Adelmann[2], Michael Merz[2], Mahmoud Abdel-Hafiez[3], Rüdiger Klingeler[1], and Christoph Meingast[2] — [1]Kirchhoff Institute of Physics, Heidelberg University, Germany — [2]Institute for Solid State Physics, Karlsruhe Institute of Technology, Germany — [3]Physikalisches Institute Goethe-Universität,Germany

The $Fe_{1+y}Te_{1-x}Se_x$ series presents one of the main families of high T_C Fe-based superconductors. To provide further insight into these materials, we present detailed thermal expansion study on high quality single-crystalline $Fe_{1+y}Te_{1-x}Se_x$ ($0 \leq x \leq 0.4$) by means of high-precision capacitance dilatometry. Clear anomalies in the thermal expansivity are observed at both the magneto/structural and superconducting transitions. Further, the electronic component of the thermal expansion is quite large and can be extracted from the data. We discuss these data in light of strong electronic correlations and possible quantum criticality.

TT 5.3 Mon 10:00 H23

Electronic structure of iron-based superconductors: BKFA and FeSe — •Volodymyr Bezguba[1,3] and Alexander Kordyuk[1,2] — [1]Kyiv Academic University, 36 Vernadsky blvd., Kyiv 03142, Ukraine — [2]G. V. Kurdyumov Institute for Metal Physics, 36 Vernadsky blvd., Kyiv 03142, Ukraine — [3]IFW Dresden, Helmholtz-Straße 20, D-01069 Dresden, Germany

The nature of high-temperature superconductivity (HTSC) remains unclear. There are many different theoretical models, which describe some of HTSC aspects and peculiarities, but none of them is neither fully predictive nor coherent enough. Because of the extremely complicated electronic structure, the iron-based superconductors (IBS) are one of the most interesting classes of HTSC to study. In particular, the effect of three-dimensionality of electronic structure on electronic properties of IBS is not clear at all.

Using angle-resolved photoemission spectroscopy (ARPES) we have measured and studied the kz-dependence of electronic structure in BKFA. We focus on peak positions of unoccupied bands in different points of Brillouin zone, Fermi surface and renormalization dependencies. A number of unexpected effects have been observed such as the swap of known excitation energy values for Γ and Z points and renormalization dependence from kz in BKFA.

In addition, temperature dependence of FeSe was carefully studied and leads to new explanation of dxy-band shift in the center of Brillouin's zone.

TT 5.4 Mon 10:15 H23

Impact of magnetic disorder and van der Waals interaction on structure parameters of FeSe and FeTe superconductors by density functional theory calculations — •Felix Lochner[1,2], Ilya Eremin[2], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany

Density functional theory (DFT) calculations for iron base superconductors often show deviations in the lattice constants compared to experiment. Therefore, we have studied the impact of the magnetic phase on the lattice parameters of FeSe and FeTe. We focus on the competition between stripe-type anti ferromagnetism (AFM) and paramagnetic disorder (PM). The PM state is implemented by using the spin-space average approach [1]. We find for both magnetic states an unphysical behavior of the structural ground state. The reason is the lack of Van der Waals (vdW) interaction in the employed PBE-GGA functional. Therefore, we have applied several approaches to include vdW. Our results show, that the additional vdW forces have a large impact on the out-of-plane lattice constant. Using the PM spin configuration together with the Van der Waals corrections we obtain lattice constants that are in excellent agreement with those obtained from experiment [2].

[1] F. Körmann, A. Dick, B. Grabowski, T. Hickel, and J. Neugebauer, Phys. Rev. B **85**, 125104 (2012)
[2] F. Ricci and G. Profetta, Phys. Rev. B **87**, 184105 (2013)

TT 5.5 Mon 10:30 H23

Magnetic fluctuations in FeSe: effect of orbital selectivity — •Andreas Kreisel[1], Johannes H. J. Martiny[2], Brian M. Andersen[3], and Peter J. Hirschfeld[4] — [1]Universität Leipzig, Germany — [2]Center for Nanostructured Graphene, Technical University of Denmark, Denmark — [3]Niels Bohr Institute, University of Copenhagen, Denmark — [4]University of Florida, USA

Recent STM experiments and theoretical considerations have highlighted the role of interaction-driven orbital selectivity in FeSe, and its role in generating the extremely anisotropic superconducting gap structure in this material. We study the magnetic excitation spectrum resulting from the coherent quasiparticles within the same renormalized random phase approximation approach used to explain the STM experiments, and show that it agrees well with the low-energy momentum and energy dependent response measured by inelastic neutron scattering experiments. We find a correlation-induced suppression of (π, π) scattering due to a small quasiparticle weight of states of d_{xy} character [1]. We compare predictions for twinned and untwinned crystals, and predict in particular a strongly $(\pi, 0)$-dominated susceptibility at low energies in untwinned systems. Since the system is known to be close to a magnetic phase transition, it is possible that impurities can pin local magnetic order in this system. Within a mean field approach in real space, we deduce the structure of such local magnetic order and predict implications of this as been visible in a STM experiment even if a non-spinpolarized technique is used [2].

[1] A. Kreisel et al., arXiv:1807.09482
[2] J. Martiny et al., arXiv:1811.01788

TT 5.6 Mon 10:45 H23

Non-local Correlations in FeSe within the Two-Particle Self-Consistent approach — •Karim Zantout[1], Steffen Backes[2], and Roser Valentí[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany — [2]CPHT, Ecole Polytechnique, 91128 Palaiseau cedex, France

In this talk we will present results on non-local correlations in FeSe obtained with the non-perturbative Two-Particle Self-Consistent approach that provides a frequency- and momentum-dependent Self energy. We will compare our calculations to results obtained by local approximation techniques as DMFT and discuss their relevance to experimental observations such as ARPES experiments.

TT 5.7 Mon 11:00 H23

Band engineering in the iron pnictides: Search for topological surface states — •Lars Lauke[1], Rolf Heid[1], Michael Merz[1], Amir-Abbas Haghighirad[1], and Jörg Schmalian[1,2] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie (KIT), 76344

Eggenstein-Leopoldshafen, Deutschland — [2]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe, Deutschland

By band engineering the iron pnictide Fe(SeTe) via ab-initio calculations, we search for topological surface states and realizations of Majorana bound states. Proposed topological states are expected to occur for non-stoichiometric compositions on a surface Dirac cone where issues like disorder scattering and charge transfer between the relevant electronic states have to be addressed. However, this surface Dirac cone is well above the Fermi-level. The goal is to make the surface Dirac cone experimentally accessible by modifying the bulk material without disturbing the surface. Going beyond conventional density functional theory (DFT), we apply the coherent potential approximation (BEB-CPA) in a mixed basis pseudopotential framework to scan the substitutional phase-space of co-substitutions on the Fe- and Se-sites. We find that substitution on the transition-metal-site is not a viable option but a number of viable candidates at the Se-site achiev the desired effect of bringing the Dirac cone into vicinity of the Fermi-level. We further seek to experimentally realize these predicted compounds.

15 min. break.

TT 5.8 Mon 11:30 H23

Temperature dependence of quasiparticle states in superconducting monolayer FeSe on STO: a theoretical study — •Fabian Schrodi, Alex Aperis, and Peter Oppeneer — Department of Physics and Astronomy, Uppsala University, Sweden

We study the temperature evolution of the quasiparticle bands of the FeSe monolayer on the $SrTiO_3$ (STO) substrate from 10 to 300 K by applying the anisotropic, multiband and full-bandwidth Eliashberg theory. To achieve this, we extend this theory by self-consistently coupling the chemical potential to the full set of Eliashberg equations. In this way, regardless of the temperature, the electron filling can be kept at a constant level with high accuracy. Solving the coupled equations self-consistently, and with focus on the interfacial electron-phonon coupling, we predict a non-trivial evolution of the global chemical potential. Focusing on the ARPES spectra, we suggest a new route to determine the energy scale of the interfacial phonon mode by measuring the energy position of second-order replica bands. Finally, our results reveal potential implications for the determination of the momentum anisotropy of the superconducting gap in ARPES measurements [1].
[1] F. Schrodi, A. Aperis, P. M. Oppeneer, Phys. Rev. **98**, 094509 (2018)

TT 5.9 Mon 11:45 H23

Cavity-enhanced electron-phonon coupling in monolayer FeSe/STO — •Michael Sentef[1], Michael Ruggenthaler[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010

Laser control of solids was so far mainly discussed in the context of strong classical nonlinear light-matter coupling in a pump-probe framework. Here we propose a quantum-electrodynamical setting to address the coupling of a low-dimensional quantum material to quantized electromagnetic fields in quantum cavities [1]. Using a protoypical model system describing FeSe/$SrTiO_3$ with electron-phonon long-range forward scattering, we study how the formation of phonon polaritons at the 2D interface of the material modifies effective couplings and superconducting properties in a Migdal-Eliashberg simulation. We find that through highly polarizable dipolar phonons, large cavity-enhanced electron-phonon couplings are possible but superconductivity is not enhanced for the forward-scattering pairing mechanism due to the interplay between coupling enhancement and mode softening. Our results demonstrate that quantum cavities enable the engineering of fundamental couplings in solids paving the way to unprecedented control of material properties.
[1] M. A. Sentef, M. Ruggenthaler, A. Rubio, Science Advances 4, eaau6969 (2018).

TT 5.10 Mon 12:00 H23

Interplay of lattice, electronic, and spin degrees of freedom in detwinned $BaFe_2As_2$: A Raman scattering study — •Andreas Baum[1,2], Ying Li[3], Milan Tomić[3], Nenad Lazarević[4], Daniel Jost[1,2], Florian Löffler[1,2], Bernhard Muschler[1], Thomas Böhm[1,2], Jiun-Haw Chu[5,6,7], Ian R. Fisher[5,6], Roser Valentí[3], Igor I. Mazin[8], 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, 60438 Frankfurt am Main, Germany — [4]Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia — [5]SIMES, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — [6]GLAM and Department of Applied Physics, Stanford University, Stanford, CA 94305, USA — [7]Department of Physics, University of Washington, Seattle WA 98195, USA — [8]Code 6393, Naval Research Laboratory, Washington, DC 20375, 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 3.1 eV with distinct differences between the antiferromagnetically and the ferromagnetically ordered direction. The E_g phonon at 130 cm^{-1} splits into two modes having B_{2g} and B_{3g} symmetry which differ by 10 cm^{-1}. Both effects can be attributed to the emergence of magnetic order, rather than the structural transition, by DFT calculations.

TT 5.11 Mon 12:15 H23

Unusual thermoelectric properties of $BaFe_2As_2$ in high magnetic fields — •Martina Meinero[1,2], Federico Caglieris[3], Gianrico Lamura[2], Ilaria Pallecchi[2], Andreas Jost[4], Uli Zeitler[4], Shigeyuki Ishida[5], Hiroshi Eisaki[5], and Marina Putti[1,2] — [1]Dipartimento di Fisica, Università di Genova, Via Dodecaneso 33, 16146 Genova, Italy — [2]CNR-SPIN, Corso Perrone 24, 16152 Genova, Italy — [3]IFW Dresden, Helmholtz Strasse 33, Dresden, Germany — [4]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Toernooiveld 7, 6525ED Nijmegen, The Netherlands — [5]National Institute of Advanced Industrial Science and Technology, Tsukuba 305-8568, Japan

Electric and thermoelectric transport properties are mutually intertangled in diffusive transport equations. In particular, in high mobility multiband systems an anomalous behavior may occur, which can be tracked down to the properties of the individual bands. Here, we present magneto-electric and magneto-thermoelectric transport properties of a $BaFe_2As_2$ high-quality single crystal, for different magnetic field directions up to 30 T. We detect a giant Nernst effect and an anomalous field dependence of the Seebeck coefficient. The extraction of the Peltier tensor coefficients α_{xx}, α_{xy} and α_{xz} allows us to disentangle the main transport mechanisms in play. The large α_{xy} and α_{xz} values and their field dependence provide evidence of the presence of a high mobility band, compatible with a Dirac dispersion band, crossing the Fermi level, and suggest a possible three-dimensional nature of the Dirac fermions.

TT 5.12 Mon 12:30 H23

Charge density wave instability in $Ba(Ni_{1-x}Fe_x)_2As_2$ probed by time-resolved optical spectroscopy. — •V. Yu. Grigorev[1,2], A. Mejas[3], T. Dong[1], Th. Wolf[4], A. A. Haghighirad[4], C. Meingast[4], M. Le Tacon[4], M. Merz[4], and J. Demsar[1] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, Mainz, Germany — [2]Graduate School of Excellence, Materials Science in Mainz (MAINZ), Mainz, Germany — [3]Institute for solid state physics, TU Wien, Vienna, Austria — [4]Institute for Solid State Physics, KIT, Karlsruhe, Germany

In Fe-based superconductor $BaFe_2As_2$, which displays the spin-density wave order, superconductivity is induced by chemical doping, reaching the maximum T_c of 24 K [1]. In its structural homologue $BaNi_2As_2$, however, superconductivity is observed even in undoped samples, yet the maximal T_c in Co-doped samples does not exceed 3 K [2,3]. Recent diffraction studies [4] suggest that superconductivity in $BaNi_2As_2$ is competing with the unidirectional charge-density-wave (CDW) order. Here we report on optical femtosecond time-resolved spectroscopy on weakly doped $BaNi_{1.93}Fe_{0.07}As_2$, aiming at investigating the CDW collective modes - see e.g. [4]. We present a clear evidence for a commensurate-to-incommensurate CDW lock-in phase transition at 45 K, and the low temperature amplitude mode at 1 THz in the commensurate CDW phase.
[1] J. Paglione and R. L. Greene, Nat. Phys. 6, 645 (2010)
[2] Z. G. Chen et al., Phys. Rev. B 80, 094506 (2009)
[3] S. Lee et al., arXiv:1801.04874
[4] H. Schäfer et al., Phys. Rev. B. 89, 045106 (2014)

TT 5.13 Mon 12:45 H23

Nematic susceptibility in heavily hole-doped iron-based superconductors — •Xiaochen Hong[1], Saicharan Aswartham[1], Igor Morozov[1,2], Steffen Sykora[1], Federico Caglieris[1], Silvia Seiro[1], Bernd Büchner[1,3,4], and Christian Hess[1,4] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden (IFW-Dresden), Dresden, Germany — [2]Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia — [3]Institute of Solid State Physics, TU Dresden, Dresden, Germany — [4]Center for Transport and Device, TU Dresden, Dresden, Germany

Unconventional superconductivity typically is closely related to the suppression of ordered states which possibly compete or coexist with superconductivity in the underdoped region. The overdoped systems are usually assumed to stay in a rather conventional Fermi liquid state. However, for iron-based superconductors, experiments indicate that the heavily hole-doped end-member KFe_2As_2, together with its sister compounds, are more complicated including the possibility of emerging electronic nematic order.

We present elasto-resistivity measurements of KFe_2As_2, revealing a divergent nematic susceptibility. The evolution of nematic susceptibility is also tracked with isovalent doping and electron doping on the K site. Our results point to unexpected nematic critical point(s) in those overdoped superconductors.