# TT 52: Superconductivity: Fe-based Superconductors - FeSe and LiFeAs

Time: Wednesday 9:30–13:00 Location: HFT-FT 101

TT 52.1 Wed 9:30 HFT-FT 101

**Interfacial phonons in the single unit cell of FeSe grown on $SrTiO_3$(001)** — •Dominik Rau[1], Tobias Engelhardt[2], Jasmin Jandke[2], Fang Yang[2], Endre Barta[2], Wulf Wulfhekel[2], and Khalil Zakeri Lori[1] — [1]Heisenberg Spin-dynamics Group, Physikalisches Institut, Karlsruhe Institute of Technology, Germany — [2]Physikalisches Institut, Karlsruhe Institute of Technology, Germany

Among all Fe-based superconductors a single unit cell of FeSe on $SrTiO_3$ exhibits the highest transition temperature $T_c$. Despite the intensive research, the physical origins of the observed high $T_c$ and the role of the interfacial phonons in superconductivity are still highly under debate. Utilizing high-resolution electron energy-loss spectroscopy we probe the phonon spectrum in a unit cell of FeSe epitaxially grown on Nb-doped $SrTiO_3$(001). The Fuchs–Kliewer interfacial phonons are observed to appear at energies of 57 and 91.5 meV near the zone center. Both modes exhibit a weak dispersion while increasing the wave vector from $\overline{\Gamma}$ towards the zone boundary ($\overline{\mathrm{X}}$-point). The intrinsic linewidth of the higher energy phonon mode is about 11.5 meV at the $\overline{\Gamma}$-point and remains nearly constant over a large fraction of the Brillouin zone. The nearly momentum-independent phonon lifetime excludes particularly strong electron–phonon coupling near the zone center. This observation indicates that other bosonic excitations, e.g. those of electronic origin, should play an important role in the formation of Cooper pairs and superconductivity in this system. This work has been supported by DFG through the Heisenberg Programme ZA 902/3-1 and DFG Grant Wu 349/12-1 and by the Alexander von Humboldt Foundation.

TT 52.2 Wed 9:45 HFT-FT 101

**Interface high temperature superconductivity in FeSe/$TiO_2$** — •Lili Wang and Qikun Xue — Tsinghua University, Beijing, China

The discovery of high temperature superconductivity with a superconducting gap of 20 meV in monolayer FeSe films epitaxially grown on $SrTiO_3$ substrate has stimulated tremendous interest in superconductivity community, for it opens new avenue for both raising superconducting transition temperature and understanding the pairing mechanism of unconventional high temperature superconductivity. In this talk, I will present the experimental progress on interface enhanced superconductivity in FeSe/$TiO_2$ interfaces, studied by scanning tunneling microscopy/spectroscopy, angle-resolved photoemission spectroscopy and transport experiments. Then I will discuss the roles of interfaces, such as charge transfer and electron-phonon coupling, inferred from those studies.

[1] Q.-Y. Wang et al., Chin. Phys. Lett. 29, 037402 (2012).
[2] W.-H. Zhang et al., Chin. Phys. Lett. 31, 017401 (2014).
[3] C. J. Tang et al., Phys. Rev. B 93, 020507(R) (2016).
[4] G. Y. Zhou et al., Appl. Phys. Lett. 108, 202603 (2016).
[5] H. Ding et al., Phys. Rev. Lett. 117, 067001 (2016).
[6] H. M. Zhang et al., Nature Communs. 8 214 (2017).

TT 52.3 Wed 10:00 HFT-FT 101

**Response of the Structural Transition of FeSe under Uniaxial Stress** — •Jack Bartlett[1,2], Alexander Steppke[1], 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

FeSe is unique as an iron-based superconductor due to its simple structure, and lack of magnetic order at ambient pressure, which offers an opportunity to disentangle the interplay of structural, magnetic and orbital degrees of freedom. Additionally, this material undergoes a structural phase transition at $T_s \sim 90$ K, in which the lattice changes symmetry from tetragonal to orthorhombic. Uniaxial stress is a conjugate field to this transition, and therefore one naively expects an increase in the transition temperature and a broadening of the transition under uniaxial stress. We observe an unexpected suppression of $T_s$ under both compressive and tensile stress, as well as a dramatic broadening of the transition. We discuss these results in the context of orbital-selective physics.

TT 52.4 Wed 10:15 HFT-FT 101

**Gap anisotropy in FeSe from ARPES** — •Yevhen Kushnirenko[1], Alexander Fedorov[1], Erik Haubold[1], Timur Kim[2], Thomas Wolf[3], Saicharan Aswartham[1], Bernd Büchner[1], and Sergey Borisenko[1] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Diamond Light Source, Didcot OX11 0DE, United Kingdom — [3]Institut für Festkörperphysik, Karlsruhe Institute for Technology, Karlsruhe 76021, Germany

There were plenty of attempts to measure superconducting gap in FeSe and related SC using different techniques: tunneling spectroscopy, photoemission spectroscopy, specific heat. But the consensus on a size and symmetry of the SC gap has not been reached. ARPES is only one technique, in which it is possible to measure SC gap in a certain part of momentum space directly. Because of this ARPES is a key tool for solving this complicated problem. Here we present results of our investigation of the superconducting gap anisotropy in FeSe using angle-resolved photoemission spectroscopy. We have measured the superconducting gap for both electron- and hole-like pockets for different kz positions. The gaps on both pockets are considerably anisotropic. Such gap anisotropy can possibly be explained in terms of orbital-selective pairing.

TT 52.5 Wed 10:30 HFT-FT 101

**Evolution of the Fermi surface across a clean nematic quantum phase transition in $FeSe_{1-x}S_x$** — •Pascal Reiss[1], David Graf[2], Amir A. Haghighirad[3], and Amalia I. Coldea[1] — [1]Clarendon Laboratory, Oxford University, UK — [2]NHMFL, Tallahassee, USA — [3]IFP, Karlsruhe Institute of Technology, GER

The interplay between superconductivity and long-range electronic orders is an intensely studied subject. Iron-based superconductors offer a fruitful field to investigate the role of magnetic order, however the concomitant instability towards nematic (orbital) order requires to be disentangled. For this purpose, the isoelectronic doping series $FeSe_{1-x}S_x$ is ideally suited. Undoped FeSe displays nematic but no long-range magnetic order, and becomes superconducting below 9 K. Applied pressure suppresses the nematic transition towards 0 K, but the nematic quantum phase transition is masked by an emerging magnetic phase stabilising superconductivity up to 37 K [1].

With sulphur doping, magnetic order is quickly suppressed, and the nematic quantum phase transition is unmasked [2,3]. We will present transport and TDO measurements as a function of pressure and fields up to 45 T, and – for the first time – we will follow the evolution of the Fermi surface and the strength of electronic correlations across a nematic quantum phase transition.

We acknowledge funding from the EPSRC UK (EP/I004475/1), the NSF and the State of Florida.

[1] S. Medvedev *et al.*, Nat. Mater. (2009)
[2] K. Matsuura *et al.*, Nat. Commun. (2017)
[3] L. Xiang *et al.*, PRB (2017)

TT 52.6 Wed 10:45 HFT-FT 101

**Domain Imaging Across the Magneto-Structural Phase Transition in $Fe_{1+y}Te$** — •Jonas Warmuth[1], Martin Bremholm[2], Philip Hofmann[2], Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Dept. of Physics, Hamburg University, Germany — [2]Depts. of Chemistry and Physics, Aarhus University, Denmark

The investigation of the magnetic phase transitions in the parent compounds of Fe-based superconductors is essential for understanding the pairing mechanism in the related superconducting compounds [1,2]. Here, we present a real space spin-resolved scanning tunneling microscopy investigation of the surface of $Fe_{1+y}Te$ single crystals with different excess Fe contents, $y$, which are continuously driven through the magnetic phase transition. For $Fe_{1.08}Te$, the transition into the low-temperature monoclinic commensurate antiferromagnetic phase [3] is accompanied by the sudden emergence of ordering into four rotational domains with different orientations of the monoclinic structure and of the antiferromagnetic order, showing how structural and magnetic order are intertwined. In the low-temperature phase of $Fe_{1.12}Te$ one type of the domain boundaries disappears, and the transition into the paramagnetic phase gets rather broad, which is assigned to the formation of a mixture of orthorhombic and monoclinic phases [4].

[1] Paglione, J. *et al*, Nature Physics **6**, 645-658 (2010)

[2] Stewart, G. R. *et al*, Reviews of Modern Physics **83**, 1589 (2011)
[3] Hänke, T. *et al*, Nature Communications **8**, 13939 (2017)
[4] Koz, C. *et al*, Physical Review B **88**, 094509 (2013)

TT 52.7 Wed 11:00 HFT-FT 101

**evidence of orbital selective cooper pairing within surface unit cell of FeSe** — •Fang Yang[1], Jasmin Jandke[1], Peter Adelmann[2], Markus Klug[3], Thomas Wolf[2], Jörg Schmalian[3], and Wulf Wulfhekel[1] — [1]Physikalisches institut, KIT, Karlsruhe, Germany — [2]Institut für Festkörperphysik, KIT, Karlsruhe, Germany — [3]Institut für Theorie der Kondensierten Materie, KIT, Karlsruhe, Germany

Numerous attempts have been made to demonstrate the multi-band nature of superconductivity in bulk FeSe in the nematic phase. To investigate this multi-band character, we determined the electronic density of states at the surface of FeSe with high energy and spatial resolution using a 40 mK dilution STM. A high spatial resolution was achieved using an STM tip with electronic p-states, which not only gives a higher lateral resolution compared to an s-state tip but also is sensitive to the surface symmetry. With this, we were able to resolve the superconducting gap of all five bands cutting the Fermi energy and, in combination with the high lateral resolution, the spatial distribution of the intensity of the quasiparticle peaks within the unit cell. By comparison with the expected d-orbital wave functions, we propose that different gaps are of particular orbital nature.

**15 min. break.**

TT 52.8 Wed 11:30 HFT-FT 101

**Structural component of an incipient ordering mode** — •Sahana Roessler[1], Alexander A. Tsirlin[2], Marco Scavini[3], Cevriye Koz[1], Ulrich Schwarz[1], Ulrich K. Roessler[4], and Steffen Wirth[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Experimental Physics VI, University of Augsburg, Germany — [3]Chemistry Department, University of Milan, Milano, Italy — [4]IFW-Dresden, Institute for Solid State Research, D-01171 Dresden, Germany

The binary compound FeSe is a multiband superconductor with fascinating properties. Unlike other Fe-based superconductors, the transition from tetragonal ($P4/nmm$) to orthorhombic ($Cmme$) structure in FeSe at $T_s \approx 87$ K at ambient pressure is not accompanied by a long-range magnetic order and the leading order parameter of the phase transition is attributed to an electronic origin. Upon further reducing temperature, two energy scales at temperatures $T^* \approx 75$ K and $T^{**} \approx 20$ K have been identified based on anomalies observed in the Hall effect, magnetotransport, thermal conductivity, and scanning tunneling spectroscopy [1]. Here we show, using a pair distribution function analysis, a local Fe-Fe atomic distortion with short-range correlations occurring at $T^{**}$. Thus, incipient ordering in FeSe occurs as a precursor state to superconductivity and is reminiscent of behavior found in several high-$T_c$ cuprates [2].

[1] S. Rößler *et al.*, Phys. Rev. B 92, 060505(R) (2015).
[2] E. Fradkin and S. A. Kivelson, Nature Phys. 8, 864 (2012).

TT 52.9 Wed 11:45 HFT-FT 101

**Unconventional pairing versus phonon mediated superconductivity in single FeSe layers** — •Jasmin Jandke[1], Fang Yang[1], Patrik Hlobil[2], Tobias Engelhardt[1], Chunlei Gao[3], Jörg Schmalian[2,4], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, KIT, 76131 Karlsruhe, Germany — [2]Institut für Theorie der Kondensierten Materie, KIT, 76131 Karlsruhe, Germany — [3]State Key Laboratory of Surface Physics and Department of Physics, Fudan University Shanghai 200433, China — [4]Institut für Festörperphysik, KIT, 76344 Karlsruhe, Germany

Both conventional [1] and unconventional [2] mechanisms have been discussed for a single layer FeSe films on $SrTiO_3$ showing a $T_c$ of 60-100 K [3,4], i.e. an order of magnitude larger than in bulk FeSe. Here we report a direct measurement of the electron-boson coupling in FeSe on $SrTiO_3$ using inelastic tunneling spectroscopy. We exclude strong electron-phonon coupling except for places near structural domain boundaries in the FeSe layer. Instead, the bosonic excitation spectrum is shown to be fully gapped below $T_c$ in agreement with an electronic pairing mechanism. By deconvolution of the experimental data, we were able to reconstruct the electron-boson coupling function, which shows beside a gap a characteristic peak at the expected resonance mode energy of paramagnons.

[1] J. J. Lee et al., Nature, 515, 245 (2014)
[2] B. Li et al., J. Appl. Phys. 115, 193907 (2014)
[3] Q.-Y. Wang et al., Chin. Phys. Lett. 29, 037402 (2012)
[4] J.-F. Ge et al., Nat. Mat., 14, 285 (2015)

TT 52.10 Wed 12:00 HFT-FT 101

**Interplay of structural properties and magnetic disorder in FeSe: Density-functional theory calculations** — •Felix Lochner[1,2], Ilya Eremin[2], Jörg Neugebauer[1], and Tilmann Hickel[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Deutschland — [2]Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Deutschland

We calculate the effect of local magnetic moments and particularly their paramagnetic disorder on the normal state of a prototype iron-based superconductor FeSe. For this purpose the spin-space averaging approach [1] for density functional theory (DFT) calculations is applied.

Here, we analyze the structural parameters of FeSe, the impact on the electronic properties as well as the interplay of electronic and phononic degrees of freedom in the paramagnetic state. In contrast to original non-magnetic DFT calculations [2], the results in the paramagnetic state agree after relaxation with experimentally observed lattice parameters with an error less than 5%. Based on this achievement a DFT based understanding of the mechanisms underlying the superconducting behavior and driving the nematic transition of FeSe seems now to be feasible.

[1] F. Körmann, A. Dick, B. Grabowski, T. Hickel, J. Neugebauer, Phys. Rev. B 85, 125104 (2012).
[2] L. Boeri, M. Calandra, I. I. Mazin, O. V. Dolgov, and F. Mauri Phys. Rev. B 82, 020506(R) (2010)

TT 52.11 Wed 12:15 HFT-FT 101

**Electron-boson interaction of LiFeAs revealed by resonantly enhanced Friedel oscillations: Experiment** — Zhixiang Sun[1], Pranab Kumar Nag[1], Steffen Sykora[1], Jose M. Guevara[1], Rhea Kappenberger[1], Sabine Wurmehl[1,2], 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

For rationalizing the Cooper pairing mechanism in a superconductor, it is central to identify bosons interacting with the conduction electrons. We determine the energy and momentum characteristics of such bosons in LiFeAs by exploiting the boson-assisted resonant amplification of Friedel oscillations by Fourier transform scanning tunneling spectroscopy (FT-STS). We show that the FT-STS signatures of the bosonic states survive in the normal state, and, moreover, that they are in perfect agreement with well-known strong above-gap anomalies in independently measured tunneling spectra at the very same energy. Thus, the small-momentum bosonic modes are promising candidates for providing the pairing interaction in LiFeAs.

TT 52.12 Wed 12:30 HFT-FT 101

**Nematic fluctuations in Li doped NaFeAs** — •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

In strongly correlated electronic systems, the electronic distribution favors local variations, often forming patterns that break the rotational symmetry of the crystal. Nematicity has special relevance in systems where competiton of different phases plays an important role, and has been observed in the most prominent families of high temperature superconductors, i.e. cuprates and iron-pnictides. The Li doped NaFeAs samples allows a new approach to explore nematicity in Iron-pnictides, given the strong differences of the phase diagram in the parents compounds, NaFeAs and LiFeAs.

In our work, we measure 3%, 4% and 5% Li doped NaFeAs samples, where longe range order is suppressed, with a low temperature scanning tunneling microscope. We visualize the real-space distribution of the nematic fluctuations, which are found to ubiquitously exist, from the superconducting state to the normal state at higher temperatures.

TT 52.13 Wed 12:45 HFT-FT 101

**Electron-boson interaction of LiFeAs revealed by resonantly enhanced Friedel oscillations: Theory** — •Steffen Sykora[1], Zhixiang Sun[1], Pranab Kumar Nag[1], Jose M. Guevara[1], Rhea Kappenberger[1], Sabine Wurmehl[1,2], 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

We present a new experimental/theoretical approach to determine bosonic modes by investigating resonantly enhanced Friedel oscillations caused by a coupling of conduction electrons to the bosons. Upon focusing on the unconventional superconductor LiFeAs we show that under particular conditions the impurity scattering potential is strongly renormalized leading to enhanced signals in the quasiparticle interference. For this a simplified model of electron-boson coupling in the presence of one single impurity is solved by a many-particle renormalization method. Comparing our theoretical results with Fourier transform scanning tunneling spectroscopy data we reveal for LiFeAs bosonic states at particular momentum and energy. The bosonic modes are promising candidates for providing the pairing interaction in LiFeAs.