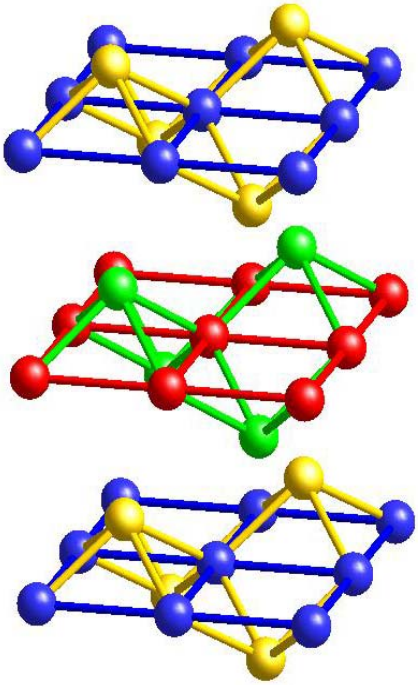
Electronic Structure of Fe-based Superconductors



Scientific Report

Program

Abstract

List of Participants

MPI-FKF Stuttgart
10-12 May 2010

Contents

Place:

Max-Planck Institute for Solid State Research, Stuttgart, Germany

Dates:

10-12 May 2010

Sponsors:

- Ψ_k, European Science Foundation;
- Max-Planck Society;
- Office of Naval Research Global (ONRG)

Workshop Organizers:

Ole Krogh Andersen (MPI Stuttgart);
Lilia Boeri (MPI Stuttgart);
Igor Mazin (Naval Research Lab, USA)
Helge Rosner (MPI Dresden);

Web page:

http://www.fkf.mpg.de/conf/fesc2010/

Scientific Report

The Fe-based superconductors (*FeBSC*) are generally considered to be the most important discovery in superconductivity since the cuprates. What sets them apart is their complex, multiband electronic structure that plays the pivotal role for both normal state properties and superconductivity. First-principles calculations have had an unprecedented impact in this field. The unusual and unexpected magnetic state of the parent compound was predicted theoretically and the now accepted unconventional s^{+-} superconducting symmetry was proposed long before any experimental evidence was found, also based on first-principles calculations. Rarely have so many people in the field of superconductivity, both theorists and experimentalists, had their ears so sharply attuned to what band theorists say.

The goal of the workshop on the *"Electronic Structure of Fe-based superconductors"* (FESC2010) was to bring together most European groups engaged in the band theory of *FeBSC*, in order to have a profound and more detailed discussion of the electronic structure of *FeBSC* than what usually takes place in more general conferences. Selected experimentalists whose work is closely related to the electronic structure was also presented in talks and posters.

In total, 84 people from Europe, USA, China and Japan attended the workshop. Of these, 29 were invited speakers; in addition, there were 25 poster contributions, which were also introduced in short oral presentations on Monday 10th 2010.

The most energetically discussed subject was the ***origin and the microscopic picture of magnetism in the parent compounds***. Three basic points of view emerged from the talks and the discussions.

1) Fully itinerant picture.

I. Eremin, S. Graser, R. Arita, C. Honerkamp (also e.g. A. Chubukov, D-H Lee)

- Magnetism is driven by nesting.
- Magnetic interaction of itinerant (RKKY) nature, defined by the Fermi surface geometry.
- Similar to 1D spin-Peierls.
- Spin fluctuations can be described by RPA/FLEX/RG.

2) Fully localized picture.

Z-Y. Lu (also e.g. J.P. Hu, Q. Si)

- Magnetism is driven by combination of Hubbard *U* and Hund's *J*.
- Magnetic interaction are local, of superexchange nature.
- Similar to cuprates and 3d oxides.
- Spin fluctuations can be described by the *J1*+*J2* model.

3) Orbital ordering picture.

Wei Ku (also e.g. R. Singh, P. Phillips)

- SOME electrons are localized, others itinerant.
- Magnetic interactions are set by competition between the orbital ordering (Jahn-Teller) in the localized orbitals, and metallic double exchange of the other electrons.
- Similar to CMR manganites.
- Spin-fluctuations can be described by orbital-dependent superexchange + double exchange?

4) Local-itinerant picture

D. Singh,M. Johannes, V. Antropov (also e.g. Yildirim), P. Hansmann, R. Arita. D. Reznik, R.Heid

- Magnetism is driven by Hund's *J*.
- Magnetic interaction of itinerant (not always RKKY) nature, affected, but not fully defined by the Fermi surface geometry, cannot be described in terms of superexchange.

- Similar to 3d metals (Cr, Mn, Fe).
- Spin fluctuations can be described, with reservations, by RPA/FLEX/RG .

The next important issue that was discussed was the ***strength of the electronic correlations and the possible proximity to the Mott-Hubbard transition***. This issue has been discussed in many details by the DMFT experts*: V. Anisimov, M. Aichorn, P. Hansmann*. A better consensus has been achieved in the sense that all parties argue that FeBSCs are in a regime of weak to moderate correlations. A. *Liebsch* also supported this conclusion, but argued that for an integer doping (one electron or one hole) a Mott transition would be observed. It was pointed out though that experiments for KFe_2As_2 do not agree with this prediction. A number of experimental talks (*Borisenko, Coldea*) raised the question of the strong bandwidth and the effective mass renormalization with respect to DFT calculations, observed in ARPES and de-Haas van Alphen experiments. What is the origin? Is the m* divergence associated to a quantum critical point (QCP)?
These questions remain a challenge to the theorists.

Further there was a discussion on the ***role of electron-phonon coupling***. *M. Calandra* showed improved first-principles calculations, which place an upper limit for the electron-phonon coupling constant $\lambda \sim 0.3$-0.4. *J. Fink* presented an experimental estimate of 0.2, while Borisenko showed a kink in the electronic dispersion corresponding to a phonon-driven Fermi velocity renormalization of 1.4 (corresponding to a conventional $\lambda = 0.4$). The ***three-dimensional dispersion*** was discussed by *D. J. Singh* and, experimentally, by *Brouet, Jensen* and by *Fink*. *Graser* emphasized the importance of this factor for superconductivity.

The ***coupling of magnetism*** (within LDA) with other degrees of freedom was addressed in several talks: *Johannes, Antropov, Yaresko, Kasinathan, Valenti*. It was discussed from the phenomenological Ginzburg-Landau point of view by *Lorenzana*. ***Methodological*** papers by *Hansmann, Buenemann/Schikling* discussed possibilities of speeding up the traditional DMFT calculations by reducing the basis set *Hansmann* or by using the Gutzwiller approximation *(Buenemann/Schikling)*.Finally, *Benfatto, Ortenzi, Plakida, Ummarino, Ciechan, Golubov* presented various results regarding ***multiband effects*** in superconductivity and normal properties.

The final program of the conference, the abstracts of presented papers, and the list of participants are attached to this report.

Program

Monday, 10th May 2010

8:15		Minibus transfer from hotel Schatten
8:45-9:00	**L. Boeri**	Opening remarks
9:00-9:30	**D. Singh**	Electronic structure of iron super-conductors: not oxides
9:30-10:00	**V. Anisimov**	Coulomb correlation effects in pnictide superconductors from LDA+DMFT calculations
10:00-10:30	**S. Graser**	Superconducting pairing in Fe-based superconductors via weak-coupling approach
10:30-10:50		*Coffee Break*
10:50-11:20	**M. Calandra**	Effects of magnetism and doping on the electron-phonon coupling in $BaFe_2As_2$
11:20-11:40	**D. Reznik**	Interplay between phonons and magnetism in 122 ferropnictides
11:40-12:00	**R. Heid**	Lattice dynamics of Fe-based superconductors from first principles
12:00-13:00		*Poster Presentations*
13:00-14:00		*Lunch Break*
14:00-14:30	**M. Johannes**	Dual character of magnetism in pnictides
14:30-15:00	**S. Borisenko**	ARPES studies of Fe-based super-conductors
14:30-15:00	**A. Coldea**	Quantum oscillation experiments in Fe-based superconductors
15:00-16:00		*Poster Presentations*
16:00-16:30		*Coffee in the canteen*
16:30-on…		*Poster Session outside lecture hall* *from 18:00 beer and sandwiches*

Tuesday, 11th May 2010

8:30		Minibus transfer from hotel Schatten
9:00-9:30	**Z. Lu**	Electronic structures and magnetic properties of iron-pnictides by the first-principles study
9:30-10:00	**M. Aichhorn**	Correlated electronic structure of iron-based superconductors from an LDA+DMFT perspective
10:00-10:30	**Wei Ku**	What does the rich magnetic structures of parent compounds tell us about the essential low-energy electronic structure?
10:30-11:00		*Coffee Break*
11:00-11:30	**A. Yaresko**	Spin-spiral calculations of the magnetic properties of Fe-based superconductors
11:30-12:00	**S. Massidda**	Magnetism in Fe-based superconductors
12:00-12:30	**R. Arita**	LDA+FLEX study for Fe-based superconductors based on *ab-initio* downfolding
12:30-13:00	**A. Boris**	Criticality-induced optical anomalies in 122 Fe pnictides
13:00-14:00		*Lunch Break*
14:00-14:30	**I. Eremin**	Magnetism, superconductivity and pairing of Fe-based superconductors in the RPA formalism
14:30-15:00	**K. Koepernik**	Bulk and surface electronic structure of Fe-pnictides: TB-models, cleavage behavior and surface states
15:00-15:30	**S. Dugdale**	Probing the Fermi surface with Compton scattering: theory and experiment
15:30-16:00		*Coffee Break*

16:00-16:30	**D. Inosov**	Normal-state spin dynamics and temperature-dependent spin resonance energy in an optimally doped iron arsenide superconductor
16:30-17:00	**D. Kasinathan**	Relation of structure, magnetism, doping and pressure in $AFe_{2-x}T_xAs_2$ (A=Ca,Sr,Ba,Eu; T=Co,Rh,Ru)
17:00-17:30	**R. Valentí**	Effect of pressure on the electronic structure of Fe-based superconductors
		Bus transfer:
17:45		*from MPI to hotel Schatten*
18:30		*from MPI to Bärenschlössle car park with*
18:35		*pickup stop at hotel Schatten*
19:00-22:00		*Conference Dinner*
22:15		*Bus transfer from Bärenschlössle car park to hotel Schatten and MPI*

Wednesday, 12th May 2010

8:30		Minibus transfer from hotel Schatten
9:00-9:30	**A. Liebsch**	Correlation induced spin freezing in FeSe and FeAsLaO: a dynamical mean field study
9:30-10:00	**C. Honerkamp**	Iron pnictides viewed by the functional renormalization group
10:00-10:30	**B. Büchner**	Nanoscale electronic order in underdoped iron pnictides
10:30-11:00		*Coffee Break*
11:00-11:20	**P. Hansmann**	Dichotomy between large local and small ordered magnetic moment in iron-based superconductors
11:20-11:40	**J. Lorenzana**	First principle Landau theory of competing orders in LaOFeAs
11:40-12:10	**A. Golubov**	Strong coupling theory of super-conducting pnictides: multiband scenario
12:10-12:40	**L. Benfatto**	Eliashberg approach to multiband pairing in pnictides
12:40-13:25	**I. Mazin**	Summary of the conference
13.25-13.30	**O.K. Andersen**	Closing remarks
13:30-14:30		*Lunch Break*

14:30	**N. Spaldin**	*MPI Seminar (Seminar room 7D2)* Oxide-oxide interfaces from first-principles: Design and understanding
15:30	**N. Plakida**	*MPI Seminar (Seminar room 7D2)* Dynamic spin susceptibility of superconducting cuprates: A microscopic theory of the magnetic resonance mode

Invited Talks

Correlated electronic structure of iron-based superconductors from an LDA+DMFT perspective

Markus Aichhorn

CPHT, Ecole Polytechnique, Palaiseau, France

The discovery of high-temperature superconductivity in iron-based compounds triggered an enormous amount of research in condensed matter physics. Not even two years after their discovery, scientists have already collected a huge amount of experimental data, due to very powerful experimental techniques that have been developed during the last decades. A very intriguing property of these new compounds is the rather high flexibility concerning elemental substitutions, leading to several families of superconductors, termed '1111', '122', '11', and so on, depending on their chemical composition. We analyse the single-particle properties of prominent iron-based supercondutors using a combination of density-functional theory with a state-of-the-art many-body technique, the Dynamical Mean-Field Theory. This approach enables us to understand also these more complex materials at a first-principle level. We will show that there are significant differences in the electronic properties, when going from more weakly correlated members as LaFeAsO, to more correlated ones like FeSe. For reasonable Coulomb parameters, the properties range from Fermi-liquid like to incoherent bad-metal like.

Coulomb correlation effects in pnictide superconductors from LDA+DMFT calculations

Vladimir Anisimov

Institute of Metal Physics, Russian Academy of Sciences, Ekaterinburg, Russia

Electronic structure of pnictide superconducting materials LaOFeAs, $BaFe_2As_2$ and LaOFeP was studied by LDA+DMFT method. Calculation results are in good agreement with PES and ARPES data. Calculated quasiparticle bands renormalization corresponding to effective mass enhancement m*/m~2 observed simultaneously with the absence of Hubbard bands show pnictide superconductors as moderately correlated systems but far from metal-insulator Mott transition.

LDA+FLEX study for Fe-based superconductors based on *ab-initio* downfolding

Ryotaro Arita

University of Tokyo and JST, TRIP and JST, CREST, Tokyo, Japan

We first derive effective Hamiltonians for LaFeAsO, LaFePO, $BaFe_2As_2$, LiFeAs, FeSe and FeTe in terms of the maximally localized Wannier functions. [1,2] Systematic dependences of the derived model parameters are elucidated, many of which are shown to be understood from the systematic variation of the covalency between Fe-3*d* and pnictogen-/chalcogen-*p* orbitals. The evaluation of the interaction parameters by means of the constrained RPA method clarifies that the family dependence has a wide variation ranging from weak correlation regime (LaFePO) to strong correlation regime (FeSe, FeTe).

We then apply the fluctuation exchange approximation (FLEX) to the derived effective Hamiltonians to study whether the Fermi-surface (FS) nesting can really give rise to high temperature superconductivity. We found that even when the FS obtained by FLEX looks quite similar to that of LDA, it does not necessarily favor the stripe antiferromagnetic order observed in experiments, especially for realistic electronic correlations. [3]

If superconductivity in iron pnictides is magnetically mediated and has fully-gapped sign-reversing s-wave symmetry, our results suggest that the pairing interaction does not arise only from FS nesting and exchange interactions between local moments in the Fe-3*d* orbitals may also play a crucial role. [4]

[1] K. Nakamura, R. Arita, and M. Imada, J. Phys. Soc. Jpn., **77**, 093711 (2008)
[2] T. Miyake, K. Nakamura, R. Arita, and M. Imada, J. Phys. Soc. Jpn., **79,** 044705 (2010)
[3] R. Arita and H. Ikeda, J. Phys. Soc. Jpn., **78,** 113707 (2009)
[4] Talk given by P. Hansmann, and P. Hansmann, R. Arita, A. Toschi, S. Sakai, G. Sangiovanni, and K. Held, arXiv:1003.2162

Eliashberg approach to multiband pairing in pnictides

Lara Benfatto

CNR-INFM Statistical Mechanics and Complexity Center, Rome, Italy

The occurrence of superconductivity in pnictides renewed in the last year the interest in the physics of multiband superconductors. However, what makes the case of pnictides very peculiar is the fact that pairing has mainly an interband character, as due to exchange of spin fluctuations between hole and electron pockets. These two characteristics make the theoretical description of pnictides much more involved than what is usually believed. In this talk I will review some of our recent results based on a four-band model with anisotropic interactions, where pairing is described within the Eliashberg theory. I will show that this approach allows us to account for several spectroscopic and thermodynamic properties of pnictides that are not directly captured by LDA+DMFT calculations.

Criticality-induced optical anomalies in 122 Fe pnictides

A. Charnukha, P. Popovich, Y. Matiks, D. L. Sun, C. T. Lin, A. N. Yaresko, B. Keimer, and A. V. Boris

Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Unlike in high-Tc cuprates, the Fermi surface of iron pnictides has been reliably determined and shows good agreement with experiments in all regions of the phase diagram. This and moderate electron correlations render LDA calculations a better approximation enabling more accurate tests of possible manifestations of pairing mechanisms. Here we report a spectroscopic ellipsometry study, extended to a spectral range $12\,\mathrm{meV} - 6.7\,\mathrm{eV}$, of a high-quality single-phase optimally-doped $Ba_{0.68}K_{0.32}Fe_2As_2$ crystal with $T_C = 38.5$ K. We observe superconductivity-induced suppression of an absorption band at a photon energy of 2.47 eV, two orders of magnitude above the superconducting gap $2\Delta \approx 19\,\mathrm{meV}$. This suggests that unconventional electronic pairing mechanisms might contribute to the formation of the superconducting condensate. Subsequent LDA calculation allowed us to confidently assign the suppressed band to a transition from As−*p* to Fe−*d* orbitals crossing the Fermi surface, whose density of states is expelled as superconductivity develops. A much larger effect was identified in parent compounds of this family at the spin-density-wave transition. This suggests that deep-lying As − *p* states contribute to the critical behaviour of iron pnictides.

ARPES studies of FeAs superconductors

Sergey Borisenko

IFW Dresden, Germany

We have studied the electronic structure of the Fe-pnictides using angle-resolved photoemission spectroscopy. Among them is a non-magnetic LiFeAs (T_c~18K) superconductor. In LiFeAs we find a notable absence of the Fermi surface nesting, strong renormalization of the conduction bands by a factor of three, high density of states at the Fermi level caused by a Van Hove singularity, strong coupling to phonons and no evidence for either a static or fluctuating order except superconductivity with in-plane isotropic energy gaps. Our observations suggest that these electronic properties capture the majority of ingredients necessary for the superconductivity in iron pnictides [1,2].

[1] S. V. Borisenko et al., arXiv:1001.1147
[2] A. A. Kordyuk et al., arXiv:1002.3149

Nanoscale electronic order in underdoped iron pnictides

Bernd Büchner

Institute for Solid State Physiks, IFW Dresden, Germany

Studying nuclear magnetic resonance and electronic transport properties we have investigated short range order phenomena in $RFeAsO_{1-x}F_x$ (R = La;Sm) pnictide superconductors. The charge distribution in the FeAs layers is probed using As nuclear quadrupole resonance [1]. Whereas undoped and optimally doped or overdoped compounds feature a single charge environment, two charge environments are detected in the underdoped region. Spin-lattice relaxation measurements show their coexistence at the nanoscale. Together with the quantitative variations of the spectra with doping, they point to a local electronic order in the iron layers, where low- and high-doping-like regions coexist on the nanometer scale. In the same doping range a pronounced increase of the relaxation rate is found signalling a slowing down of Fe spin fluctuations with decreasing temperatures [2]. This clearly shows the proximity of static magnetic order, which is, however, absent according to our high sensitive μSR studies [3]. The appearance of the slow magnetic fluctuations as signalled by the NMR data correlates with clear-cut anomalies of the electronic transport properties resistivity [4] and Nernst coefficient [5]. On the basis of these data the possibility of nematic-like order of charges- orbitals – and/or spins in underdoped pnictides is discussed.

[1] G. Lang et al., Phys. Rev. Lett. **104,** 097001 (2010)
[2] H.J. Grafe et al., Phys. Rev. Lett. **104**, 097001 (2010), unpublished
[3] H. Luetkens et al., Nature Mater. **8**, 305 (2009)
[4] C. Hess et al., Europhys. Lett. **87**, 17005 (2009)
[5] C. Hess, A. Kondrat et al., to be published

Effects of magnetism and doping on the electron-phonon coupling in $BaFe_2As_2$

Matteo Calandra

CNRS and Institut de Minéralogie et de Physique des Milieux Condensés, Paris, France

In this talk I present the result of first-principles calculations in the framework of linear-response theory and pseudopotentials to address the role of local magnetic moments on the electron-phonon coupling in $BaFe_2As_{2+\delta}$.
I show that the magnetism enhances the total electron-phonon coupling by ~ 50%, up to λ . 0.35, still not enough to explain the high critical temperature, but strong enough to have a non-negligible effect on superconductivity, for instance, by frustrating the coupling with spin fluctuations and inducing order parameter nodes. The enhancement comes mostly from a renormalization of the electron-phonon matrix elements. We also investigate, in the rigid band approximation, the effect of doping, and find that λ versus doping does not mirror the behavior of the density of states; while the latter decreases upon electron doping, the former does not, and even increases slightly.

Quantum oscillation experiments in Fe-based superconductors

Amalia I. Coldea

H. H. Wills Physics Laboratory, Bristol University, and Clarendon Laboratory, Oxford University, United Kingdom

Quantum oscillations is a bulk probe which allows to map out the Fermi surface and its three-dimensional shape. Quantum oscillations are determined by the Landau quantization in high magnetic fields and are usually observed at very low temperatures and in very clean samples. The mass of the quasiparticles in the normal state is extracted from the temperature dependence of the oscillation amplitude and the degree of electronic correlations is estimated by comparison with band structure calculations. I will present measurements of quantum oscillations in iron-based superconductors and metals and I will discuss the effect of structure and magnetism on the Fermi surface shape and the strength of electronic correlations in superconducting systems [1-4].

[1] A. I. Coldea, J. D. Fletcher, A. Carrington et al., Phys. Rev. Lett. **101**, 216402 (2008)
[2] J. G. Analytis, C. M. J. Andrew, A. I. Coldea et al., Phys. Rev. Lett. **103**, 076401 (2009)
[3] A. I. Coldea, C. M. J. Andrew, J. G. Analytis et al., Phys. Rev. Lett. **103**, 026404 (2009)
[4] H. Shishido, A. F. Bangura, A. I. Coldea et al., Phys. Rev. Lett. **104**, 057008 (2010)

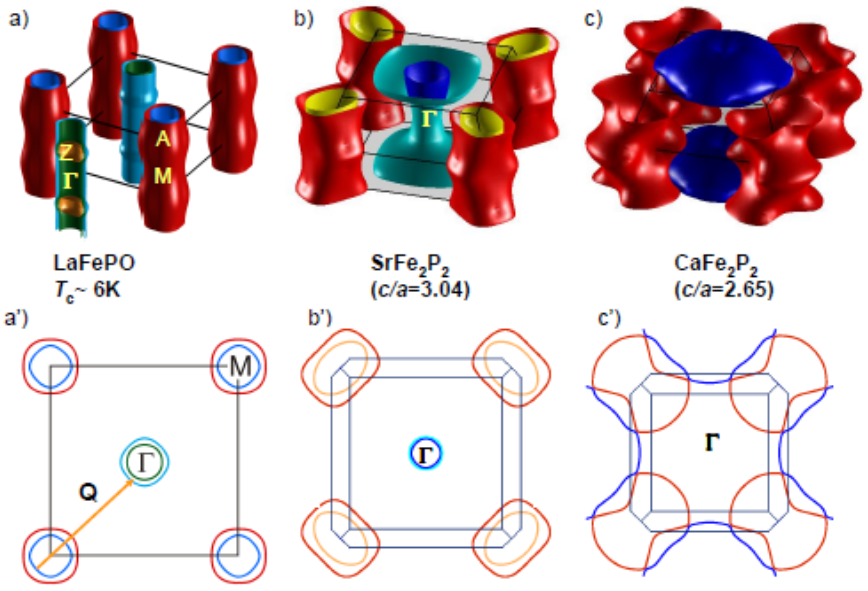


Fig. 1: The Fermi surface and the corresponding in-plane cross sections at kz = 0 (Γ point) of a) quasi-two dimensional LaFePO,
b) quasi-three dimensional $SrFe_2P_2$ and c) three dimensional system, $CaFe_2P_2$.

Probing the Fermi surface with Compton scattering: theory and experiment

Stephen Dugdale

University of Bristol, United Kingdom

When other methods for mapping the Fermi surface are excluded (for example, owing to sample quality, concerns about the surface, substitutional disorder, or simply the temperature at which the phase of interest exists), then the Fermi surface can be accessed through measurements of the momentum distribution via x-ray Compton scattering. By measuring the energy distribution of x-ray photons which have been inelastically scattered by the electrons in the sample, it is possible to measure their momentum distribution.

The momentum distribution contains information about the occupied momentum states, and therefore about the Fermi surface.

Results are presented of recent Compton scattering measurements performed on optimally Co-doped $BaFe_2As_2$. When compared to ab-initio calculations which have been adjusted through small shifts of the bands with respect to the Fermi energy, the Compton scattering results can only be understood if those calculations were performed at the LDA-relaxed As position, rather than at the experimental one. [1]

[1] D.J. Singh , Phys. Rev. B **78**, 094511 (2008)).

Magnetism, superconductivity and pairing of Fe-based superconductors in the RPA formalism

I. Eremin[1], J. Knolle[2], A. Akbari[1], A.V. Chubukov[3], and R. Moessner[2]

[1] Institute for Theoretical Physics III, Ruhr-Universität Bochum, Germany
[2] Max Planck Institute for Physics of Complex Systems, Dresden, Germany
[3] Department of Physics, University of Wisconsin-Madison, USA

Recent discovery of superconductivity in the iron-based layered pnictides with Tc ranging between 26 and 56 K generated enormous interest in the physics of these materials. Like the cuprates, the iron-based superconductors are quai-two-dimensional, their parent material shows antiferromagnetic long-range order below 2000 K and superconductivity occurs upon doping of either electrons or holes into the FeAs layers. In my talk I will analyze antiferromagnetism and superconductivity within the renormalization group (RG) technique in novel Fe-based superconductors using the itinerant model of small electron and hole pockets near (0, 0) and (π,π), respectively, originating from the two strongly hybridized orbitals. We find that, for this model, the bare interactions in the Cooper channel are repulsive, and superconductivity does not occur at the mean-field level. However, under RG the effective interaction in the superconducting channel changes sign and becomes attractive. Furthermore, the effective interactions in antiferromagnetic and superconducting channels logarithmically flow towards the same absolute values at low energies, i.e., both must be treated on equal footings.

I will further discuss the selection of the stripe magnetic order in the unfolded BZ within itinerant description. Selecting one hole and two electron pockets we found that SDW order is highly degenerate if electron pockets are circular and interactions involved are between holes and electrons only. Repulsive charge interactions between two electrons as well as ellipticity of the electron pockets break the degeneracy and select metallic (0, π) [(π,0)] SDW state in the unfolded BZ – the same order as seen in the experiments. We found that the SDW state remains a metal even for the case of a perfect nesting because one combination of the two hole operators and one combination of two electron operators decouple from the SDW mixing. We further discuss the resulting spin wave spectrum in the SDW state and the resulting quasiparticle interference patterns.

Strong coupling theory of superconducting pnictides: multiband scenario

A.A. Golubov[1], O.V. Dolgov[2], D. Parker[3], P. Popovich[2], and A.V. Boris[2]

[1] Faculty of Science and Technology and MESA+ Institute of Nanotechnology, University of Twente, The Netherlands
[2] Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
[3] Naval Research Laboratory, Washington, DC, USA

We consider a two-band superconductor with relative phase ¼ between the two order parameters as a model for the superconducting state in ferropnictides. Within this model we calculate the microwave response and the NMR relaxation rate. The influence of intra- and interband impurity scattering beyond the Born and unitary limits is taken into account. We show that, depending on the scattering rate, various types of power law temperature dependencies of the magnetic field penetration depth and the NMR relaxation rate at low temperatures may take place.
The model is further generalized to the case of four bands. We show that an Eliashberg model with two hole and two electron bands gives the correct values of the critical temperature, the superconducting gaps, and the temperature dependence of the free-energy difference in optimally hole-doped $Ba_{0:68}K_{0:32}Fe_2As_2$ single crystals. The results indicate strong coupling with intermediate bosons, in good agreement with an Eliashberg analysis of a spin-fluctuation model.

Superconducting pairing in Fe-based superconductors via weak-coupling approach

Siegfried Graser

University of Augsburg, Germany

A comparison of the new high-T_C superconductors of the iron pnictide and chalcogenide family to the cuprates reveals startling similarities between the two classes: both are layered materials with mainly 2D character, a conductivity that is dominated by *d*-electrons, and an antiferromagnetic or spin-density wave phase in proximity to the superconducting state.
However, the pronounced multiband character of the iron pnictides that becomes manifest in several disconnected Fermi surface sheets, distinguishes them from the cuprates and requires a multiorbital description of its electronic properties. This multiorbital character of the bands at the Fermi level together with the rich momentum structure of the Fermi surface allows for a wide variety of possible superconducting ground states.
We have explored the symmetry of the superconducting state assuming a pairing mechanism based on the exchange of spin fluctuations using a 5-orbital tight-binding Hamiltonian fitted to the LDA band structure of LaOFeAs. We could show that not only the symmetry but also the anisotropy of the pairing state depends sensitively on the inter- and intraorbital interaction parameters. In addition we have compared the pairing ground state calculated from a two dimensional model appropriate for materials with a mainly 2D electronic structure, e.g. the 1111 compounds, to the ground state obtained from a full 3D calculation necessary to describe the characteristics of the 122 or 11 materials.

Dichotomy between large local and small ordered magnetic moment in iron-based superconductors

Philipp Hansmann

Institute for Solid State Physics, Vienna University of Technology, Vienna, Austria

We study a four band model for iron-based superconductors within local density approximation + dynamical mean field theory (LDA+DMFT). This successfully reproduces the results of models which take As *p* degrees of freedom explicitly into account and has several *physical* advantages over the standard five *d*-band model. Our findings reveal that the new superconductors are more strongly correlated than their single-particle properties suggest. Two-particle correlation functions unveil the dichotomy between local and ordered magnetic moments in these systems, calling for further experiments to better resolve the short time scale spin dynamics.

[1] P. Hansmann, R. Arita, A. Toschi, S. Sakai, G. Sangiovanni, and K. Held, arXiv:1003.2162

Lattice dynamics of Fe-based superconductors from first principles

Rolf Heid

Karlsruhe Institute of Technology, Institute for Solid-State Physics, Karlsruhe, Germany

A prominent feature of all families of the pnictide superconductors is the complex interplay of structural and magnetic degrees of freedom, which has a significant impact on the bonding properties and thus on the lattice dynamics. In this talk, first-principles studies of the phonon dispersion of 122 pnictides using density functional perturbation theory within a mixed-basis pseudopotential approach will be presented. Focus will be on the dependence of the phonon spectra on structural parameters and magnetic order, and also the impact of pressure and doping will be considered. The accuracy and potential shortcoming of this first-principles approach will be discussed in the light of experimental phonon measurements on $CaFe_2As_2$ (both at ambient pressure and in the collapsed phase [1,2]) and on $BaFe_2As_2$ (both pure and doped [3]).

[1] R. Mittal et al., Phys. Rev. Lett. **102**, 217001 (2009)
[2] R. Mittal et al., arXiv0911.1665 (2009), to appear in Phys. Rev. B
[3] D. Reznik et al., Phys. Rev. B **80**, 214534 (2009)

Iron pnictides viewed by the functional renormalization group

Carsten Honerkamp

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The superconducting iron pnictides are prominent examples for the interplay of magnetic and superconducting ordering. This competition can be studied theoretically using the functional renormalization group in an unbiased and flexible way. Furthermore, with this method, the superconducting gap structure can be analyzed in detail. Here the multi-band character of the iron pnictides enriches the picture considerably and is the source of some interesting features. We also discuss attempts to clarify the parameter and material dependence of the superconducting energy gap and describe the possibilities for time-reversal symmetry-breaking superconducting states.

Normal-state spin dynamics and temperature-dependent spin resonance energy in an optimally doped iron arsenide superconductor

D. S. Inosov[1], J. T. Park[1], P. Bourges[2], D. L. Sun[1], Y. Sidis[2], A. Schneidewind[3,4], K. Hradil[5,4], D. Haug[1], C. T. Lin[1], B. Keimer[1] and V. Hinkov[1]

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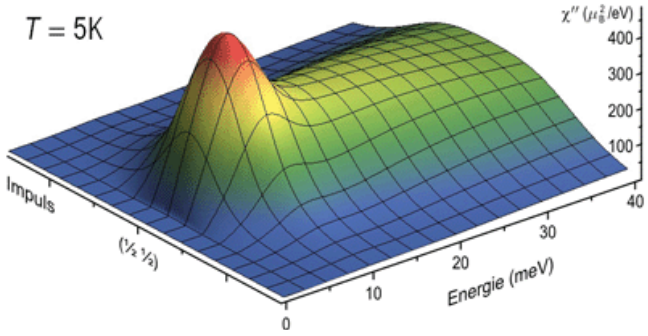
The proximity of superconductivity and antiferromagnetism in the phase diagram of iron arsenides, the apparently weak electron-phonon coupling and the "resonance peak" in the superconducting spin excitation spectrum have fostered the hypothesis of magnetically mediated Cooper pairing. However, since most theories of superconductivity are based on a pairing boson of sufficient spectral weight in the normal state, detailed knowledge of the spin excitation spectrum above the superconducting transition temperature Tc is required to assess the viability of this hypothesis. Using inelastic neutron scattering we have studied the spin excitations in optimally doped $BaFe_{1.85}Co_{0.15}As_2$ (Tc = 25 K) over a wide range of temperatures and energies [1]. We present the results in absolute units (see figure) and find that the normal state spectrum carries a weight comparable to underdoped cuprates. In contrast to cuprates, however, the spectrum agrees well with predictions of the theory of nearly antiferromagnetic metals [2], without complications arising from a pseudogap or competing incommensurate spin-modulated phases. We also show that the temperature evolution of the resonance energy follows the superconducting energy gap, as expected from conventional Fermi-liquid-based approaches. Our observations point to a surprisingly simple theoretical description of the spin dynamics in the iron arsenides and provide a solid foundation for models of magnetically mediated superconductivity.



[1] D. S. Inosov, J. T. Park, P. Bourges, D. L. Sun, Y. Sidis, A. Schneidewind, K. Hradil, D. Haug, C. T. Lin, B. Keimer and V. Hinkov, Nature Phys. **6**, 178–181 (2010).
[2] T. Moriya, *Spin Fluctuations in Itinerant Electron Magnetism* (Springer-Verlag, Berlin Heidelberg, 1985)

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Dual character of magnetism in pnictides

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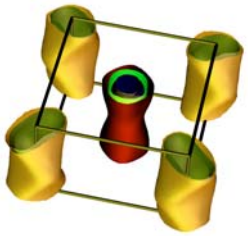
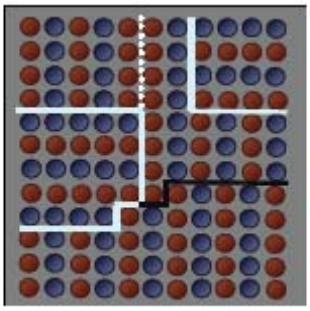


Since the discovery of a high temperature superconducting transition in ferropnictides approximately two years ago, the highly magnetic character of these compounds and the close relationship between superconductivity and magnetism has been widely recognized and intensely studied. Initially, debate about the nature of the magnetism was split into two camps: localized moments (as in cuprates) and pure itineracy (a spin-Peierls type transition). We argue that the magnetism in pnictides and in the related chalcogenides is between these two extremes, consisting of Hund's rule (or Stoner) derived moments on the Fe atoms. Using density functional theory (DFT) calculations, we show that the ordering mechanism is not Fermi surface driven and is also unlikely to be of superexchange origin. We explain, from a computational perspective, how the magnetic and structural transitions are related and compare calculated doping and pressure dependent quantities to experiment. We discuss which quantities are well reproduced and explainable using DFT and what remaining questions need to be answered before magnetism, superconductivity and their relationship can be considered as understood. We argue that spin fluctuations are the driving force behind the superconductivity and that magnetic order is a competing, and therefore detrimental, phase. We propose a particular spin fluctuation scheme that could explain why the structural transition appears either in conjunction with or before the magnetic transition.



Relation of structure, magnetism, doping and pressure in $AFe_{2-x}T_xAs_2$ (A=Ca,Sr,Ba,Eu; T=Co,Rh,Ru)

Deepa Kasinathan

MPI-CPfS, Dresden, Germany

In a joint experimental and theoretical study we present an overview of recent results for the '122' compound family. We show thermodynamical measurements and band structure results for the undoped Sr-compound under ambient conditions, and also the influence of hydrostatic pressure and doping on the A site as well as the Fe site on the magneto-structural and superconducting transitions.
The magnetism is weakened upon the application of pressure as indicated by resistivity, X-ray data and density functional band structure calculations.
Similar to substitution on the Sr site, substitutions on the Fe-site quench the magnetic transition and induce bulk superconductivity with T_c up to 20 K for ambient pressure and up to 27 K for underdoped $SrFe_{2-x}Co_xAs_2$ for pressures of 2.6 GPa. In our analysis, we attempt to disentangle the interplay of charge doping and structural changes induced by the substitution and by external pressure.

Bulk and surface electronic structure of Fe-pnictides: TB-models, cleavage behavior and surface states

Klaus Koepernik

IFW Dresden, Germany

The similarities and differences among the Fe-pnictides with respect to the bulk and surface electronic structure and chemical bonding is discussed on the basis of density functional theory. The implications for TB-models are shown. In order to help to understand the angle resolved photo emission data we investigate the cleavage behavior and the emergence of surface states in the 111 and 1111 compounds.

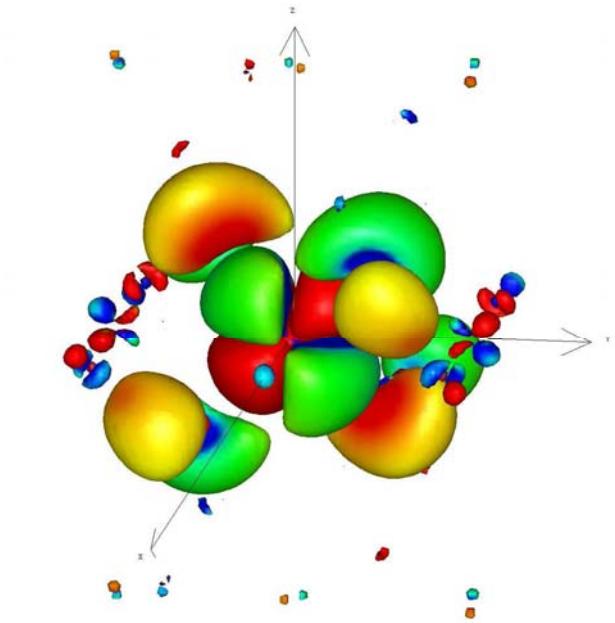
What does the rich magnetic structures of parent compounds tell us about the essential low-energy electronic structure?

Chi-Cheng Lee, Weiguo Yin, and Wei Ku

CMPMSD, Brookhaven National Lab, Upton, NY, USA

The proximity of the superconducting phase to the magnetic phase in the newly discovered Fe-based high-Tc superconductors suggests strongly an intimate relationship between the magnetism and superconductivity. Indeed, the mainstream efforts of the community have been focusing on the roles of spin fluctuation in pairing the electrons. Yet, currently, there exists little consensus on the nature of the long-range magnetic order in the parent compounds. A comprehensive understanding of the rich magnetism of both the "collinear" structure in the 1111 and 122 families and the "bi-collinear" structure in the 11 families will be presented in this talk, based on first-principles Wannier function analysis of the electronic structure. The rich magnetism can be unified in a simple model that highlights the essential role of the orbital freedom in Fe-based high-Tc superconductors and how the low-energy electronic structure of this class of materials differs fundamentally from that of the cuprates and the manganites. Finally, a few remarks/implications on superconductivity will be presented.

[1] Phys. Rev. Lett. **103**, 267001 (2009)
[2] arXiv:1003.0512



Correlation induced spin freezing in FeSe and FeAsLaO: a dynamical mean field study

Ansgar Liebsch

Research Center Jülich, Germany

The recent discovery of high-temperature superconductivity in iron-based pnictides and chalcogenides has led to an intense discussion regarding the role of Coulomb correlations in these materials. Although compounds such as FeAsLaO, $BaFe_2As_2$, LiFeAs, and FeSe have rather similar one-electron properties, a variety of experiments suggest significant differences.

Using an accurate single-particle description of the electronic structure together with appropriate interaction parameters calculated within constrained RPA [1], and evaluating the effect of local Coulomb correlations within five-band ED/DMFT, we show that the formation of 3*d* local moments in FeSe gives rise to non-Fermi-liquid behavior [2]. Thus, electronic states at the Fermi energy exhibit a reduced lifetime associated with a finite onset of the imaginary part of the 3*d* self-energy.

These bad-metallic properties are caused by a spin-freezing transition which was recently discovered in a fully degenerate three-band model [3]. Using the same approach for FeAsLaO we show that Coulomb interactions are not strong enough to give rise to spin freezing, so that this compound merely exhibits moderate effective mass enhancement [2,4].

[1] T. Miyake, K. Nakamura, R. Arita, and M. Imada, J. Phys. Soc. Jpn **79**, 044705 (2010).
[2] A. Liebsch and H. Ishida, arXiv:1004.2851.
[3] P. Werner, E. Gull, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **101**, 166405 (2008).
[4] H. Ishida and A. Liebsch, Phys. Rev. B **81**, 054512 (2010).

First principle Landau theory of competing orders in LaOFeAs

José Lorenzana

SMC-ISC-CNR and Dipartimento di Fisica, Università di Roma "La Sapienza", Rome, Italy

Magnetism in FeAs superconductors appears sometimes through a first order transition and sometimes through a second order transition which suggest that these systems are close to a tricritical point. A Landau analysis close to the tricritical point identifies all possible phases competing with superconductivity [1]. Apart from the well know columnar phase we find a non-collinear phase and a spin and charge ordered phase. A first principle computation in LaOFeAs [2] confirms the proximity to the tricritical point, determines the Landau coefficients and the zero temperature phase diagram. Schemes to tune the materials exactly at the tricritical point at zero temperature to produce a quantum tricritical point and the consequences for the normal and superconducting properties will be analysed.

[1] J. Lorenzana, G. Seibold, C. Ortix, and M. Grilli, Phys. Rev. Lett. **101** 186402 (2008).
[2] G. Giovannetti, C. Ortix, M. Marsman, M. Capone, J. van den Brink and J. Lorenzana, in preparation.

Electronic structures and magnetic properties of iron-pnictides by the first-principles study

Zhong-Yi Lu

Department of Physics, Renmin University of China, Beijing, China

The first-principles electronic structure calculations play an important role on study of high Tc superconductor iron-pnictides. Iron-pnictides were first predicted by theoretical calculations to be antiferromagnetic semimetals [1]. Based on the calculations, Arsenic-bridged antiferromagnetic superexchange interaction was proposed [2]. The bi-collinear antiferromagnetic order was predicted on alpha-FeTe as well [3]. In this talk, we will present our study on the phase diagram of iron-pnictides under pressures. And we also will present our calculations on surfaces of iron-pnictides to clarify the surface electronic structures and magnetic properties.

[1] Physical Review B **78**,033111 (2008)
[2] Physical Review B **78**, 224517 (2008)
[3] Phys. Rev. Lett. **102**, 177003 (2009)

Magnetism in Fe-based superconductors

S. Sharma, S. Shallcross, J.K. Dewhurst, A. Sanna, C. Bersier, Sandro Massidda[1], E.K.U. Gross

[1] Physics Department, University of Cagliari, Italy

Magnetic properties of Fe-based superconductors are extremely important, due to their connections with superconductivity. In particular, the role of the rare earth element (R) in ROFeAs deserves attention. We will report the results of firstprinciples calculations of the magnetic behavior of CeOFeAs. We find the Ce layer moments oriented perpendicular to those of the Fe layers. An analysis of incommensurate magnetic structures reveals that the Ce-Ce magnetic coupling is rather weak with, however, a strong Fe-Fe and Fe-Ce coupling. Comparison of the origin of the tetragonal to orthorhombic structural distortion in CeOFeAs and LaOFeAs shows marked differences; in CeOFeAs the distortion is stabilized by a lowering of spectral weight at the Fermi level, while in LaOFeAs by increase in Fe spin moment. Finally, we will report on the impact of electron doping upon CeOFeAs and LaOFeAs and show that for $CeO_{1-x}F_xFeAs$ the moment is *almost unchanged* upon electron doping, whereas in $LaO_{1-x}F_xFeAs$ we found a strong suppression of the moment.

Interplay between phonons and magnetism in 122 ferropnictides

Dmitri Reznik

University of Colorado, Boulder, USA

I will present results of neutron and x-ray scattering measurements and density functional theory (DFT) calculations of phonon dispersions in doped and undoped $CaFe_2As_2$ (Ca122) and $BaFe_2As_2$ (Ba122). Density functional theory predicts that the frequencies of some phonons depend strongly on the Fe moment and the relative orientation between the Fe moment and the phonon propagation vector. Thus a comparison of experimental phonon frequencies and the DFT calculations can serve as a probe of magnetism. The calculation gives correct frequencies of most phonons in both compounds for the experimental crystal structure. However in Ba122 some phonons are softer in the experiment than calculated. The agreement is improved if a large Fe magnetic moment is included into the calculation. However, this Fe moment would result in phonon peak splitting that is not observed. The talk will focus on how these already published results relate to our understanding of the physics of the pnictides and the coupling between phonons and magnetic fluctuations. I will also present many new unpublished results on Ba122 under hydrostatic pressure, phonons in $FeSe_xTe_{1-x}$, will discuss novel magnetic excitations, and will reexamine phonon peak assignments of our previous neutron scattering measurements.

Electronic structure of iron superconductors: not oxides

David J. Singh

Materials Science and Technology Division, Oak Ridge National Laboratory, USA

The electronic structure plays a fundamental role in understanding superconductivity. In this talk I discuss the electronic structure of the iron-based superconductors based on first principles results and comparison with experimental data. These materials are high density of states, low carrier density metals with itinerant magnetism. In fact, at the mean field level, as in standard density functional calculations, they are rather strongly magnetic. There is accumulating evidence for strong spin fluctuations that suppress the ordered magnetism and may be central to understanding the superconductivity. There is also evidence for momentum dependent renormalization of the electronic band structure, which may be connected with spin-fluctuations. Superconductivity is discussed in this context as are implications for the discovery of new materials. We emphasize the point that these materials are fundamentally not oxides, and that this leads to differences in behavior from traditional correlated oxides.

This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

Effect of pressure on the electronic structure of Fe-based superconductors

Roser Valentí

Institute for Theoretical Physics, University of Frankfurt, Germany

Within the framework of density functional theory and molecular dynamics calculations we investigate the nature of magnetism as well as the origin of structural and magnetic phase transitions under pressure in some 122 and 1111 families [1,2,3]. In the talk we will discuss the comparison with experimental observations and the implications of the study on the superconducting behavior of these materials.

[1] A. Simon, J. Kimber et al., Nature Materials **8**, 471 (2009)
[2] Zhang et al. Phys. Rev. B **80**, 094530 (2009)
[3] Zhang et al. Phys. Rev. B **81**, 094505 (2010)

Spin-spiral calculations of the magnetic properties of Fe-based superconductors

Alexander Yaresko

Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The wave-vector (**q**) and doping (δ) dependences of the noninteracting susceptibility, magnetic energy, iron moment, and effective exchange interactions in novel iron-based superconductors LaFeAsO and MFe$_2$As$_2$ (M=Ba, Sr) are studied by performing LSDA band structure calculations.

The real part of the static noninteracting susceptibility, $\chi_0(\mathbf{q}, 0)$, obtained from linear-response calculations for undoped ($\delta = 0$) compounds based on their paramagnetic LDA band structure has a maximum at $\bar{X}$ point with $\mathbf{q}=(\pi,0)$ corresponding to stripe anti-ferromagnetic (AF) ordering of Fe moments. The maximum appears due to a prominent peak of $\mathrm{Im}\chi_0(\mathbf{q})$ at the same wave vector, which evidences efficient nesting of hole-like Fermi surfaces centered at the Γ point with electron-like sheets at the Brillouin zone corners. The nesting is rapidly suppressed by either electron or hole doping and the maximum of $\mathrm{Re}\chi_0(\mathbf{q})$ shifts to incommensurate **q** already at $|\delta| = 0.1$.

The minimum of the LSDA total energy, $E(\mathbf{q})$, of the undoped compounds calculated self-consistently as a function of a wave vector **q** of co-planar spin spirals is also found at $\mathbf{q}=(\pi,0)$, with the calculated Fe moment being $\sim 1.3\mu_B$. In contrast to the doping dependence of $\mathrm{Re}\chi_0(\mathbf{q})$, the effects of electron and hole doping on $E(\mathbf{q})$ are remarkably different. As FeAs layers are doped with electrons ($\delta > 0$) to simulate F doping in $LaFeAsO_{1-x}F_x$ or Co doping in $M(Fe_{1-x}Co_x)_2As_2$, the minimum of $E(\mathbf{q})$ shifts at an incommensurate wave vector $\mathbf{q}_{min}$ along the $(\pi,0)$-(π,π) line and the collinear AF solution becomes unstable. On the other hand, when MFe$_2$As$_2$ is doped with holes, stripe AF order remains stable up to the doping level of $\delta \sim -0.3$, which corresponds to K content y=0.6 in $M_{1-y}K_yFe_2As_2$. The stabilization energy of the stripe-ordered solution is, however, strongly reduced by hole doping. Calculations for LiFeAs give a magnetic solution which exists in a narrow range of q around $\bar{X}$. The Fe moment and stabilization energy in LiFeAs are significantly smaller than in 1111 and 122 compounds.

Posters

Like in this booklet, the posters are displayed in alphabetical order according to the presenting author.

The rare earth impurity and the symmetry of superconducting gap in iron-based superconductors

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[2] Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

We study some aspects of the Ce rare-earth impurity in iron-based superconductors. In particular, we analyze the evolution of the crystalline electric-field (CEF) excitations in the superconducting state, and the local quasiparticle density of states of conduction electrons in $CeFeAsO_{1-x}F_x$ systems.
We show that resonant magnetic excitations of the conduction electrons that have been observed in these systems below Tc [1] may result in the formation of the bound state in the 4*f*-electron susceptibility at energies well below the CEF excitation energy. We find that the feedback of unconventional superconductivity on the CEF excitations results in two characteristic features. If the coupling between the CEF excitations and conduction *d*-electrons is large, the resonant excitations in the conducting electrons susceptibility centered at ω_r yield an additional bound state in the *f*-electron susceptibility at energies $\omega \leq \omega_r$. At the same time, the CEF excitations shifts towards higher energies and acquire an additional damping below T_c. If the coupling between the *d*-electrons and CEF excitations is weak the additional pole does not occur and the only effect of the unconventional superconductivity is the anomalous damping of the CEF excitations and their slight upward shift below T_c. We argue that the latter effect is observed in iron-based superconductors and supports strongly the $s^{\pm}$ gap function which changes sign between electron and hole pockets[2].
For investigation the effect of magnetic impurities on the local quasiparticle density of states (LDOS) in iron-based superconductors, we employ the twoorbital Anderson model within slave boson approximation, where 3*d* electron and hole conduction bands hybridize with the localized *f*-orbital of the impurity spin. We investigate how various symmetries of the superconducting gap and its nodal structure influence the quasiparticle excitations and the impurity bound states. We show that the bound states behave qualitatively different for each symmetry. Most importantly we find that the impurity-induced bound states can be used to identify the nodal structure of the extended s-wave symmetry ($S^{\pm}$) that is actively discussed in ferropnictides[3].

[1] S. Chi, et al., Phys. Rev. Lett. **101**, 217002 (2008).
[2] A. Akbari, I. Eremin, P. Thalmeier, and P. Fulde, Phys. Rev. B **80**, 100504(R) (2009).
[3] A. Akbari, I. Eremin, and P. Thalmeier, Phys. Rev. B **81**, 014524 (2010).

Coexistence of localized and itinerant magnetisms in iron pnictides.

V.P. Antropov, M. van Schilfgaarde, L. Ke and J.J. Pulikkotil

Ames Laboratory, Ames, IA, and Arizona State University, Tempe, AZ, USA

This presentation will consist of three parts:
Part one: LSDA total energy calculations and spin dynamical simulations to search for low energy magnetic structures in iron pnictides. In addition, the analysis of magnetic stability of the different phases is performed using static linear response technique. Correspondingly, the transversal (exchange coupling) and longitudinal elements of susceptibility are obtained for a wide range of pnictides as a function of magnetic moment, pressure and concentration. We found a large continuum of nearly degenerate states lying very close to the magnetic "striped" structure. The presence of non-collinearity seems to be a generic feature of iron pnictides when the Fe moment is small. At small R_{FeAs} the system is itinerant: long ranged interactions create incommensurate orderings and strong biquadratic coupling violates the applicability of Heisenberg model. There is a smooth transition to more localized behavior as R_{FeAs} increases: stable magnetic orbital order develops which favor long range AFM stripe ordering with strongly anisotropic in-plane exchange couplings. The stabilization of the stripe magnetic order is accompanied by the inversion of the exchange coupling.
Part two: Magnetic excitations in the striped phase of $CaFe_2As_2$ are studied with dynamic spin susceptibility calculations. Several types of itinerant particle-hole (Stoner) excitations, some of which originate largely from a narrow band of Fe *d* states, are found to coexist with the usual antiferromagnetic spin waves. While a multiplicity of elementary excitations are found, the Stoner excitations appear to predominate for energies below the Néel temperature, which is the energy range physically significant for magnetism and superconductivity. The band responsible for them is highly sensitive to lattice structure; thus there is a strong interaction between lattice vibrations and these spin dependent particle-hole excitations. A weakness of Heisenberg model is shown in details. The influence of spin zero-point fluctuations on stability of local magnetic moment and long range magnetic order is discussed. We provide a detailed comparison with neutron scattering experiments and discuss existing experimental controversies.
Part three: Using density functional approach we construct a general spin Hamiltonian for these materials. The Heisenberg model parameters are obtained using generalized 'inverse susceptibility' approach which produces parameters beyond commonly accepted long wave approximation. Biquadratic exchange parameters have been obtained using non-collinear total energy calculations beyond linear response approximations. The resulting Hamiltonian consists of anisotropic 1nn exchange couplings (J_{1a} and J_{1b}), 2nn coupling ($J_2 > J_{1a} + J_{1b}$), c-axis exchange ($J_z \approx 0.1\ J_2$), biquadratic exchange ($K_1 \approx 0.2\ J_2$) and magnetic anisotropy term (D). At small moments (when $J_{1a} = J_{1b}$), more distant exchanges have to be added to the description. While this Hamiltonian can reflect many experimental features there are numerous cases when this localized spin description is totally not applicable. At the end we discuss a possible nature of magneto-structural transition in these materials.

Comparison of Fermi surface and band structure measured with ARPES of $Ba(Fe_{0.65}Ru_{0.35})_2As_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$

Véronique Brouet[1], M. Marsi[1], B. Mansart[1], M.F. Jensen[1], A. Taleb-Ibrahimi[2], P. Le Fèvre[2], F. Bertran[2], A. Nicolaou[2], D. Colson[3], A. Forget[3], F. Rullier-Albenque[3]

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[2] CASSIOPEE beamline, Synchrotron SOLEIL, France
[3] SPEC, CEA Saclay, France

We present a compared investigation of the electronic structure of two families of iron pnictides, where superconductivity is achieved either by electron doping or by isovalent substitution. We observe that Co substitution leads to an electron doping of the electronic structure, in good agreement with a rigid band filling picture [1]. We also observe that Ru substitution yields a coherent electronic structure, with the same number of holes and electrons, i.e. with no induced doping [2]. However, these two numbers are about twice larger than in $BaFe_2As_2$, suggesting the absolute number of carriers is an adjustable parameter of the electronic structure. Simultaneously, we observe a large increase of the Fermi velocities, probably exceeding the increase expected in band structure calculations. These observations present interesting analogies with those observed by de Haas-Van Alphen oscillations in $BaFe_2(As_{1-x}P_x)_2$. These studies show that superconductivity can take place in quite different environment in doped and undoped superconductors.

[1] V. Brouet *et al.*, Phys. Rev. B **80**, 165115 (2009)
[2] V. Brouet *et al.*, cond-mat/1002.4952

Magnetic order in the iron pnictides

Jörg Bünemann and Tobias Schickling

Philipps-Universität Marburg, Germany

We present results on the electronic and magnetic properties of five-band Hubbard models which are assumed to capture the relevant physics of the iron pnictides [1,2]. In our calculations, we employ the Gutzwiller variational theory which, unlike, e.g., a Hartree-Fock (HF) approximation, is a genuine many-particle approach. The numerical efforts of this method, however, are still modest and it is therefore possible to carry out rather accurate calculations for complex multi-band systems.
We will present results both on the paramagnetic and the antiferromagnetic phases of our model systems. A comparison with recent paramagnetic DMFT calculations [3] shows very good agreement. In our studies on the antiferromagnetic phases, we find huge differences between the Gutzwiller- and the HF-theory. While the magnetic moment is significantly overestimated in HF, in Gutzwiller theory we find relatively small values of the moment over a reasonably large range of Coulomb- and exchange interaction parameters. Our findings therefore raise the question whether effective single-particle approaches are sufficient to describe the normal phase physics of the iron pnictides.

[1] K. Kuroki, S. Onari, R. Arita, H. Usudi, Y. Tanake, H. Kontani, and H. Aoki, Phys. Rev. Lett. **101**, 087004 (2008).
[2] S. Graser, T. A. Maier, P. J. Hirschfeld, and D. J. Scalapino, New J. Phys. **11**, 025016 (2009).
[3] H. Ishida and A. Liebsch, Phys. Rev. B **81**, 054513 (2010).

Inter-orbital effects in the impure pnictide superconductors

Anna Ciechan and Karol Izydor Wysokiński

Institute of Physics and Nanotechnology Centre, M. Curie-Skłodowska University, Lublin, Poland

We study the local properties of the iron oxypnictides by means of the real space Bogolubov–de Gennes equations. Starting with the realistic energy spectrum and assuming small amount of impurities we calculate the energy dependence of the local density of states and spatial distribution of the local values of the superconducting energy gap. We pay particular attention to the role of the inter-orbital scattering of pairs and the effect of impurity scattering on the superconducting state. The effect of inter-orbital impurities depends on the relative signs of the order parameters related to two orbitals in question. For opposite signs impurities produce bound states inside the gap, while for the same sign of the order parameters they hardly affect the superconductor. The results obtained for impure systems have been shown as a maps of the order parameters and local density of states. They well compare with the existing STM spectra of the iron pnictides.

Implications of electronic structure and lattice dynamics of NaFeAs

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In this work, we will discuss the implications of electronic structure and lattice dynamics of NaFeAs as established from first-principle FP-LMTO method. The global double degeneracy of bands along $X-M$ and $R-A$ (see Fig. 1) has been shown to be an universal characteristic for the new superconducting Fe pnictides. A tight-binding model has been proposed to explain the origin of the double degeneracy as due to a reduction of the unit cell along the diagonal directions. This global double degeneracy implies an instability of the electronic structure, which is quantitatively addressed by calculating the generalized susceptibility $\chi(\mathbf{q}, \omega = 0)$. The calculated values of $Re\ \chi(\mathbf{q}, 0)$ indeed show a rather sharp peak at $\mathbf{Q}_M$, (1/2, 1/2, 0) suggesting a spin density wave (SDW) ground state, however, competing orders, such as charge density wave (CDW), may exist. By using the calculated electron-phonon (e-p) interaction matrix elements, and a discriminat for the occurrence of SDW and CDW as derived from a restricted Hartree-Fock approximation, we have excluded the possibility of a CDW instability related to the nesting vector $\mathbf{Q}_M$. The peak-like structure of e-p coupling also present in NaFeAs (see Fig. 2) will be compared with those of other superconductors such as Hg, MgB_2 and $Li_{1-x}BC$ etc.. The A_{1g} phonon involving only the z-direction vibration of As and Na couples to steep band electrons, however, too weakly to explain the superconductivity on the basis of a conventional e-p coupling mechanism. The large transfer of spectral weight from Fe-$3dx^2-y^2$ to Fe-$3dz^2-r^2$ due to electron correlation may enhance the e-p coupling for Fe states.

[1] S. Deng, J. Köhler and A. Simon, Phys. Rev. B **80**, 1(2009)

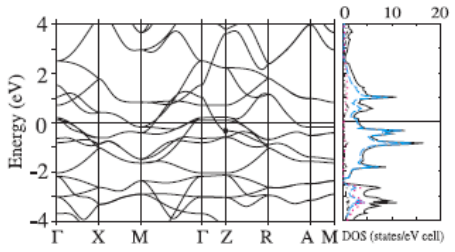

Fig. 1: Band structure and DOS curves (solid for total DOS, blue broken line for Fe-3*d*, red broken line for As-4*p*, and black broken line for NaFeAs.

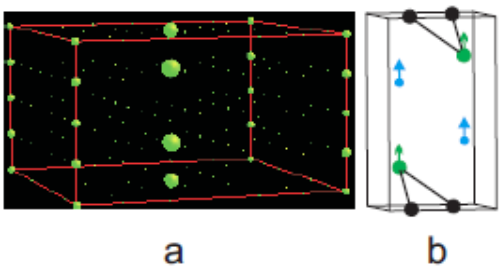

Fig. 2: a) **q** dependence of e-p coupling constant, $\lambda(\mathbf{q})$, in the first BZ of phonons revealing a peak-like structure, b) the most important A_{1g} phonon in e-p coupling.

Insights into the physics of pnictides from optical, penetration depth, upper critical field and NMR data

S.-L. Drechsler[1], R. Schuster[1], F. Roth[1], M. Grobosch[1], H. Rosner[2], I. Eremin[3], M. Korshunov[3], K. Koepernik[1], J. Málek[1], H.-H. Klauss[4], M. Rotter[5], D. Johrendt[5], S. Elgazzar[6], G. Fuchs[1], G. Behr[1], D. Singh[7], L. Zhang[7], N. L. Wang[8], B. Gorshunov[9], M. Dressel[9], D. Wu[9], J. van den Brink[1], S. Haindl[1], B. Holzapfel[1], V. Grinenko[1], F. Hammerath[1], H.J. Grafe[1], B. Büchner[1], M. Knupfer[1]

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The optical spectra of more than 12 Fe-pnictides at room temperature are analyzed within the Drude-Lorentz model with respect to the unscreened plasma frequency Ω_p, the back ground dielectric constant ε_∞ and anomalous mid-infrared absorption below 1eV and compared with the corresponding quantities as derived from standard LDA calculations and calculations within the RPA within a wide frequency region up to 10eV. From the measured Ω_p we estimate a moderate mass enhancement in between 2 and 3 as in ordinary transition metals ruling out strong correlations caused by a sizable on-site Coulomb interaction $U_d \approx 4$eV at Fe-sites sometimes proposed in the literature. From the estimated large $\varepsilon_\infty \approx 10 \div 12$ a sizable polarization can be derived which yields a considerable screening of Coulomb interactions. In particular, $U_d \leq 2$ eV can be estimated in accord with various electron spectroscopy data. However, details of that screening mechanism as well as the origin of an intense interband transition near 0.6 eV remain unclear within the frame of LDA-based RPA calculations for the dielectric function. We compare these anomalies with similar features for α-iron near 0.2 eV and discuss the relevance of spin-orbit effects and a mixture of charge, spin and orbital degrees of freedom. Possible contributions for the pairing mechanism are mentioned. From the superconducting penetration depth at $T=0$ a further mass renormalization at low T is observed which is ascribed to the coupling of various bosons within the framework of the Eliashberg theory and moderate total coupling strength $\lambda \sim 1$ is estimated for the La-1111 system.
Upper critical field and As-NMR data [1] point to unusual disorder effects caused for instance by As-vacancies and other defects: leading to improved superconducting properties at low magnetic fields and to Pauli paramagnetism at high fields as well as to a change of the As-spin lattice relaxation rate from a T^3 in clean to a T^5-behavior in disordered samples.
These data are discussed within the framework of the popular unconventional $s_\pm$ – as well as the conventional s_{++} scenarios for multiband superconductivity and a complex competition of superconductivity with *several* magnetic instabilities strongly affected by the local disorder.

[1] F. Hammerath *et al.* , Phys. Rev. B, Rapid. Commun. in press (2010)

Electronic structure studies of ferropnictide superconductors and their parent compounds by angle and time-resolved photoemission spectroscopy

J. Fink[1,2], S. Thirupathaiah[1], E. Rienks[1], H. A. Dürr[1], S. de Jong[3], E. van Heumen[3], E. Slooten[3], Y. Huang[3], R. Huisman[3], M. S. Golden[3], R. Cortes[4], L. Rettig[4], U. Bovensiepen[5], M. Wolf[4], A. Erb[7], T. Wolf[8], H.S. Jeevan[9], P. Gegenwart[9]

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We report high-resolution ARPES studies of the electronic structure of ferropnictide high-T_c superconductors and their parent compounds. The results are compared with DFT calculations in the paramagnetic phase. Here we focus on undoped and doped Ba/$EuFe_2As_2$ compounds. Upon variation of the polarization of the incident photons, important information on the orbital character of the states close to the Fermi level is obtained. [1] Using variable photon energies, information on the band dispersion perpendicular to the FeAs layers is derived. In the case of chemically n-type (p-type) doped systems, e.g. replacing Fe by Co (Ba by K), we observe a filling of the hole pockets (electron pockets) at the Γ (X)-point due to a shift of the Fermi level to higher (lower) energies in an almost rigid band system. These changes of the electronic structure upon doping cause a more three-dimensional electronic structure together with a reduction of the nesting conditions, possibly yielding a microscopic explanation of the generic phase diagrams in which antiferromagnetic (AF) order is destroyed followed by the appearance of the superconducting dome. [2] Regarding the almost equivalent phase diagram detected upon chemically pressurizing the compound (e.g. replacing As by P), one expects a similar change of the electronic structure. However, here with increasing P concentration, we observe a non-rigid-band-like change of the electronic structure in the centre of the Brillouin zone (BZ) (a disappearance of the hole pockets at Γ but an increase of the hole pockets at Z) while the size if the electron pockets does almost not change. ARPES studies on the undoped compound $EuFe_2As_2$ in the AF state reveal droplet-like Fermi surfaces caused by the partial opening of gaps of the order of 50 to 70 meV, similar to Cr metal in the AF state. These changes of the electronic structure in the AF state are related to a back folding and hybridization of the bands and indicate a strong interaction of magnetic and the electronic degrees of freedom in ferropnictides. Interestingly a Dirac cone-like dispersion of bands is observed near the X-point. [3] Finally, we have performed femtosecond time-resolved ARPES studies on $EuFe_2As_2$ and $BaFe(Co)_2As_2$ after excitation by 1.5 eV photons. The excitation of coherent photons, not yet detected in Raman spectroscopy, is observed. Attempts to evaluate the strength of electron-phonon coupling for phonons at the centre and at the corner of the BZ are discussed.

[1] J. Fink et al. Phys. Rev. B **79**, 155118 (2009)
[2] S. de Jong et al. EPL **89**, 27007 (2009)
[3] S. Thirupathaiah et al. Phys. Rev. B **81**, 104512 (2010)

The anti-ferromagnetic phase of $BaFe_2As_2$ investigated with ARPES

Maria Fuglsang Jensen[1], V. Brouet[1], M. Marsi[1], B. Mansart[1], A. Taleb-Ibrahimi[2], P. Le Fèvre[2], F. Bertran[2], A. Nicolaou[2], D. Colson[3], A. Forget[3], F. Rullier-Albenque[3]

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In this poster we will present a study of the difference in electronic structure between the paramagnetic (PM) phase and the anti-ferromagnetic (AFM) phase of the undoped $BaFe_2As_2$. The Fermi surface of the PM phase using the folded Brillouin zone is believed to have 3 circular hole pockets (where two are degenerate) around the Γ-point and two oval electron pockets around the X-point. Band folding is expected in the AFM phase as a result of the larger unit cell due to the magnetic ordering and gap openings should in principle take place by considering hybridisation between the back-folded electron bands onto the hole bands. Band folding has been clearly observed by angle-resolved photoemission spectroscopy (ARPES), but the resulting gap openings have not yet been fully clarified. There are many reasons for this. First of all, the many different bands crossing the Fermi level lead to a complex Fermi surface of multi orbital nature. Secondly, it is necessary to investigate how these bands depend on the photon energy as some may disperse with k_z. Matrix element effects also cause some bands to be suppressed and therefore the experimental settings highly influence the obtained results. At last, the electronic structure undergoes a structural transition at a temperature close to the transition from the PM phase to the AFM phase and it is not always easy to know which changes in the electronic structure are caused by the structural reconstruction, the magnetic interactions, or maybe even both. We present data measured in different experimental conditions, which allow us to resolve two bands constituting the electron pockets, with clearly different orbital symmetries. We study how these bands evolve as a function of the temperature and the results are compared to the structures measured at the hole pocket.

Structure and magnetism in electron-doped $SrFe_2As_2$

Jack Gillett, Sitikantha D. Das, Paul Syers, Alison K. T. Ming, Suchitra E. Sebastian, Gil G. Lonzarich

University of Cambridge, United Kingdom

A phase diagram of Co-doped $SrFe_2As_2$ is constructed as a function of doping using high purity single crystalline samples, and the evolution of magnetism into superconductivity studied. Similarities and differences with Co-doped $BaFe_2As_2$ are extracted and the underlying origin discussed, providing insight into possible factors that enhance superconductivity in these families of materials.

Could pnictidetype superconductivity occur in FeAs/GaAs superlattices?

Sinead Griffin and Nicola Spaldin

UC Santa Barbara, USA

A recurring feature in the iron pnictide superconductors is the existence of an FeAs layer. Here we use firstprinciples density functional calculations to examine whether the electronic structure characteristics believed to correlate with superconductivity in the pnictides are reproduced in superlattices containing alternating FeAs/GaAs layers. Both the effect of varying the FeAs structure and the number of zincblende GaAs layers is considered. Such superlattices could offer important advantages in ease of fabrication using MBE techniques and integration with semiconductor devices.

Inelastic x-ray scattering investigations of iron pnictide superconductors

M. Le Tacon[1], T. R. Forrest[2], Ch. Rüegg[2], A. Bosak[3], A. C. Walters[2,3], N. D. Zhigadlo[4], J. Karpinski[4], J. P. Hill[5], M. Krisch[3], and D. F. McMorrow[2]

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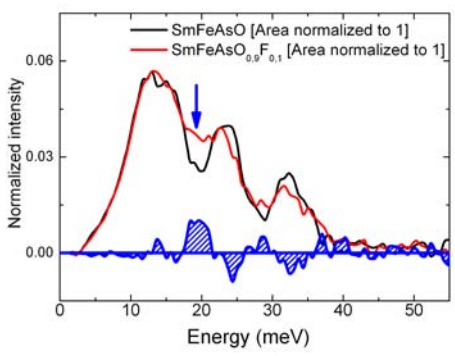
I will present measurements of the phonon density of states (PDOS) and dispersion in iron oxypnictide superconductors by inelastic x-ray scattering.
In the PDOS, we observe softening of phonon branches under fluorine doping in $NdFeAsO_{1-x}F_x$ and $SmFeAsO_{1-x}F_x$, and Raman-scattering experiments lead us to conclude that this softening is not related to zone-center phonons. It consequently implies an important softening of the relevant phonon branches at finite-momentum transfer Q [1]. Further experiments on the parent SmFeAsO and superconducting $SmFeAsO_{0.60}F_{0.35}$ single crystals have been carried out in order to map the phonon dispersion. Particular attention was paid to the dispersions along the 100 and 110 directions of three optical modes close to 23 meV, polarized out of the FeAs planes. Remarkably, two of these modes are strongly renormalized upon fluorine doping [2].
These results provide significant insight into the energy and momentum dependence of the coupling of the lattice to the electron system and underline the importance of spin-phonon coupling in the superconducting iron pnictides.



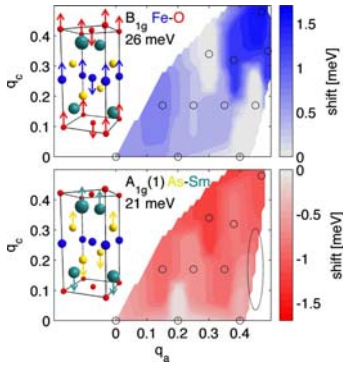


Fig. 1: Doping dependence of the phonon density of in $SmFeAsO_{1-x}F_x$.
Fig. 2: Momentum dependence of the doping induced renormalization of the 26 meV, $B1_g$ (upper panel) and 21 mV, A1*g* (lower panel) modes in the (q_a 0 q_c) plane. The dashed ellipse indicates the q-resolution. The insets show schematics of the respective q=0 eigenvectors, with the atoms color coded as indicated.

[1] M. Le Tacon, M. Krisch, A. Bosak, et al., Physical Review B **78**, R140505 (2008)
[2] M. Le Tacon, T. R. Forrest, C. Rüegg, et al., Physical Review B **80**, R220504 (2009)

A comparative study of $Fe_{1+\delta}Te_{1-x}Se_x$ single crystals grown by Bridgman and self flux techniques

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Single crystals of $Fe_{1+\delta}Te_{1-x}Se_x$ ($0 \leq x \leq 0.5$) were grown via both Bridgman and self flux techniques. Large crystals of size ø 10 x 50 mm could be obtained with the Bridgman method. The excess of iron, $\delta \geq 0.07$, at interstitial sites was observed to deteriorate the superconductivity of the samples. Study of semiconducting and Curie-Weiss-like behavior indicates that an appearance of a hump for $Fe_{1+\delta}Te_{0.60}Se_{0.40}$ ($\delta \leq 0.04$) is more pronounced for the self flux growth than for the Bridgman method. This was observed via measurement of the normal state of resistivity and magnetic susceptibility, which decrease with lower temperature. Furthermore, our results give evidence that the phase with x~0.40 is readily formed in the self flux method despite the use of various ratios of initial mixtures.

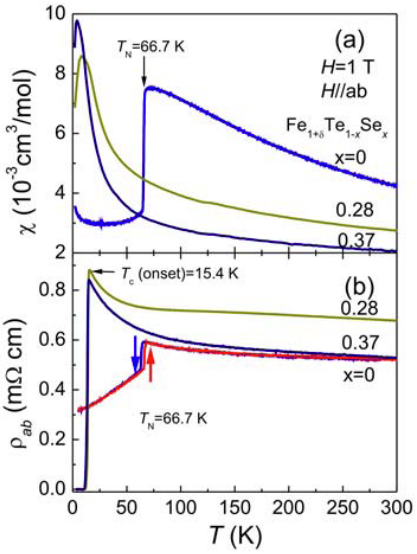

Fig. 1
(a) Magnetic susceptibility displays a Curie-Weiss-like behavior at high temperatures for $Fe_{1+\delta}Te_{1-x}Se_x$ crystals (x=0, 0.28, and 0.37) grown with the Bridgman method.
(b) Temperature dependence of resistivity for $Fe_{1+\delta}Te_{1-x}Se_x$ crystals (x=0, 0.28, and 0.37). The thermal hysteresis behavior is observed at T_N~66.7 K, indicating the existence of the first order structure phase transition. The arrows of blue and red indicate the directions of cooling and warming processes, respectively.

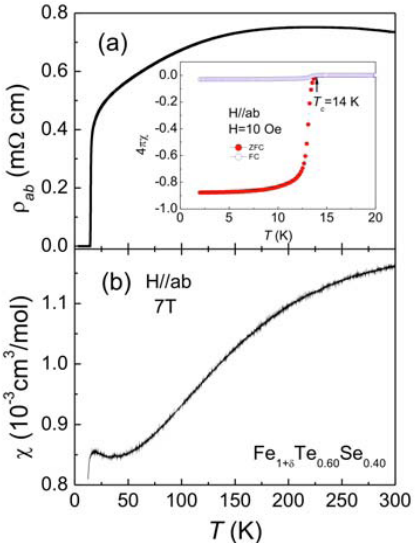

Fig. 2
(a) Temperature dependence of resistivity of a $Fe_{1+\delta}Te_{0.60}Se_{0.40}$ crystal grown with the self flux method. Inset shows the magnetic susceptibility displaying a superconducting transition at T_C~14 K.
(b) Magnetic susceptibility decreases with decreasing temperature and exhibits an upturn behavior below 40 K.

Infrared spectroscopy study on Fe-based superconducting single crystals

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The presence of superconductivity in hole- and electron-doped Fe-based pnictides has triggered strong research efforts since its discovery in 2008.
The undoped parent compounds show an antiferromagnetic metallic ground state due to the development of a spin density wave (SDW) state around a characteristic temperature T*. Superconductivity appears when the antiferromagnetic ordering for the Fe-layer is suppressed by doping with electrons or holes.
Upto now several questions are still open: in particular origin and nature of superconductivity in these systems are not yet clearly established. Moreover the role of the correlation effects in doped pnictides is still unknown.
We present an infrared spectroscopy study of undoped and doped compounds of a member of the Pnictides family, FeTeSe.
In particular we present optical conductivity obtained from absolute reflectivity measurements via Kramers-Kronig transformations at several temperatures above and below transition temperatures (T* and T_c for the undoped and doped compounds respectively).
The integral of the optical conductivity, the optical spectral weight W(W,T), is proportional to the number of carriers participating in the optical process in the frequency range of integration, from the minimum measured frequency to a high frequency cut-off W. Studying its evolution with the frequency of the temperature dependence of W(W,T) gives information about the strenght of correlation in these class of materials in comparison with conventional metal and cuprates.
On doped compounds through the ratios Rs/Rn between the superconducting (Rs) and normal state (Rn) reflectance at THz frequencies is possible to study the opening of the superconducting gap and its evolution for $T < T_c$.

The (*anti*) PbFCl structure family: from ionic insulators to superconductors

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The relationship between the details of the two-dimensional arrangements of transition-metals in the series of PbFCl- and "filled" PbFCl-type pnictides and their physical properties deserve particular attention, because some of them are superconducting with relatively high critical temperatures (T_c).
All in all, about 990 compounds are referred to crystallize in the PbFCl (*anti*-PbFCl) type of structure [1-3]. It is most frequently formed by ionic compounds with the formula *MXY*. Usually, a large cation *M* and two anions *X* and *Y*, which differ in size significantly, are the constituents needed. Such preconditions, based on a simple hard sphere model, would no longer apply if different kinds of interactions, like covalent or metallic bonding gain more importance. Numberless examples of the same atomic arrangement with partial covalent or metallic bonding have been reported. Among them are ZrSiS, and also intermetallic phases of general formula A_2B (*A*1*A*2*B*). One (*A*) or two different metals (*A*1, *A*2) occupy the sites of F and Cl in PbFCl, while a metalloid (*B*), which is often a heavy element of group 14 or 15, substitute for Pb. Besides the prominent example of the "111" iron arsenide superconductor, LiFeAs, some further interesting representatives with *anti*-PbFCl-type structures are Cu_2Sb, Fe_2As, Sc_2Sb, ScDySb.
The bonding properties of the PbFCl-type representatives, including LiFeAs, are compared on the basis of a structure field diagram and the Electron Localization Function (ELF). The combination of both methods allows a classification of the bonding characteristics into ionic, covalent, and metallic.

[1] J. Nuss, M. Jansen, Z. Anorg. Allg. Chem. **628,** 1152 (2002)
[2] J. Nuss, U. Wedig, M Jansen, Z. Kristallogr. **221,** 554 (2006)
[3] J. Nuss, U. Wedig, M. Jansen, Z. Anorg. Allg. Chem. 2010, in press, doi:10.1002/zaac.201000095

Fermi surface shrinking and interband coupling in iron-based pnictides

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Measurement of Fermi surface with de Haas-van Alphen oscillations in LaFePO [1,2] showed a shrinking of the Fermi pockets with respect to first-principle LDA calculations, suggesting an energy shift of the hole and electrons bands with respect to LDA calculations. In this POSTER I will show that these shifts are a natural consequences of the strong particle-hole asymmetry of electronic bands in pnictides, and that they provide an indirect experimental evidence of a dominant interband scattering in these systems [3]. Recent measurement in 122 systems confirm this picture.

[1] A. I. Coldea et al., Phys. Rev. Lett. **101**, 216402 (2008)
[2] A. Carrington et al. arXiv:0901.3976
[3] L. Ortenzi et al., Phys. Rev. Lett. **103**, 046404 (2009)

Two-band strong coupling superconductivity theory

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A microscopic strong-coupling theory of superconducting pairing induced by an arbitrary electron interaction with bosons is formulated for the two-band model:

$$H = \sum_{p,\alpha=1,2} \varepsilon_\alpha(p) a^\dagger_{\alpha p} a_{\alpha p} + \sum_{p,p',\alpha,\beta} W_{\alpha\beta}(p,p')\, a^\dagger_{\alpha p}\, a_{\beta p'} + H_b\,, \tag{1}$$

where $p = (\mathbf{p}, \sigma)$ and $\varepsilon_\alpha(p)$ is the electron energy in the band $\alpha = 1, 2$. The matrix $W_{\alpha\beta}(p, p')$ describes electron interaction with various types of collective excitations: phonons, spin-fluctuations, charge-fluctuations, described by the Hamiltonian H_b.
We consider the two-time thermodynamic Green functions (GF) in terms of the four-component Nambu operators $(\bar\sigma = -\sigma)$

$$\mathsf{G}_{\mathbf{p}\sigma}(\omega) = \langle\langle \begin{pmatrix} \hat a_{\mathbf{p},\sigma} \\ \hat a^\dagger_{-\mathbf{p}\bar\sigma} \end{pmatrix} \mid \begin{pmatrix} \hat a^\dagger_{\mathbf{p},\sigma} & \hat a_{-\mathbf{p}\bar\sigma} \end{pmatrix} \rangle\rangle_\omega = \begin{pmatrix} \hat G_{\mathbf{p}\sigma}(\omega) & \hat F_{\mathbf{p}\sigma}(\omega) \\ \hat F^\dagger_{\mathbf{p}\sigma}(\omega) & -\hat G_{-\mathbf{p}\bar\sigma}(-\omega) \end{pmatrix}, \tag{2}$$

$$\hat G_{\mathbf{p}\sigma}(\omega) = \langle\langle \begin{pmatrix} a_{1,p} \\ a_{2,p} \end{pmatrix} \mid \begin{pmatrix} a^\dagger_{1,p} & a^\dagger_{2,p} \end{pmatrix} \rangle\rangle_\omega, \quad \hat F_{\mathbf{p}\sigma}(\omega) = \langle\langle \begin{pmatrix} a_{1,p} \\ a_{2,p} \end{pmatrix} \mid (a_{1,-p}\ a_{2,-p}) \rangle\rangle_\omega. \tag{3}$$

The system of equations for the two-component GFs (3) can be written as

$$\hat G_{\mathbf{p}\sigma}(\omega) = \left(\hat G^N_{\mathbf{p}\sigma}(\omega)^{-1} + \hat\Phi_{\mathbf{p}\sigma}(\omega)\, \hat G^N_{\mathbf{p}\sigma}(-\omega)\, \hat\Phi^\dagger_{\mathbf{p}\sigma}(\omega)\right)^{-1}. \tag{4}$$

$$\hat F^\dagger_{\mathbf{p}\sigma}(\omega) = -\hat G^N_{\mathbf{p}\sigma}(-\omega)\, \hat\Phi^\dagger_{\mathbf{p}\sigma}(\omega)\, \hat G_{\mathbf{p}\sigma}(\omega). \tag{5}$$

$$\hat G^N_{\mathbf{p}\sigma}(\omega) = \left(\omega\hat\tau_0 - \hat\varepsilon(\mathbf{p}) - \hat M_{\mathbf{p}\sigma}(\omega)\right)^{-1}, \quad \hat\varepsilon(\mathbf{p}) = \begin{pmatrix} \varepsilon_{1\mathbf{p}} & 0 \\ 0 & \varepsilon_{2\mathbf{p}} \end{pmatrix} \tag{6}$$

where $\hat M_{\mathbf{p}\sigma}(\omega)$ and $\hat\Phi^\dagger_{\mathbf{p}\sigma}(\omega)$ are the self-energy for the normal and anomalous GFs (3), respectively. By using the Mori projection technique and the mode-coupling (noncrossing) approximation we derive the following equations for these self-energies:

$$M^{\alpha\beta}_{\mathbf{p}\sigma}(\omega) = \frac{1}{N}\sum_{\mathbf{p}'}\sum_{\gamma\delta}\int_{-\infty}^{+\infty} dz\, K_{\alpha\gamma,\delta\beta}(\omega, z|p,p')\left\{-\frac{1}{\pi}\mathrm{Im}G^{\gamma\delta}_{\mathbf{p}'\sigma'}(z)\right\}, \tag{7}$$

$$\Phi^{\alpha\beta}_{\mathbf{p}\sigma}(\omega) = \frac{1}{N}\sum_{p'}\sum_{\gamma\delta}\int_{-\infty}^{+\infty} dz\, K_{\alpha\gamma,\delta\beta}(\omega, z|p,p')\left\{-\frac{1}{\pi}\mathrm{Im}F^{\gamma\delta}_{\mathbf{p}'\sigma'}(z)\right\}, \tag{8}$$

$$K_{\alpha\gamma,\delta\beta}(\omega, z|p,p') = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\Omega}{\omega - z - \Omega}\left(\tanh\frac{z}{2T} + \coth\frac{\Omega}{2T}\right)\chi_{\alpha\gamma,\delta\beta}(p,p'|\Omega), \tag{9}$$

$$\chi_{\alpha\gamma,\delta\beta}(p,p'|\Omega) = -(1/\pi)\,\mathrm{Im}\langle\langle W_{\alpha\gamma}(p,p')|W_{\delta\beta}(p',p)\rangle\rangle_{\Omega+i\delta}. \tag{10}$$

The self-consistent system of equations (4)–(9) can be solved numerically for a particular choice of the interaction matrix $W_{\alpha\gamma}(p,p')$ in the boson susceptibility (10).

Spin excitations in solids from *ab-initio* many-body perturbation theory

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Spin excitations in solids are of fundamental interest for a wide variety of phenomena. For example, in high-temperature superconductors the spin waves have been proposed as a possible mediator for the attractive electron-electron interaction [1]. To study spin excitations in solids from first principles we have developed a computational scheme based on many-body perturbation theory within the full-potential linearized augmented plane-wave (FLAPW) method and implement it in the SPEX code [2,3]. The main quantity of interest is the dynamical transverse spin susceptibility, from which magnetic excitations, including single-particle spin-flip Stoner excitations and collective spin-wave modes as well as their lifetimes, can be obtained. In order to describe spin waves we include appropriate vertex corrections in the form of a multiplescattering T-matrix, which describes the coupling of electrons and holes with different spins. To reduce the numerical cost for the calculation of the four-point T-matrix we exploit a transformation to maximally localized Wannier functions that takes advantage of the short spatial range of electronic correlation in the partially filled *d* or *f* orbitals of magnetic materials [4]. As an illustration, we present spin-wave spectra and dispersions for the elementary ferromagnets Fe, Co, and Ni as well as their alloys FeCo, FePd, and FePt calculated with our scheme. The results are in good agreement with available experimental data.

[1] D. J. Scalapino, Phys. Rep. **250**, 329 (1995)
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[3] C. Friedrich, S. Bl¨ugel, and A. Schindlmayr, Phys. Rev. B **81**, 125102 (2010)
[4] F. Freimuth, Y. Mokrousov, D. Wortmann, S. Heinze, and S. Blügel, Phys. Rev. B **78**, 035120 (2008)

Electronic, magnetic and transport properties of Co_2TiZ (Z=Si, Ge and Sn) Heusler alloys

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We have studied the electronic structure, magnetic and transport properties of some Co based full Heusler alloys, namely Co_2TiZ (Z=Si, Ge and Sn), using FP-LAPW method. The calculation show that Co_2TiZ (X=Si, Ge and Sn) are to be half-metallic compounds with a magnetic moment of 2 μ_B, well consistent with the Slater-Pauling rule. The electronic structure results reveal that Co_2TiZ have the high density of states at the Fermi energy in the majority-spin state and show 100% spin polarization. Our results also suggest that both the electronic and magnetic properties in these compounds are intrinsically related to the appearance of the minority-spin gap. The origin of energy gap in the minority-spin states is discussed in terms of the electron splitting of Z (Z=Si, Ge and Sn) and 3*d* Co atoms and also the *d*-*d* hybridization between the Co and Ti atoms. The transport properties of these materials are discussed on the basis of Seebeck coefficients, electrical conductivity coefficients and thermal conductivity coefficients. The linear temperature dependence of Seebeck coefficients suggests that these half-metallic compounds can be promising candidates for future thermoelectric devices.

Superconductivity in nickel analogues of iron superconductors

Alaska Subedi

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The iron superconductors and their nickel analogues have similar structure based upon Fe/Ni square lattice. Since Ni and Fe are ambient temperature ferromagnets and many Fe and Ni compounds show magnetism, it is plausible to expect that Ni can fill in the role of Fe in these compounds. However, Ni compounds seem to lie further from magnetic instabilities and have lower superconducting transition temperature. We use first principles calculations on LaNiPO and $BaNi_2As_2$ to show that unlike the Fe supercondutors, superconductivity in Ni based materials is readily explained by standard electron-phonon mechanism.

Multiband strong-coupling Eliashberg theory and phenomenology of iron pnictides

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The experimental critical temperatures and the gap values of the superconducting materials $LaFeAsO_{1-x}F_x$, $SmFeAsO_{1-x}F_x$ and $Ba_{1-x}K_xFe_2As_2$, which are exponent of the most important families (1111 and 122) of iron pnictides, can be reproduced by a *s*-wave three-band Eliashberg model. According to the most widely accepted theoretical proposals for the coupling mechanism in pnictides, in this model the dominant role is played by interband interactions and the order parameter undergoes a sign reversal between hole and electron bands (*s*±-wave symmetry). The values of all the gaps and their temperature dependence can be obtained by using high values of the electron-boson coupling constants and small typical boson energies (in agreement with neutron diffraction experiments). The upper critical field, the penetration depth, the density of states and other physical quantities can be calculated as well. Finally, the energy-dependent gap functions $\Delta_i(\omega,T)$, obtained by solving the three-band Eliashberg equations, can be inserted in the Blonder-Tinkham-Klapwijk model to calculate the Andreev-reflection spectra.

[1] G. A. Ummarino et al, Phys. Rev. B **8**0, 172503 (2009)
[2] G. A. Ummarino, Advances in Condensed Matter Physics **2010**, 1-6 (2009)

Spectroscopic imaging scanning tunneling microscopy study of an iron-chalcogenide superconductor

S. C. White, U. R. Singh, Y. Liu, C. T. Lin, P. Wahl

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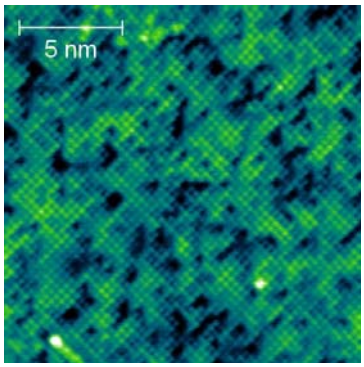
SI-STM has become a useful method for simultaneous study of the r- and k-space electronic structure of correlated electron systems such as the unconventional Fe-based superconductors. Interplay between local (r-space) and itinerant (k-space) electrons is believed to be critical in these materials. We measure variations in the local density of states at atomic resolution via differential tunneling conductance, which allows for comparative analysis of spacial modulations of the superconducting energy gap. Fourier transform scanning tunneling spectroscopy (FT-STS) is used on the same differential conductance data set to investigate k-space electronic structure. [1] We designed and constructed an SI-STM optimized to allow for high stability over measurement times up to 100 hours. A quality $Fe_{1.08}Te_{0.72}Se_{0.28}$ single crystal (T_C=14K) was cleaved in cryogenic vacuum at low temperature and characterized by SI-STM. An FeTe-based superconductor was chosen over the 122 Iron-Pnictides due to the favorable cleaving properties of the former. Preliminary analysis suggests strong electronic structure variation around the Fermi energy in r-space in this material. We expect further investigation of the $Fe_{1+\delta}Te_xSe_{1-x}$ system and other Fe-based superconductors to yield new information on the order parameter and mechanism of high-T_c superconductivity.

[1] Shen and Davis, Materials Today, Vol. **11**, Number 9, (2008)



$Ba(Fe_{1-x}Co_x)_2As_2$: crystal growth, structural and superconducting properties

Th. Wolf, P. Schweiss, R. Fromknecht, P. Adelmann, D. Ernst, F. Hardy, Ch. Meingast

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Among the FeAs superconductors discovered recently, crystal growth of large and perfect single crystals is most promising in the 122 system. Here, the easiest way to achieve superconductivity is replacing Fe by Co. Due to the toxicity and high vapor pressure of As, the growth has to be carried out in closed SiO_2 ampoules, in which the temperature is limited to T < 1200°C. Therefore, in this paper the flux method has been used to grow crystals. To do this, prereacted FeAs and CoAs, together with Ba and flux, have been filled into Al_2O_3, ZrO_2 or glassy carbon crucibles, which were then sealed in a SiO_2 ampoule under a low pressure of Ar. Various metals like Al, Pb, Sb, In, Mg, Zn, and Ag were tried as flux. These growth experiments demonstrated that the 122 phase possesses a strong tendency to grow in a dendritic manner. This led to an incorporation of large amounts of flux into the growing crystals. Reducing the supersaturation by decreasing the cooling rate to below 1°C/h finally resulted in crystals exhibiting minor flux inclusions and a reasonable habit. As all fluxes used were incorporated into the 122 phase, leading to solid-solution crystals with altered physical properties, FeAs was used as a self-flux. Starting mixtures with a ratio Ba:(Fe+Co):As = 1:4:4 allowed growth temperatures below 1200°C. However, with self-flux the tendency to grow in a dendritic manner was even more pronounced than in the cases of metallic flux. Even a reduction of the cooling rate to below 0.3°C/h did not lead to the formation of crystal faces other than (001). Instead large platelike crystals with lobed edges and thicknesses of several 100 µm were formed (Figure 1).

Figure 1: $Ba(Fe_{0.80}Co_{0.20})_2As_2$ single crystal: cleavage plane and lobed edges

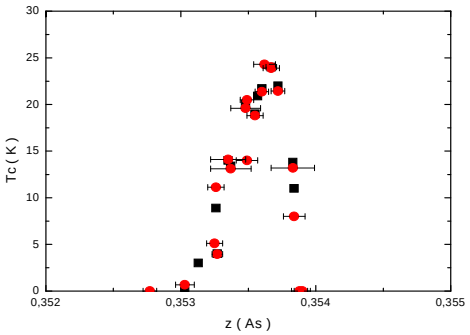

Figure 2: T_c versus z parameter

EDAX analysis of the grown crystals showed that for $x < 0.2$ the Co concentration can be calculated using a distribution coefficient of $K = 0.75$. Above $x = 0.2$ K increases to about 1. As it is not expected that the activity of Co in the flux changes abruptly, this behavior of K has to be attributed to a change in chemical bonding in the 122 phase.

The structural characterization of the crystals was carried out with a 4-circle x-ray diffractometer using Mo radiation. It was found out that both the a- and c-axes show a linear decrease with increasing Co concentration. However, the z parameter, which is the position of the As atom above the Ba atom, splits into two Vegard lines with a kink at $x \sim 0.2$.

T_c values of the crystals have been determined inductively and by measuring their specific heat and thermal expansion. The resulting phase diagram is very similar to published data with a maximum T_c value of 24.0K at $x = 6.0\%$. In the overdoped region, however, ac susceptibility detected superconductivity up to $x = 0.3$ which could not be verified by the bulk measurements. This seems to be a hint for spurious superconductivity at surfaces or inter-faces, possibly due to a change in chemical composition or to stresses.

In figure 2, bulk T_c values are plotted as function of z. T_c increases and decreases again in a very narrow interval. However, at $z = 0.3537$, where T_c attains its maximum value the corresponding angle of the FeAs tetrahedron is still far from being ideal.

Importance of Fermi surface nesting and quantum fluctuations for the magnetism in iron pnictides

Y.-Z. Zhang, H. Lee, I. Opahle, H. O. Jeschke, and R. Valentí

Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität Frankfurt, Germany

Since the discovery of high-Tc Fe-based superconductors in 2008, great effort has been devoted to understanding the mechanism of the stripe-type antiferromagnetic metallic state with small magnetic moment observed experimentally in iron pnictides. While it is still under debate whether the magnetism comes from Fermi surface nesting or exchange interaction of local spins, various mechanisms for a reduced magnetic moment have been proposed, such as negative on-site Hubbard interaction, magnetic multi-pole contributions, proximity to a magnetic instability and spin frustration. By applying density functional theory to various families of iron pnictides like 1111, 122 and 111 compounds, we find strong evidence of a close relationship between Fermi surface nesting and magnetism. Furthermore, we attribute the appearance of magnetism or superconductivity to the competition of the instabilities at nesting vectors of (π, π) and (0,0). Based on the widely believed argument that pairing in Fe-based superconductors is most probably mediated by spin-fluctuation, we predict the superconducting transition temperature T_c for several hypothetic 1111 compounds from a phenomenological relation. Our results suggest that LaOFeSb could be a good candidate for a high-Tc superconductor with transition temperature of around 60 K. Meanwhile, by employing dynamical mean field theory with continuous time quantum Monte Carlo as an impurity solver, we propose that the antiferromagnetic metal with small magnetic moment naturally arises if coupling between unfrustrated and frustrated bands is taken into account. Our results suggest a consistent scenario for the appearance of the antiferro-magnetic metal with small magnetic moment: magnetism in the iron pnictides originates from a strong instability at a nesting vector of (π, π) in weakly frustrated bands while it is reduced by quantum fluctuations due to the coupling between weakly and strongly frustrated bands.

Participants

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Psi-k Network : Towards Atomistic Materials Design

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PSI-K WORKSHOP FINANCE REPORT

Title of the Workshop	Electronic Structure of Fe-based Superconductors
Workshop Organisers	O.K. Andersen, L. Boeri, I.I. Mazin, H. Rosner
Location of the Workshop	Max-Planck-Institute for Solid State Research, Stuttgart, Germany
Dates of the Workshop	10-12 May 2010
Total Grant from Psi-k	110000 euro

EXPENDITURE

(Please complete the tables using numbers ONLY in the amounts fields - the spreadsheet will calculate the totals for you)

WORKSHOP DELEGATES / SPEAKERS			
Name and Country of Claimant	**Travel**	**Accommodation**	**Total (€'s)**
See attached list			€ -
		€ 6,495.00	€ 6,495.00
			€ -
			€ -
			€ -
			€ -
			€ -
			€ -
			€ -
			€ -
		Total Travel & Accommodation	**€ 6,495.00**

WORKSHOP REFRESHMENTS / CONFERENCE DINNERS			
Date	**Tea / Coffee**	**Lunch / Dinner**	**Total (€'s)**
11/5/2010		€ 3,120.00	€ 3,120.00
10/5-12/5		€ 1,045.00	€ 1,045.00
			€ -
			€ -
			€ -
		Total Refreshments	**€ 4,165.00**

MISCELLANEOUS EXPENDITURE	
Details	**Total (€'s)**
Bus for conference dinner	€ 340.00
Total Miscellaneous	**€ 340.00**

Total Travel & Accommodation	**€ 6,495.00**
Total Refreshments	**€ 4,165.00**
Total Miscellaneous	**€ 340.00**

TOTAL EXPENDITURE	**€ 11,000.00**

Name	Surname	Reimbursement (per day)	Number of days	Total
Aichorn	Markus	75	3	225
Akbari	Alireza	52.5	3	157.5
Anisimov	Vladimir	75	3	225
Antropov	Vladimir	52.5	7	367.5
Arita	Ryotaro	75	4	300
Benfatto	Lara	75	3	225
Bersier	Christophe	52.5	3	157.5
Borisenko	Sergey	75	3	225
Brouet/Fuglsang	Veronique/Maria	105	3	315
Buczek	Pawel	52.5	3	157.5
Buechner	Bernd	75	2	150
Buenemann	Joerg	52,5	3	157.5
Calandra	Matteo	75	3	225
Ciechan/Griffin	Anna/Sinead	105	4	420
Coldea	Amalia	75	3	225
Das/Gillet	Sitikantha/Jack	105	3	315
Drechsler	Stefan-Ludwig	75	3	225
Dugdale	Stephen	75	3	225
Eremin	Ilya	75	3	225
Fink	Joerg	75	3	225

Graser	Siegfried	75	3	225
Honerkamp	Carsten	75	2	150
Hott	Roland	52.5	3	157.5
Johannes	Michelle	75	4	300
Koepernik/Kasinathan	Klaus/Deepa	105	3	315
Ku	Wei	75	3	225
Liebsch	Ansgar	75	3	225
Liechtenstein	Alexander	75	2	150

TOTAL **6495**