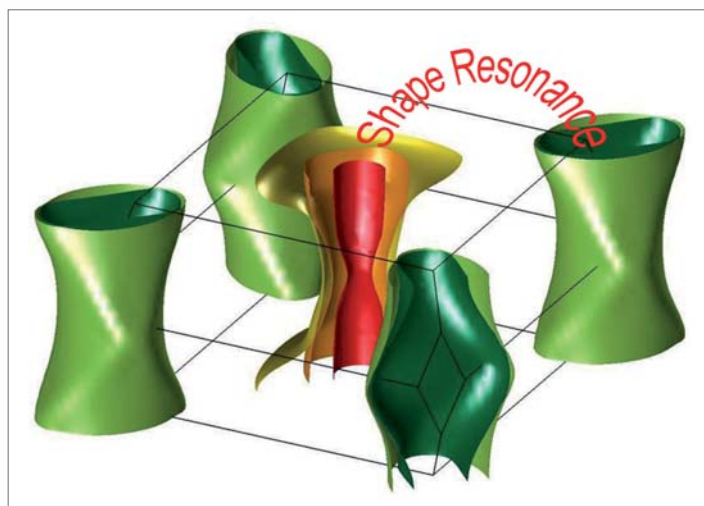

SUPERSTRIPES

2015



edited by
Antonio Bianconi

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2015

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Superconductivity, Magnetism & Ferroelectricity

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CHAPTER 1

SESSION 1

Introduction to Superstripes

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At the first Stripes conference on Dec 1996 it was clear that the universal material architecture of cuprate high temperature superconductors was a hetero-structure at atomic limit made of a superlattice of active atomic layers, CuO_2 , intercalated by a large variety of spacer layers. In the last 20 years a new field of science of nanomaterials has grown looking for new hetero-structures at atomic limit where the flat atomic CuO_2 layer, has been replaced by graphene, (intercalated graphite) boron, (MgB_2) FeAs, FeSe, (iron based superconductors) and today other monolayers like silicene, intercalated by a large variety of spacer layers with defects inserted to optimize the superconducting critical temperature.

In these 20 years experiments have shown that the electronic structure of the 2D electron gas in the active atomic layers show the coexistence and the interplay of two types of quasi one-dimensional defects called stripes due to different mechanisms:

1) the so called “extrinsic effects” which have high technological interests since they allow stripes synthesis and manipulation by material design: i) the lattice misfit strain between active atomic layers, and the spacer layers, and ii) the spatial self-organization of defects in the spacer layers inserted to optimize the critical temperature. These effects give a nanoscale phase separation with stripes in the active 2D electron gas, i.e., characterized by different charge density, different lattice distortions, different orbital symmetry [2].

2) the so called “intrinsic effects” are due to electronic instability by tuning the chemical potential in the active 2D electron gas either away from half filling in a Mott insulator or approaching a topological Lifshitz transition in a multi-bands Hubbard system (cuprates), by approaching a topological “neck disrupting” Lifshitz transition (in diborides and in iron superconductors).

In this complex scenario the system is out of equilibrium with a quenched disorder due to misfit strain and defects self organization and arrested electronic and magnetic phase transitions forming multiple short range stripes orders: periodic lattice distortion (PLD), orbital density wave (ODW), charge density wave (CDW), spin density wave (SDW),

which shows up at different critical temperature with different time scales, segregated into different portions of the k-space and real space.

PLD, ODW, CDW in high temperature superconductors [1,2] were first been observed using fast (10^{-15} s) and local (1 nm) probes: XANES [3] and EXAFS [4] joint with x-ray diffraction [5,6] and recently by scanning nano x-ray diffraction [7]. The new word "superstripes" was coined in 2000 [6] to describe a phase with the spontaneous breaking of both translational symmetry and gauge symmetry [6]. In the nanoscale phase separation landscape of superstripes localization and delocalization coexist in different portions of the k-space and real space with percolating superconducting pathways [8]. In high T_c percolating superconducting nano-puddles a first condensate in the BCS regime coexists with a second polaronic condensate at the BEC-BCS crossover coupled by the shape resonance in the superconducting gaps [9] due to exchange interaction between pairs in the different condensates. Finally the emergence of high temperature superconductivity need tuning the chemical potential near a neck disrupting topological Lifshitz transition in presence of quenched disorder to generate both nanoscale phase separation [10-12], percolation [7,8] and shape resonances [9].

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Nanoscale superconducting systems and potential for room temperature superconductivity: theory and experiment

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Keywords: high T_c, nano-clusters, shell structure, ionization

The nanoclusters form a new family of high temperature superconductors [1-3]. We focus on small metallic nanoclusters Mn (n is a number of atoms) which contain delocalized electrons (NH 102-103 ; N is a number of free carriers). The electronic states form energy shells similar to those in atoms or nuclei (e.g., s, p, d, ...) [4]. Presence of the shell structure and corresponding orbital degeneracy 2(2L+1) leads to great strengthening of the pairing interaction. Under special, but perfectly realistic conditions, the superconducting pairing is very strong and leads to high T_c. For some specific clusters, there arise T_c ~ 150-200 K and the energy spectrum becomes strongly modified. With a realistic sets of parameters, it should be possible to raise T_c up to room temperature. Specific experiments capable of detecting this phenomenon can be identified. Recent experimental measurements [5] of the ionization potential will be described. The measured temperature dependence is directly related to the electronic density of states and is caused by the presence of the temperature dependent gap parameter. According to the data, for the nano-clusters Al-66 the pairing persists up to T_{cH} 120K. This is the first spectroscopic observation of the phenomenon. Delocalized electrons in other nano-scale systems, such as quantum dots, aromatic molecules as well as biologically active systems also represent an example of superconducting systems. Pairing raises the possibility to observe the Josephson tunneling between the clusters. The phenomenon is promising for building nano-based tunneling networks transferring the superconducting current at high temperatures [6].

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Exploiting nanoribbons to enhance electron-hole superfluidity in double graphene systems



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Keywords: Graphene, Fermi-Bose systems, High Tc Superfluid, Nanoribbons

Interest in electron-hole superfluidity in spatially separated conducting sheets of electrons and holes [1–6] stems partly from the fact that high transition temperatures are predicted for these systems because the Coulomb pairing is very strong compared with conventional superconductors.

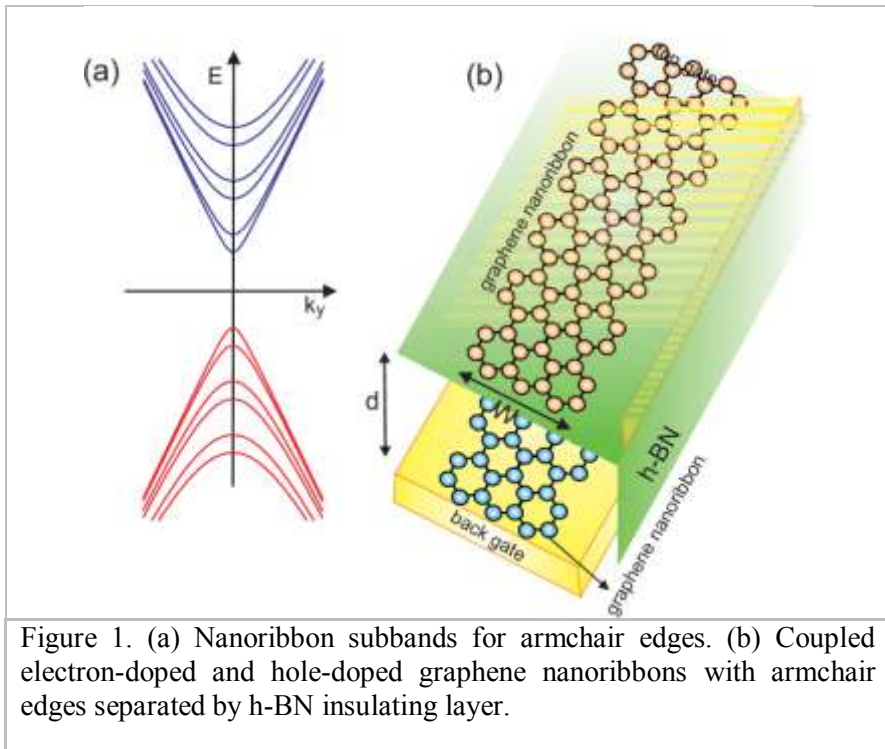
We propose a novel graphene-based device designed to boost the electron-hole pairing attraction and to reduce the effects of the screening of this attraction. The electrons and holes are confined in nanometer-scale wide nanoribbons, each ribbon etched from bilayer sheets of electron-doped or hole-doped graphene. By confining the electrons and holes close together on top of each other, the nanoribbons increase the average Coulomb interaction, which should enhance superfluid properties. Nanoribbons with armchair edges exhibit gapped parabolic-like energy bands (Fig. 1(a)). This contrasts with monolayer sheets of graphene with their familiar gapless linear spectrum. Graphene nanoribbons with controlled edges can be fabricated using mechanical and chemical techniques [7]. The nanoribbons are separated by a thin barrier of hexagonal Boron Nitride (h-BN) that is an excellent insulating barrier in graphene for thicknesses as small as 1 nm [8]. The insulating barrier permits the electrons and holes to be extremely close to each other without recombination, resulting in a very strong average Coulomb attraction. The electrons and holes are induced in the two separately electrically contacted graphene nanoribbons using top and back gates (Fig. 1(b)).

We use mean field theory for nanometer-scale wide nanoribbons with multiple electronic bands to evaluate the zero temperature superfluid energy gaps and the electron and hole chemical potentials. With finite-width ribbons, fluctuations should not destroy a mean field coherent quantum state.

We present results for the zero-temperature momentum-dependent superfluid energy gaps Δ_k and maximum gaps Δ_{max} , as functions of equal electron and hole densities. The system parameters are the width of the nanoribbons, the number of occupied electronic subbands, and the thickness of the insulating barrier separating the nanoribbons.

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Coherence in the High T_c cuprates

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The issue of coherence in the High T_c cuprates is crucial for our understanding of the underlying pairing mechanism in these materials. This issue is intimately related to the pseudo-gap phenomenon. Originally introduced by Mott to describe the impact of strong disorder on the DOS of band insulators, the idea of a pseudo-gap was applied by Friedel and Alloul to explain the decrease of the spin susceptibility at temperatures substantially higher than T_c . Later the same term was applied to the large tunneling gap opening up above T_c and apparently merging at lower temperatures with what appeared to be a superconducting gap. While the authors of the original NMR spin susceptibility measurements considered the pseudo-gap as reflecting the existence of anti-ferromagnetic fluctuations unrelated to superconductivity, most groups doing tunneling and also ARPES work considered the pseudo-gap as a precursor of superconductivity. However direct coherence probes of Bogoliubov –de Gennes quasi-particles, originally Andreev – Saint-James reflections and more recently interference effects observed by STM indicate that the coherence energy scale is different from and smaller than the tunneling gap, particularly in the underdoped regime. The co-existence of a coherent state and of localized pseudo-gap states will be discussed in detail.

SESSION 2

Oxygen Isotope Effects on Lattice Properties of $\text{La}_{2-x}\text{Ba}_x\text{CuO}$ ($x = 1/8$)



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Keywords : stripes in cuprates, isotope effects in cuprates, lattice effects in cuprates, structural properties of cuprates

A novel negative oxygen-isotope ($^{16}\text{O}/^{18}\text{O}$) effect (OIE) on the low-temperature tetragonal phase transition temperature T_{LTT} was observed in the stripe phase of the cuprate $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ ($x = 1/8$) using high-resolution neutron powder diffraction. The corresponding OIE exponent $\alpha(T_{\text{LTT}}) = -0.36(5)$ has the same sign as $\alpha(T_{\text{SO}}) = -0.57(6)$ found for the spin-stripe order temperature T_{SO} [1]. The fact that the LTT transition is accompanied by charge ordering (CO) implies the presence of an OIE also for the CO temperature T_{CO} . Furthermore, a temperature dependent shortening of the c-axis with the heavier isotope is observed. These results in combination with the previously observed OIE on the spin-stripe order temperature T_{SO} [1] indicate that all transitions observed in the stripe phase of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ ($x = 1/8$) are sensitive to oxygen lattice vibrations. Theoretical lattice dynamical calculations based on a dynamic anharmonic electron lattice interaction Hamiltonian consistently reproduce the experimental results. This structural instability is driven by phonon mode softening stemming from anharmonic electron-lattice interactions, and these interactions are essential for the stripe formation in the cuprates. The present findings may contribute to a better understanding of the complex microscopic mechanism of stripe formation and of high-temperature superconductivity in the cuprates in general.

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The Polaronic Condensate in $\text{UO}_{2(+x)}$: Dynamical Polarons and Feshbach Resonances



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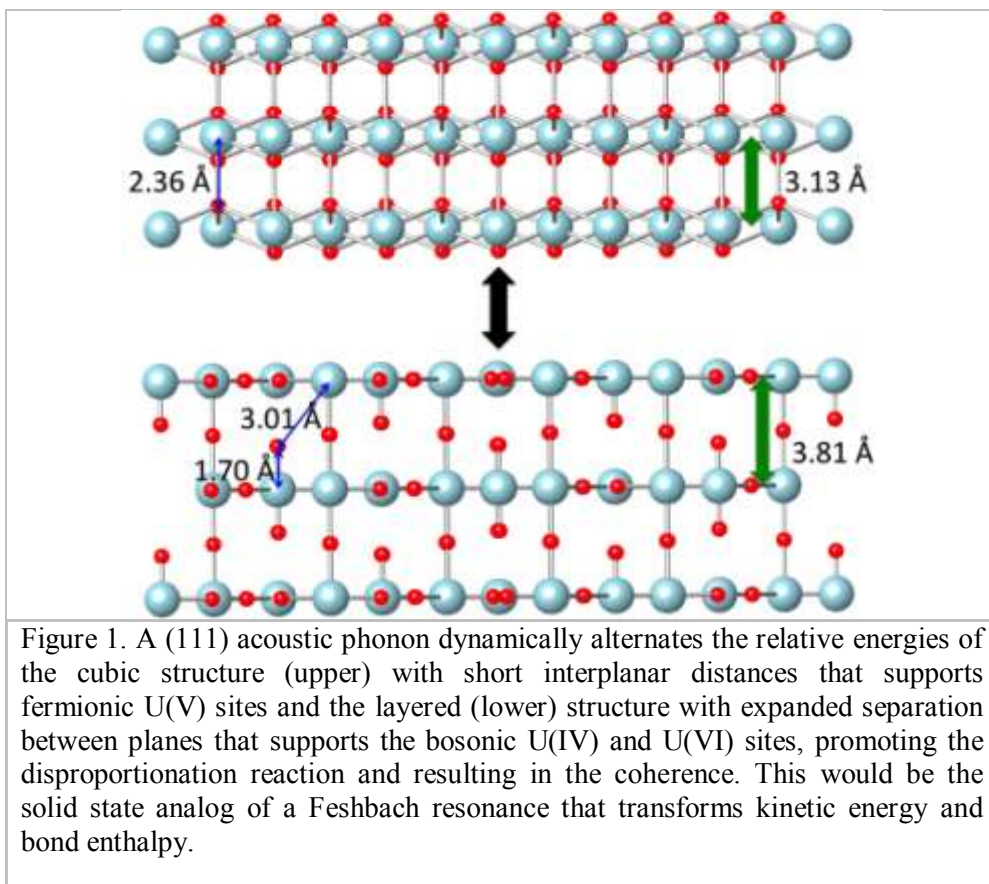
Keywords : condensates – dynamical polarons – Feshbach resonance

Bose-Einstein condensates have been made from atoms, polaritons, magnons, and excitons, posing the question of whether they can also be composed of polarons so as to combine coherently charge, spin, and a crystal lattice. Following our earlier report of unique structural and spectroscopic properties best interpreted as BEC-like behavior [1], we now definitively identify polaronic condensates in photo- and chemically doped $\text{UO}_{2(+x)}$ on the basis of the relatively high energy ultrafast time dependent terahertz and microwave absorbance spectroscopy results that show extreme coherence and additional collective properties including microwave dissipation patterns whose sole precedents are condensate vortex and defect disorder and condensate excitations. That some of these signatures of coherence in an atom-based system extend to ambient temperature indicates that it is not a ground state property. Combining the results of these current experiments with the structural characteristics suggests a novel mechanism that could be a synchronized, dynamical, charge transfer or disproportionation excitation involving the confluence of the non-degenerate valence-lattice dynamics of these polarons with the structural chemistry of uranium oxides (Fig. 1), possibly via the solid state analog of a Feshbach resonance that could automatically give the coherence [2]. A macroscopic quantum object that can be created by chemical doping, persist to ambient temperature, and resides in a bulk solid would be revolutionary.

This type of mechanism could be of more global interest because it relates the BEC in $\text{UO}_{2(+x)}$ to the BCS condensate in cuprates via the dynamical polaron that is common to both. In $\text{UO}_{2(+x)}$ the polaron aggregate forms planes, whereas in cuprates it is the dynamical stripes [3]. Although the effects of these stripes on the structure measurements were understood [4] and predictions made for the consequences on the electronic structure, in the absence of any more direct association with the properties interest was lost. However, multiphase fermionic liquids have now been found to not only involve dynamical molecule formation, but the Feshbach resonance that promotes dimerization has been implicated directly in the formation of the condensate [2]. A solid state analog of this process could therefore also be the origin of the condensates in these mixed valence oxides.

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Nanoscale competition between multiple phases in high-temperature superconductors



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Functional materials like high temperature superconductors (HTS) and complex oxides are characterized by an intrinsic complexity. Indeed, they show a coexistence of multiple phases like Charge-Density-Wave (CDW), Spin-Density-Wave (SDW) and the defects that get organized in different nano-domains and exhibit a strong dynamic competition. The understanding of the interplay among these multiple phases is challenging because their complex spatial competition and dynamics are strongly connected to the emerging of functional properties at the macroscopic scale. The interpretation at the nanoscale of these processes will open the way to the development and optimization of new functional materials. In order to clarify the phase's coexistence it is important to understand their spatial-organization. On this purpose we developed innovative techniques like scanning micro X-ray diffraction ($S\mu$ XRD) and resonant scanning micro X-ray diffraction ($rS\mu$ XRD) to directly visualize the spatial-organization of the SDW, CDW and defects nano-domains. By the use of $S\mu$ XRD on several High temperature superconductors (HTS) we evidenced a common nanoscale phase separation scenario, characterized by the coexistence of competing scale-free networks of self-organized nano-domains [1-7]. Moreover, we found that an optimum inhomogeneity is needed to promote the percolation process and the emergence of properties like superconductivity at the macroscopic scale [8]. In this process, the way how the nano-domains interact and evolve in time is still a fundamental missing point. For this reason a new experimental approach that combines temporal and spatial resolution with bulk sensitivity has been developed [9]. Combining a time-resolved scattering technique like X-ray Photon Correlation Spectroscopy (XPCS) with resonant X-ray scattering (RIXS), we were able to find peculiar slow dynamics in the nano-domains competition with high temperature superconductivity.

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Orbital-Spin Fluctuation Theory for Cuprate and Fe-based Superconductors: Impact of Aslamazov-Larkin type Vertex Correction



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Keywords : vertex correction – mechanism of superconductivity – orbital order

In this paper, we study the electronic states in multi-orbital Hubbard models for cuprate and Fe-based high- T_c superconductors. To understand the normal-state phase-diagrams in these systems, the mean-field-level approximations (such as the random-phase-approximation (RPA)) are insufficient. For example, these approximations cannot explain the axial CDW formation and orthorhombic structure transition observed in cuprate and Fe-based superconductors, respectively. To explain these unsolved phenomena, decisive role of the "Aslamazov-Larkin type vertex correction (AL-VC)", which is dropped in the RPA, had been clarified in Refs. [1-5]. We analyze the AL-VC based on both the perturbative method and the functional RG (fRG) method, and find that the spin-fluctuation-driven orbital orders are realized in cuprate and Fe-based superconductors thanks to the AL-VC.

In Fe-based superconductors, the evidences of orbital order and fluctuations have been accumulated. Recently, we have shown that strong orbital and spin fluctuations mutually develop in multiorbital systems due to the AL-VC, which is dropped in the mean-field approximations. In Ref. [3], we study the phase diagram of $\text{LaFeAsO}_{1-x}\text{H}_x$, in which the isostructural (C_4) transition is realized at $x \sim 0.5$, due to the order parameter $O_{x^2-y^2} = n_{xz} - n_{yz}$. In addition to the conventional orthorhombic (C_2) structure transition at $x \sim 0$, due to the order parameter $Q_{3z^2-r^2} = (n_{xz} + n_{yz}) - 2n_{xy}$. It is found that the trigger of the C_4 (C_2) structure transition is the non-nematic (nematic) orbital order [1,3,4].

Also, we propose a mechanism of the nematic charge-density-wave (CDW) formation in cuprate superconductors by investigating the AL-VC in the three-orbital d-p Hubbard model [5]. Due to the strong charge-spin interference driven by the AL-VC, the CDW instability at $q = (\Delta_{FS}, 0)$, $(0, \Delta_{FS})$ is enhanced significantly when the spin fluctuations are strong. Here, Δ_{FS} is the wavenumber between the neighboring hot spots. The obtained spin-fluctuation-driven CDW is described as the "intra-unit-cell orbital order" accompanied by the charge transfer between the neighboring atomic orbitals. The obtained nematic-type charge pattern is similar to the STM results. The CDW in cuprates will be closely related to the nematic orbital order in Fe-based superconductors.

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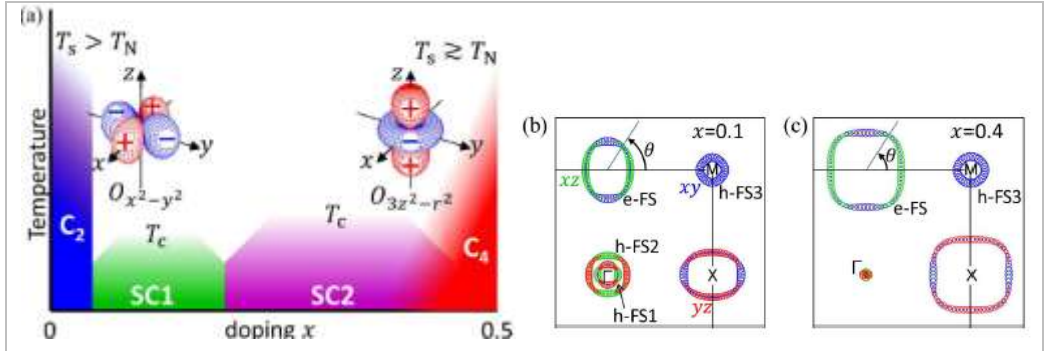


Figure 1: (a) Phase diagram in $\text{LaFeAsO}_{1-x}\text{H}_x$. Both C_2 and C_4 orbital order are reproduced on the basis of FSs at (b) $x=0.1$ and $x=0.4$, respectively. The quadrupole order parameters are given as $O_{x^2-y^2} = n_{xz} - n_{yz}$ and $Q_{3z^2-r^2} = (n_{xz} + n_{yz}) - 2n_{xy}$.

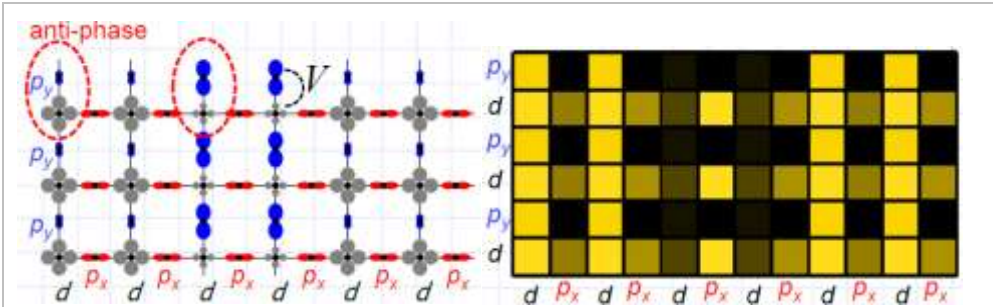


Figure 2: (left) Theoretically predicted orbital-order in real space. (right) Theoretically obtained STM signal.

Electron correlations effect on the ARPES in cuprates



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In many cases the standard perturbation approach appears to be too simple to describe precisely the angle resolved photoemission spectrum of strongly correlated electron system. In particular, to describe the momentum asymmetry observed in photoemission spectra of undoped high-T_c cuprates a phenomenological approach based on extremely correlated Fermi-liquid model has been recently introduced [1]. Here we analyze the general structure of the Green function of quasiparticles in strongly correlated electron systems and stress that it is defined not only by the self-energy of Hubbard quasiparticles but also by a strength operator. The later leads to an additional odd momentum contribution to the spectral function and alone can explain the observed asymmetry. So, the asymmetry of the ARPES spectra can be a measure of the strength of electron correlations[2].

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CHAPTER 2

SESSION 3

Optical Spectroscopy of Fermi Liquids

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Metallic materials are normally characterized as Fermi liquids if their low temperature dc resistivity has a T^2 temperature dependence. It was shown by Gurzhi that there is also a frequency dependence and the overall resistivity is given by $\rho(\omega, T) = C(\omega^2 + b\pi^2 T^2)$, where the scaling constant $b=4$ for a Fermi liquid with umklapp scattering[1]. A survey of literature shows that, where spectroscopic experiments exist, $b=4$ has not been observed[2]. We will present new spectroscopic data on LiFeAs, Sr_2RuO_2 , $\text{Sr}_3\text{Ru}_2\text{O}_7$ and Nd_xTiO_3 , four materials that show T squared resistivity at low temperatures and discuss their excitation spectra and their deviation from the canonical Fermi liquid form.

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Mott transitions with phase separations in RENiO_3 , $(\text{Ca,Sr})_2\text{RuO}_4$, $(\text{Sr,Lu})_2\text{IrO}_4$ and overdoped Na(Fe,Cu)As



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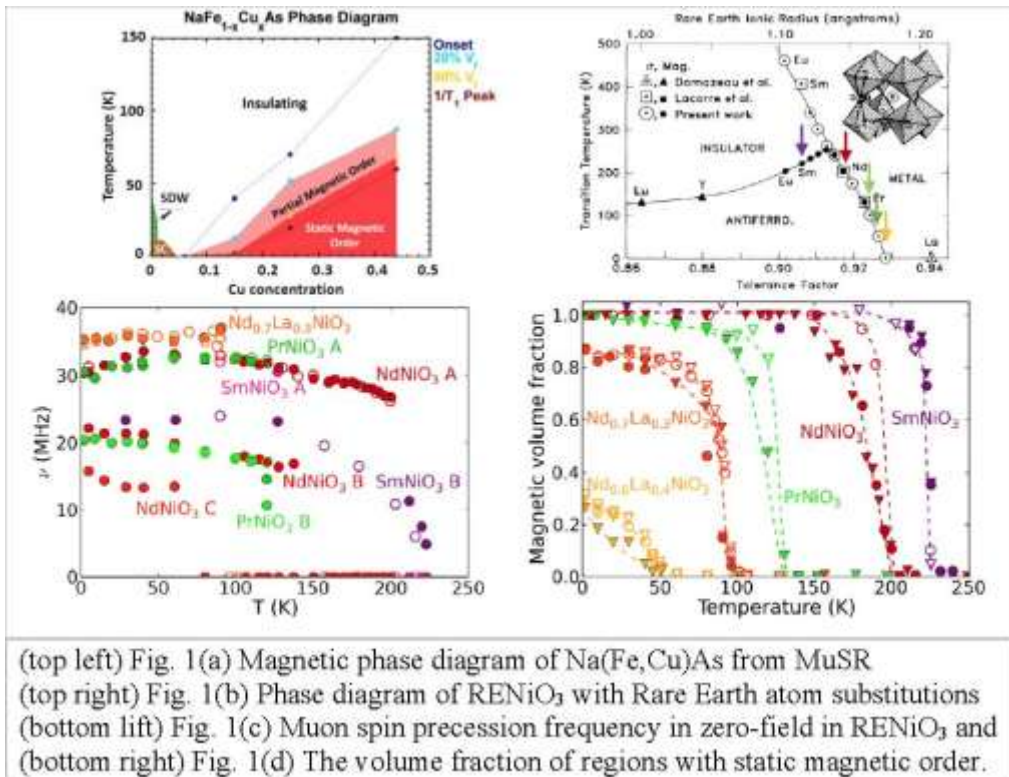
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Keywords: Mott transitions, phase separation, first-order quantum evolution, FeAs superconductors, quantum criticality

In this talk, we will present two novel results on Mott transitions. In 2013, an insulating state was detected in highly overdoped $\text{NaFe}_{1-x}\text{Cu}_x\text{As}$. STM studies of Yayu Wang found signatures similar to underdoped cuprates, the dc magnetic susceptibility χ_{dc} hinted static magnetic order, and neutron studies of Pengcheng Dai found an antiferromagnetic (AF) Bragg peak in the $x=0.44$ system. We performed muon spin relaxation (MuSR) measurements on single crystals of $\text{NaFe}_{1-x}\text{Cu}_x\text{As}$ with $x=0.06, 0.15, 0.25$, and 0.44 at TRIUMF. The zero-field MuSR spectra revealed static magnetic order in the $x=0.25$ and 0.44 specimens with sharp transitions at $T_F \sim 20\text{K}$ and 60K , followed by rapid developments of magnetic order in the entire volume fraction upon cooling. The 0.15 compound exhibits a gradual transition starting below 20K , with phase separation between the paramagnetic and magnetically ordered volumes. The moment size at $T \rightarrow 0$ was an order of magnitude smaller than those of the 0.25 and 0.44 systems. The $x=0.06$ compound is paramagnetic down to 2K . These results are shown in Fig. 1(a). The absence of sustained precession signals in ZF-MuSR, together with the cusps and history dependences in χ_{dc} , suggests possible spin-glass-like freezing similar to the behavior found in cuprates between the AF and SC phases. This is the first clear case of Mott transition in iron based superconductors.

We also performed MuSR studies of three other Mott transition systems. In RENiO_3 (RE=rare earth Sm, Nd, Pr, La), we studied five compounds shown by the arrows in the phase diagram of Fig. 1(b). In all these compounds, the muon spin precession frequency in zero field, proportional to the Ni ordered moment size, does not depend on systems (Fig. 1(c)). The RE=Pr, Sm, and Nd compounds achieve the full ordered volume fraction below the antiferromagnetic T_N , while the other two systems closer to the magnetic quantum critical point exhibit phase separation between paramagnetic and antiferromagnetic volumes, and the volume fraction diminishes as the magnetic order disappears (Fig. 1(d)). The temperature dependence of the MuSR frequency in Fig. 1(c) shows second order transition in the Sm compound and first-order transition in all other systems, as also indicated by the history dependences of the ordered volume fraction in Fig. 1(d).

Similar results were obtained in $(\text{Ca,Sr})_2\text{RuO}_4$ and $(\text{Sr,Lu})_2\text{IrO}_4$. In all these Mott systems, magnetic transitions are spread in wide temperature regions with gradual buildup of the ordered volume fraction near the quantum critical point. This first-order magnetic quantum evolution is common to the case of the overdoped $\text{Na}(\text{Fe,Cu})\text{As}$, as well as to the phase evolution found in metallic $\text{Ba}(\text{Fe,Ni})_2\text{As}_2$.



(top left) Fig. 1(a) Magnetic phase diagram of $\text{Na}(\text{Fe,Cu})\text{As}$ from MuSR
 (top right) Fig. 1(b) Phase diagram of RENiO_3 with Rare Earth atom substitutions
 (bottom left) Fig. 1(c) Muon spin precession frequency in zero-field in RENiO_3 and
 (bottom right) Fig. 1(d) The volume fraction of regions with static magnetic order.

Theory of disorder and quasiparticle interference in superconductors



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Keywords : disorder, quasiparticle interference, STM

I present a novel theoretical approach to the theoretical calculation of STM real-space images and quasiparticle interference (QPI) patterns in high-temperature superconductors. The usual Bogoliubov de-Gennes eigenvalues and eigenvectors are used, together with first-principles Wannier functions for a given material, to calculate images of impurities on the surface with atomic-scale resolution comparable to experiment.

These images automatically reflect local symmetries of the system, including those away from the high-symmetry plane traditionally calculated. Phenomenological “filter” effects are discussed and critiqued from this perspective. Representations of both real-space defects and QPI patterns are shown to be vastly improved relative to experiments on Fe-based systems and cuprates. Finally, I discuss ideas about how QPI can be used *qualitatively* to probe gap sign changes in multiband systems.

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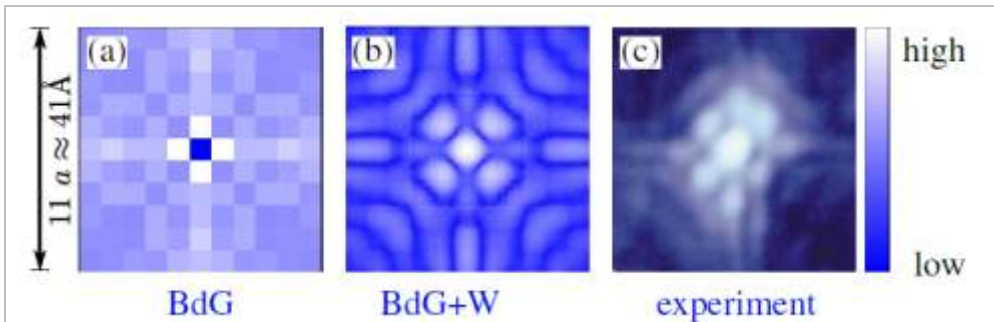


Figure 1: From Ref. 1: (a) Resonant state real space BdG patterns at $\Omega_0 = -3.6$ meV as obtained from conventional BdG calculations in logarithmic scale, (b) xy cut through continuous 3D LDOS ($x; y; z = 5 \text{ \AA}$; ω) in $(\text{eV bohr}^3)^{-1}$ at Ω_0 , (c) measured conductance maps on BSCCO-2212.

Critical dynamics and domains' motion from permittivity of the electronic ferroelectric (TMTTF)₂AsF₆



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Keywords : ferroelectricity, charge order, Mott insulator, permittivity, dynamical scaling, domains, walls

The electronic ferroelectricity was discovered [1] in quasi-1D organic conductors (TMTTF)₂X via observation of the dielectric permittivity ϵ' which diverges approaching the transition temperature T_C , reaching astonishing values $\sim 10^6$. The ferroelectricity coexists with a low-activated spinless conductivity which gives rise to the unusual material “ferroelectric Mott semiconductor”. The intrinsic conductivity provides the screening of outgoing electric field which eliminates the equilibrium domain structure and the resulting hysteresis which are common to ferroelectrics. That can lead to complete repolarisation under the ac field, and even to an unusual mono-domain state of the whole sample.

We shall present and interpret the experimental data allowing to reach profoundly the critical dynamics and to single out (below T_C) the contribution of domain walls [2]. By analysis of the inverse $1/\epsilon = \mu = \mu' + i\mu''$ of the complex permittivity $\epsilon = \epsilon' + i\epsilon''$ as a function of frequency f , we determine the critical slowing-down when approaching T_C , and the low frequency absorption features coming from the creep of domain walls. We are able to distinguish several regimes:

A) Critical slowing down near T_C characterized by anomalous powers n in the dependence of $\epsilon''(f) \sim f^n$ which are found as $n=0.86$ and $n=0.78$ - above and below T_C . That might be the ever first observation of the dynamical scaling in ferroelectrics, in Mott insulators and in electronic systems in general.

B) Low frequency response associated to sweeping of domain walls below T_C . Crossing T_C recovers the aggregation of solitons into macroscopic domain walls.

C) Thermally activated low temperature viscosity of the ferroelectric polarization which follows the concentration of particles – presumably the solitons which are the incarnations of holons in the Mott state.

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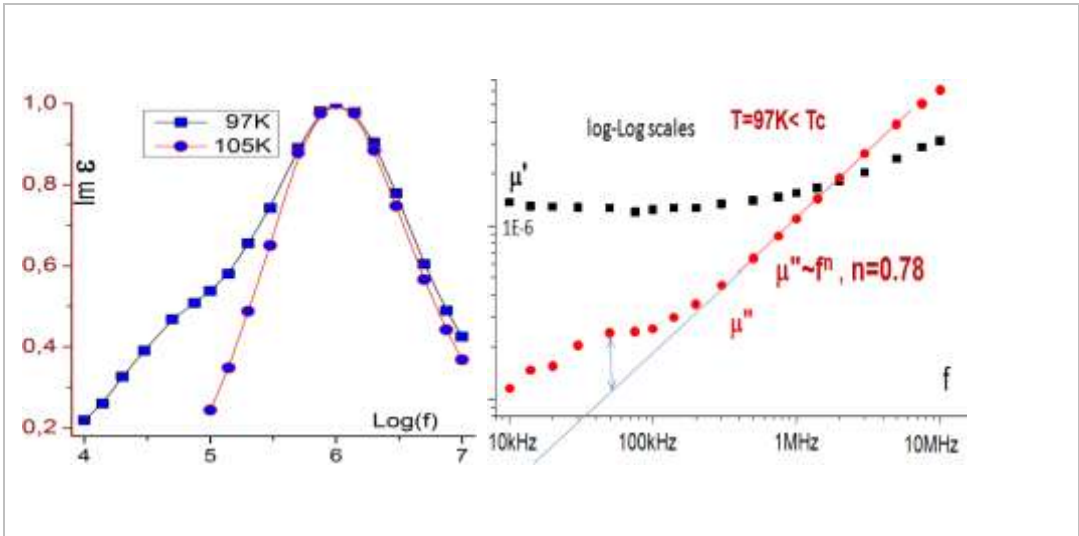


Figure: Deconvolution of the critical behavior and the creep by going from the complex susceptibility ϵ to its inverse μ .

Left panel: lin-log plot of $\epsilon''(f)$ just above and just below T_C .

Right panel: Frequency dependences of μ' (black squares) and μ'' (red circles) just below T_C . The blue line is the low f extrapolation of the power law dependence at higher frequency (the red line). The vertical blue arrow indicates the contribution from the creep of domain walls.

Interface enhanced superconductivity in one unit-cell FeSe films grown on SrTiO₃

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Heterostructure based interface engineering has been proved an effective method for finding new superconducting systems and raising superconducting transition temperature (T_C). Recently discovered high temperature superconductivity in one unit-cell (UC) FeSe films on SrTiO₃ (Nb-STO) substrate grown by molecular beam epitaxy has attracted intensive attention. In sharp contrast to FeSe films on graphene where a 2.2 meV superconducting gap is observed on thick (~ 16.5 nm) films and no superconducting gap on 1-UC FeSe down to 2.3 K, 1-UC FeSe films on STO substrate exhibit unexpected large superconducting gaps of 15-20 meV. Interestingly, the anomalously large superconducting gap is only found in the first UC FeSe but not on 2-UC or thicker layers, indicating that interface plays a crucial role in the enhanced superconductivity in 1-UC FeSe films on STO substrate. Another interesting point of this system is its simple band structure that consists only of electron Fermi pockets at M points, which is different from that of bulk FeSe. In this talk, a comprehensive study of 1-UC FeSe films by *in situ* scanning tunneling microscopy/spectroscopy (STM/STS) and angle-resolved photoemission spectroscopy (ARPES) and *ex situ* transport measurements will be presented to discuss the possible superconducting mechanism in this well-defined heterostructure.

SESSION 4

Novel Spin-Orbital Phases Induced by Orbital Dilution



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Keywords: spin-orbital order – orbital dilution – superexchange – orbital polarons

Strong coupling between spins and orbitals leads to spin-orbital entanglement in transition metal oxides [1]. The spin and orbital superexchange interactions in a Mott insulator lead to spin-orbital order which can be destabilized by spin-orbital quantum fluctuations [2], being particularly strong in systems with active t_{2g} orbitals. For instance, in ruthenates (e.g. in Sr_2RuO_4) spin-orbital superexchange [3] couples $S=1$ spins and t_{2g} orbitals including one doublon at each Ru^{4+} ion. It is intriguing how the spin-orbital order is modified by d^3 defects with $S=3/2$ spins and no orbital degree of freedom (orbital dilution), see Fig. 1. We focus here on this challenging situation with finite spin-orbit coupling, but the conclusions are more general [4]. The superexchange on the host $4d-4d$ bonds J competes with local $3d-4d$ superexchange J' which depends in a crucial way on the type of doubly occupied t_{2g} orbital. One finds that in some cases, due to the quench of the orbital degree of freedom at the $3d$ impurity, the spin-orbital order within the host is drastically modified by doping. The impurity acts either as a spin defect accompanied by an orbital vacancy in the spin-orbital structure when the host-impurity coupling is weak, or it favors doubly occupied active orbitals along the $3d-4d$ bond leading to antiferromagnetic or ferromagnetic spin coupling (orbital polarons [5]) (Fig. 1). This competition between different magnetic couplings generates quite different ground states. In particular, for the case of a finite and periodic distribution of $3d^3$ impurities ($x=1/8, 1/5, 1/9$ doping) it leads to striped patterns either with alternating ferromagnetic (antiferromagnetic) domains or with islands of saturated ferromagnetic order [4]. Here we explore in addition the consequences of quantum fluctuations for $x=1/4$ doping. We find that magnetic frustration and spin degeneracy can be lifted by the quantum orbital flips of the host but they are robust in special regions of the incommensurate phase diagram. Orbital quantum fluctuations modify quantitatively spin-orbital order imposed by superexchange. In contrast, the spin-orbit coupling can lead to anisotropic spin and orbital patterns along the symmetry directions and cause a radical modification of the order imposed by the spin-orbital superexchange. Our findings [4] are expected to be of importance for future theoretical understanding of experimental results for $4d$ transition metal oxides doped with

$3d^3$ ions. We suggest how the local or global changes of the spin-orbital order induced by such impurities could be detected experimentally.

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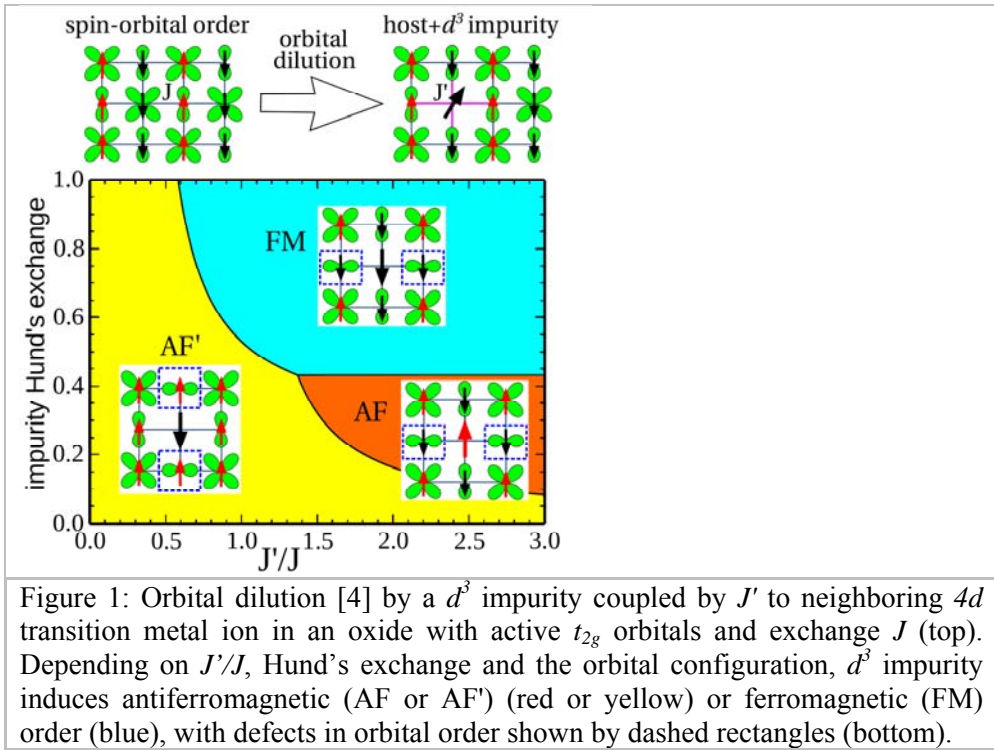


Figure 1: Orbital dilution [4] by a d^3 impurity coupled by J' to neighboring $4d$ transition metal ion in an oxide with active t_{2g} orbitals and exchange J (top). Depending on J'/J , Hund's exchange and the orbital configuration, d^3 impurity induces antiferromagnetic (AF or AF') (red or yellow) or ferromagnetic (FM) order (blue), with defects in orbital order shown by dashed rectangles (bottom).

Phase separation, commensurate and incommensurate antiferromagnetic phases in the systems with imperfect nesting



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Keywords: electronic phase separation – imperfect nesting – commensurate and incommensurate phases

We present here a review of our recent results concerning the electronic properties of the systems having an electron- and a hole-band with imperfect nesting. Such electronic structure is observed in a number of important materials, for example, in superconducting iron pnictides, chromium and its alloys, AA-stacked graphene bilayers, some borides, etc. We discuss model Hamiltonians appropriate for the description of these systems and analyze their phase diagrams taking into account the effects of doping and applied magnetic field. We show that the instability of the uniform ground state with respect to nano-scale electronic phase separation is a common feature of such systems. It is known that the commensurate and incommensurate antiferromagnetic states can exist in the systems with imperfect nesting. The pairing of one electron and one hole band due to the electron-electron interaction leads to the formation of the spin-density-wave order with a nesting vector \mathbf{Q}_0 commensurate with lattice period. Upon doping the commensurate antiferromagnetic phase is changed to the incommensurate one with $\mathbf{Q} = \mathbf{Q}_0 + \mathbf{q}$, where $|\mathbf{q}| \ll |\mathbf{Q}_0|$. The incommensurate antiferromagnetic phase is mathematically equivalent to the Fulde-Ferrel-Larkin-Ovchinnikov state in superconductors. Under definite conditions, the phase separation occurs due to the competition between these two antiferromagnetic phases and/or paramagnetic phase. Depending on the system parameters, the inhomogeneous state could be a mixture of the commensurate and incommensurate antiferromagnetic phases or paramagnetic phase and one of the antiferromagnetic phases. The phase separation, in particular, gives rise to the specific behavior of the magnetoresistance of the system and in some cases to the insulator-metal transition with change of temperature or magnetic field. We discuss the experimental data, which can confirm the existence of the phase-separated state in the considered systems.

Weak crystallization theory of metallic alloys.



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Keywords : charge density waves – crystallization – quasicrystals

Crystallization is probably the most familiar phase transition, but one of the hardest to analyze. The workhorse of the theory of phase transitions, the Ginzburg-Landau theory, cannot be easily applied to many of the crystallization transitions since they tend to be strongly first order, i.e. the order parameter experiences a large jump at the transition.

What is the order parameter of a crystal? The crystal is characterized most naturally in the reciprocal space, with the long-range ordering being identified with the appearance of resolution-limited Bragg peaks. Most often the reciprocal lattice is as simple as the real space one; however, for a material family known as *quasicrystals* the symmetry of the Bragg peaks is inconsistent with the simple periodic real space arrangement of atoms.

Weak Crystallization theory [1] applies Ginzburg-Landau machinery to crystallization by assuming that only the Bragg peaks on a single momentum shell are significant enough to affect energy. It has been used to predict ubiquity of BCC crystals at high temperatures [2], to study effects of fluctuations [3], and even attempt to explain stability of quasicrystals [4]. As such, it has been a useful symmetry-based tool to study the crystallization transition, even beyond its immediate range of validity.

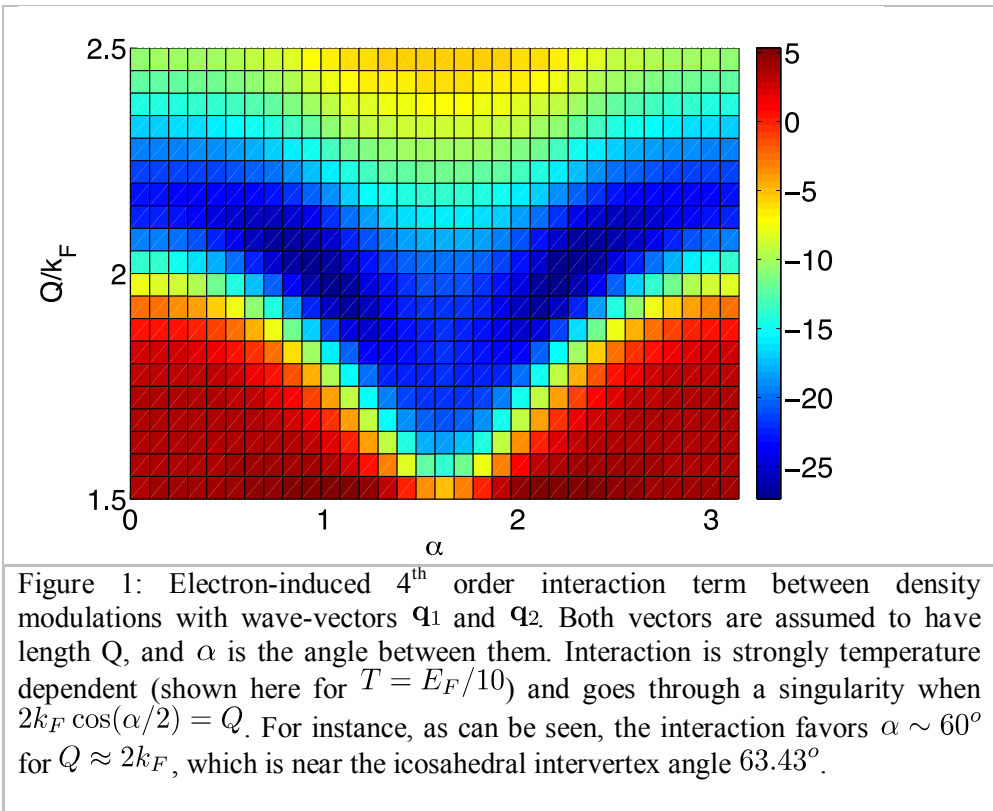
Here we extend the Weak Crystallization theory to metallic systems. Starting from the basic model of electrons weakly interacting with ions, and perturbatively integrating electrons out leads to the appearance of singular (as $T \rightarrow 0$) angular dependencies in the interaction terms of weak crystallization theory (see Figure 1). This leads to drastic modifications of the phase diagram, stabilizing FCC, rhombohedral, and most notably icosahedral quasicrystals (iQC) states.

The condition for stability of iQC that we find very closely corresponds to the Hume-Rothery rules known empirically for majority of stable iQC; namely, the wave vector of the primary Bragg peaks is approximately equal to the diameter of the Fermi surface. Our approach is conceptually analogous to Mermin and Troian [2], where we identify Fermi

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Sea as the auxiliary component driving interaction anisotropy.



SESSION 5

Magnetic order and spin excitations in anisotropic Heisenberg antiferromagnets



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Keywords: spin excitations – compass model – Heisenberg antiferromagnet

A spin-rotation-invariant Green-function theory for the dynamic spin susceptibility in the anisotropic non-frustrated J_1 - J_2 model for the iron pnictides AFe_2As_2 ($A = \text{Ca}, \text{Sr}, \text{Ba}$) is presented [1]. The two-spin correlation functions, the spin-excitation spectrum, and the staggered magnetization are calculated self-consistently. The temperature dependence of the uniform magnetic susceptibility, in particular the linear increase with T in a wide temperature region, is in good quantitative agreement with experiments. The values of the Néel temperature resulting from the localized spin model are found to be higher than the measured ones that suggests to take into account the itinerant electron degrees of freedom. The layered spin-1/2 antiferromagnetic Heisenberg model with compass-model interaction in the plane proposed for iridates is considered [2]. The spin-wave excitation spectrum, the magnetization, and the Néel temperature T_N are calculated both in the ordered and in the paramagnetic states. The spin-wave spectrum agrees well with data of Lanczos diagonalization. We find that T_N is enhanced by the compass-model interaction and is close to the experimental value for Ba_2IrO_4 . T_N can be even nonzero for the 2D lattice due to the compass-model interaction.

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Spin-spiral to spin-stripe phase transition driven by fluctuations



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Keywords : spin spiral, spin stripe.

We consider behavior of spin spiral systems in the vicinity of a critical point separating the spin ordered and the spin disordered states.

We demonstrate that generically the critical point splits in two close but separate critical points. In the first one the spin spiral is transformed to the spin stripe, and in the second point the spin ordering disappears altogether.

Specifically we address TbMnO₃ multiferroic and cuprate superconductors.

Universal Features of Local Charge Modulations in a Cuprate Superconductor



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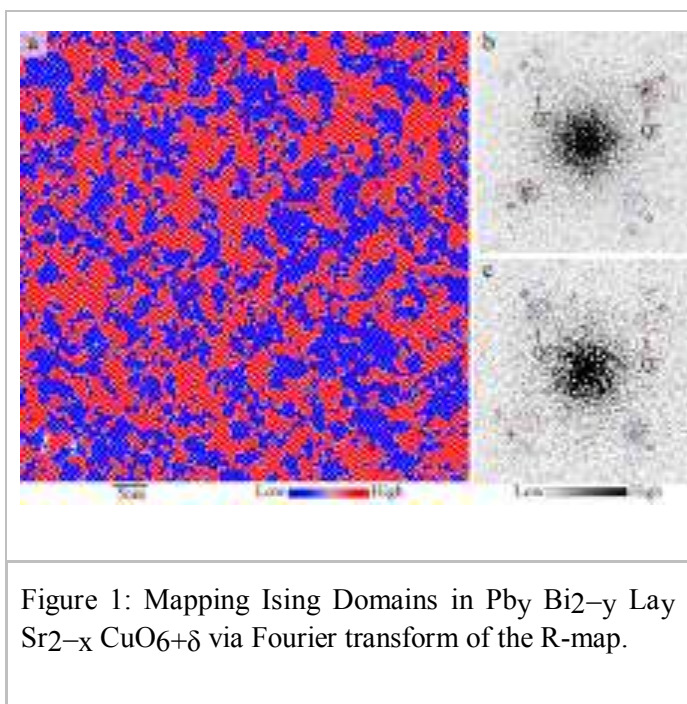
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Keywords : charge order , cuprate superconductor, nematicity.

In unconventional superconductors, real-space orders such as charge or spin density modulations can coexist with superconductivity. In the cuprate superconductors, it has recently been recognized that local charge modulations are a ubiquitous feature and likely important for understanding the superconductivity in these materials. However, there are still open issues surrounding the dimensional profile of these charge modulations, including whether the modulation wave-vector is unidirectional or bidirectional, and also whether the charge modulations extend seamlessly from the surface of the material into the bulk. In bismuth-based cuprates, material disorder is a severe enough effect so as to preclude a full understanding of the charge modulations through bulk scattering techniques. In order to resolve these issues, we use a local technique, scanning tunneling microscopy, to image the static charge modulations in $\text{Pb}_y\text{Bi}_{2-y}\text{La}_y\text{Sr}_{2-x}\text{CuO}_{6+\delta}$. We find that the charge modulations are more consistent with an underlying tendency to a unidirectional charge density wave than a bidirectional charge density wave. Using recently developed cluster analysis techniques, we show that these locally 1D structures are more than surface deep, extending into the bulk of the material throughout the doping range. The universal nature of these charge modulations makes them a viable candidate as a prerequisite of the superconductivity in cuprates.



Soft electronic matter in underdoped cuprates



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Keywords : magnetism –charge order – chiral symmetry-phase diagram-cuprates

Empirical evidence in heavy fermion, pnictide, and other systems suggests that unconventional superconductivity appears associated to some form of real-space electronic order [1]. For the cuprates, despite several proposals, the emergence of order in the phase diagram between the commensurate antiferromagnetic state and the superconducting state is not well understood. Here we show that in this regime holes assemble in “electronic polymers” [2,3]. Within a Monte Carlo study [Fig.1] we find, that in clean systems by lowering the temperature the polymer melt condenses first in a smectic state and then in a Wigner crystal both with the addition of inversion symmetry breaking thus with “ferro” order. Disorder blurs the positional order leaving a robust inversion symmetry breaking and nematic order accompanied by vector chiral spin order and with the persistence of a thermodynamic transition. Such electronic phases, whose properties are reminiscent of soft-matter physics, produce charge and spin responses in good accord with experiments including anomalous ferroelectricity [4].

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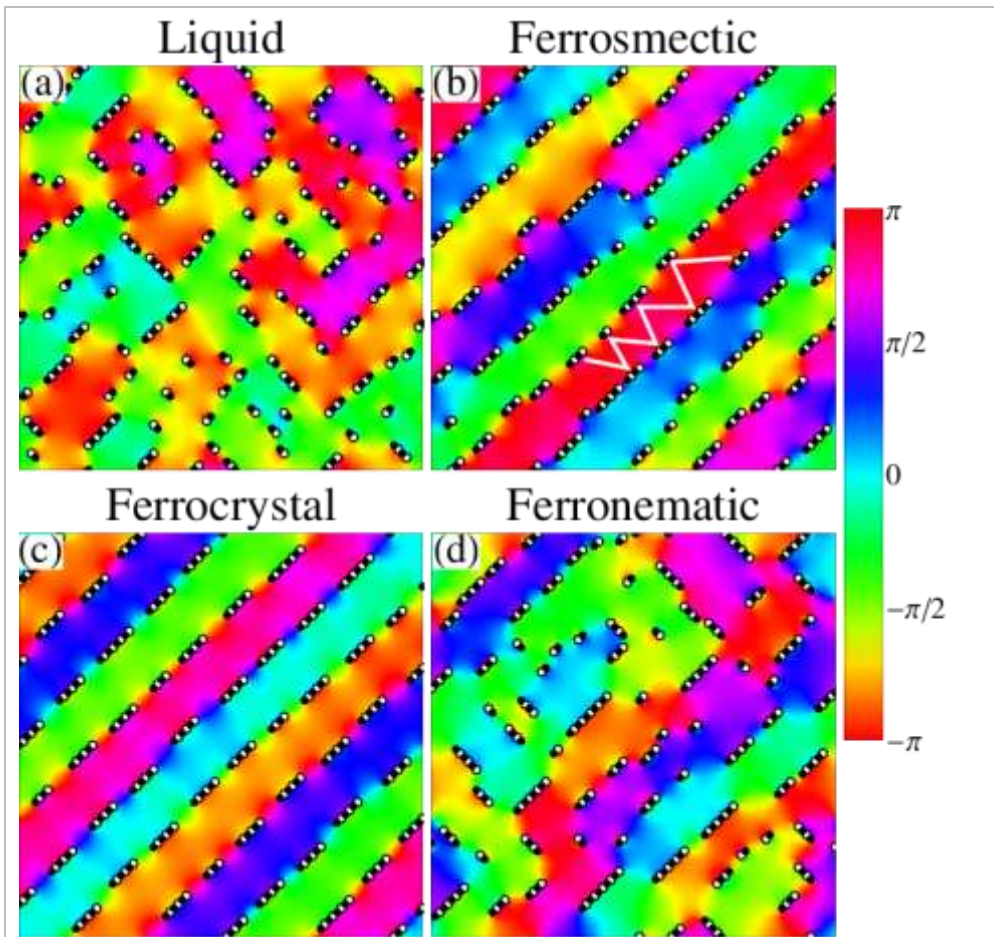


Figure 1: Charge and spin configurations in the different phases obtained in a model of heavily underdoped cuprates. White and black circles represent the positive and negative topological charges of the antiferromagnetic background, respectively. The different colours denote the angle of the staggered magnetization. The images are Monte Carlo snapshots in the absence of quenched disorder (a-c) in the thermally disordered phase with $T = 50$ K (a), in the ferrosmectic phase at $T = 38$ K (b), in the ferrocrystal phase at $T = 8$ K (c) and in the ferronematic phase at $T = 40$ K (d) which appears in the presence of quenched disorder due to the dopand ions.

SESSION 6

Electric Field Effect Studies in High- T_c Cuprates and Related Materials



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We overview our systematic studies on electric field effect with ionic liquid gating applied to a range of electronic materials, including high- T_c cuprates. Such an approach may be crucial to modulate the carrier concentration in systems where chemical doping proved itself unpractical or failed. Initially we studied thin film devices that were made in an electrical double layer gating (EDLG) configuration on gated LSCO-214 monolayers grown by Molecular Beam Epitaxy. The shifts in T_c of up to 30 K were induced in films by an external electric field, reversibly driving the insulator-to-superconductor quantum phase transition. We have measured the critical resistance, and it turned out to be precisely equal to the quantum resistance for pairs, $R_Q = h/(2e)^2 = 6.5 \text{ k}\Omega$. This is suggestive of a phase transition driven by quantum phase fluctuations. It implies the existence of 2D (interface) superconductivity, as well as of the ‘Bose’ insulator state with localized pairs. Furthermore, we have extended our studies to other related materials, including $\text{Sr}_{0.9}\text{La}_{0.1}\text{CuO}_2$, SrCuO_2 , SrFeO_3 , SrRuO_3 , WO_3 , FeTe, highly ordered pyrolytic graphite and grapheme. So far, we have observed field-induced metallicity only in WO_3 . We have also developed a method to apply Coherent Bragg Rod Analysis (COBRA) to LSCO-214 samples while they are exposed to the EDLG. We discuss the implications of our results in light of emerging physics of high- T_c cuprates and related quantum materials.

Strong effects of impurities on superconductivity and stripe order in cuprates



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Keywords: superconductivity, stripes, impurity effects

It is now well established that in high- T_c superconducting cuprates nonmagnetic Zn ions suppress T_c even stronger than magnetic Ni ions. This behavior, which is in sharp contrast to that of conventional superconductors, led to the formulation of an unconventional pairing mechanism and a symmetry of the order parameter for superconductivity in cuprates. However, up to now surprisingly little is known concerning impurity effects on static stripe phase in cuprates.

We performed muon spin rotation (μ SR) and neutron scattering experiments in Zn- and Ni-doped $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ and $\text{La}_{1.48}\text{Nd}_{0.4}\text{Sr}_x\text{CuO}_4$ ($x=1/8$) samples to systematically study the effects of magnetic and nonmagnetic impurities on static stripe order. It was found that the static spin-stripe ordering temperature T_{so} strongly decreases linearly both with Zn and Ni doping. Observed strong effect of in-plane impurities on stripe order might provide important clue for better understanding of stripes formation and their relation with superconductivity in cuprates.

Fermi-Bose mixture in Ba(K)BiO₃ superconducting oxide



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Keywords: superconducting oxides, spatially separated Bose-Fermi mixture, double-well potential, low temperature anharmonicity, charge density waves

We present the results pointed to the possibility of a two band Fermi–Bose mixture scenario in a class of superconducting oxides with cubic perovskite structure and relatively high critical temperature $T_c \sim 30$ K, namely, in the barium bismuthates $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$. The key issue is the possibility of the existence of spatially separated subsystems of fermionic and bosonic quasiparticles in these materials. The cubic perovskites $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$ (BPBO) and $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ (BKBO) have been known and extensively studied since 1975 and 1988, respectively, however the mechanism of superconductivity in these compounds is not clear up today, so as in cuprates. Moreover, the most of the unusual properties of the BaBiO_3 -family compounds mentioned in the early review by Uchida *et al.* [1] still remain unexplained. There are a lot of common properties of bismuthate and cuprate family compounds, but essential more simple structure of bismuthates gives the important advantages in the interpretation of the experimental data.

Based on the low-temperature EXAFS study of the BKBO and BPBO compounds, the motion of the local electron pairs correlated with the lattice vibrations was established [2]. We found that different electron fillings of the upper antibonding $\text{Bi}6s\text{-O}2p_{\sigma^*}$ orbital of the BiO_6 octahedra lead to vibration of part of the oxygen ions in a double-well potential in according with dynamical exchange $\text{Bi}\underline{L}^2\text{O}_6 \leftrightarrow \text{BiO}_6$ (here \underline{L}^2 means the presence of two holes in the upper antibonding orbital). Later on the existence of the double-well potential of oxygen ion vibrations was observed also both for electron ($\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_{4-\delta}$) and hole doped ($\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$) cuprates [3]. The observed anomalies allowed us to proposed a phenomenological model of the relationship between the local crystal and the local electron structures, which explained the insulator - metal transition with doping of parent insulators as for bismuthates (see Fig. 1), so for cuprates [3].

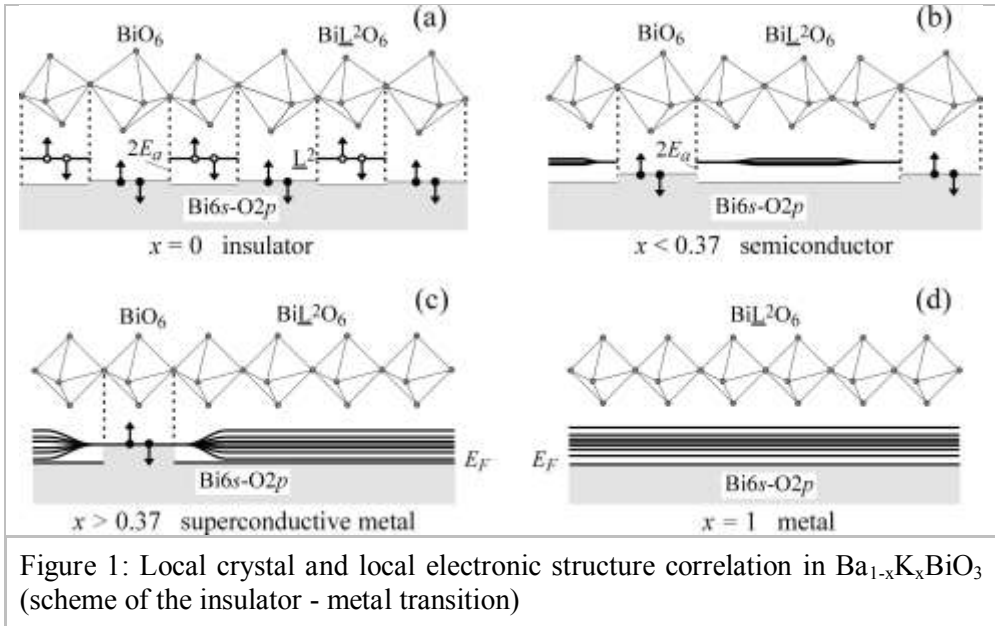
We have shown that two types of the charge carriers: the local pairs (real-space bosons) and the itinerant electrons exist in the metallic $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ ($x > 0$, 37). Bosons and fermions occupy different types of the octahedral BiO_6 complexes, so they are separated in real space. A new type of spatially separated Fermi–Bose mixture is likely to be realized in

bismuthates. The likeness of the local peculiarities of BiO_6 complexes in bismuthates and CuO_n complexes in cuprates allows one to discuss the applicability of this scenario for all high- T_c perovskite-like oxides.

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Magnetization and critical current of calcium-doped $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ composite films



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Keywords: high T_c superconductors – Ca doping – magnetization – critical current

The possibility of increase in critical current of high-temperature superconductors $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ through doping by calcium has been widely discussed (see, for example [1-6]). In particular, it was shown that the adding Ca leads to increased J_c [1, 2], which is generally attributed to excess holes introduced by Ca^{2+} substituting for Y^{3+} [3]. However, bulk samples which as a rule used for investigation consist of a network of randomly oriented grains separated by un-oriented, high-resistance grain boundaries which complicate the interpretation of the results. It is, therefore, important to understand the effects of calcium doping on more intrinsic samples such as single crystals or epitaxial thin films. Single-crystal studies show that Ca^{2+} substitutes for Y^{3+} where it acts as a hole dopant [3]. In Ref. [4] have been found that Ca segregates in grain boundaries, and it was generally believed that Ca replaces Y there as well.

It should be noted that the previous studies have been performed at temperatures near 77 K. In our report we present new results of influence of Ca doping on magnetization and critical current of HTSC composite film deposited on metallic substrate. Architecture of the composites is hastelloy/ $\text{Al}_2\text{O}_3/\text{Y}_2\text{O}_3/\text{MgO}/\text{LaMnO}_3/\text{CeO}_2/\text{Y}_{1-x}\text{Ca}_x\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}/\text{Ag}$.

The measurements were carried out in a wide temperature range 4 – 77 K and magnetic fields up to 14 T. It was obtained that the substitution of yttrium by calcium for 2 and 4 atomic percents leads to decrease in magnetisation and critical current density as well (see Figure 1). It was also found that at lower temperatures and/or higher magnetic fields the effect of calcium concentration on magnetization and critical current becomes weaker. The origins of observed effects are discussed.

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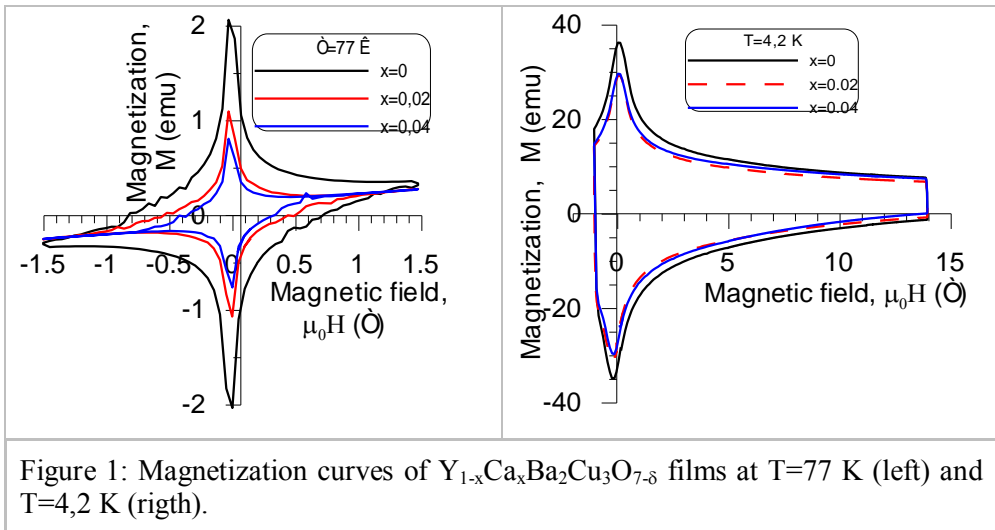


Figure 1: Magnetization curves of $\text{Y}_{1-x}\text{Ca}_x\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ films at $T=77$ K (left) and $T=4,2$ K (right).

Excitonic Fano resonance and possible BEC-BCS crossover in ternary chalcogenides Ta_2NiS_5 and Ta_2NiSe_5



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Keywords: excitonic insulator, BEC-BCS crossover, Fano interference, electron-phonon interaction, ellipsometry

Electron-hole Cooper pairs in direct-gap semiconductors, including the crossover between the excitonic BEC and the electron-hole BCS state have been predicted and extensively studied theoretically [1-3], but experimental observation of such a system has not been reported so far. Recent ARPES studies have considered Ta_2NiSe_5 as a candidate for an excitonic insulator, a material in which the exciton binding energy (E_{ex}) exceeds the band gap energy (E_G), which could lead to the observed flattening of the valence band top [4-5]. In order to explore the excitonic states we perform a comparative optical study of the ternary chalcogenides Ta_2NiSe_5 and Ta_2NiS_5 , two closely related compounds bearing a quasi-one-dimensional structure with single chains of nickel and double chains of tantalum atoms coordinated by chalcogenide atoms. The decrease of the band gap energy with the increase in size of the chalcogenide atom presumably shifts the system from a BEC state towards a BCS state. By means of wide-band spectroscopic ellipsometry we directly measured the complex dielectric function and unambiguously identified the excitonic doublet in both the compounds. The determined exciton binding energy decreases with increase in size of the chalcogenide atom and remains comparable with the optical gap energy. A gradual closing of the optical gap is observed in Ta_2NiSe_5 with increasing temperature. Furthermore, many-body interactions in these systems manifest themselves as a Fano interference of the discrete excitonic states with a band continuum that is a general feature of the exciton absorption in low-dimensional semiconductors. There are sharp and strongly temperature dependent absorption peaks above the energy scale of the excitonic Fano resonances, which correspond to the interband transitions. The character of their temperature dependence corroborates strong electron-phonon interaction with a modification of the peak energies and widths proportional to the filling factor of optical phonon modes. The electron-phonon coupling may significantly reduce the effect of the local Coulomb attraction and stabilize the condensation of the spin-singlet excitons in the system [6].

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SESSION 7

BCS-BEC crossover in multi-band and multi-gap superconductors



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Keywords: BCS-BEC crossover, multigap superconductivity, shape resonances, band edge

Superconductivity in iron-based, magnesium diborides, and other novel superconducting materials has a strong multi-band and multi-gap character [1,2] and recent experimental evidences support the possibility for a BCS-BEC crossover induced by strong-coupling and proximity of the chemical potential to the band edge of one of the bands [3, 4]. BCS-BEC crossover at the band edge has been also predicted in superconducting stripes [2]. Here we study the simplest theoretical model which accounts for the BCS-BEC crossover in a two-band / two-gap superconductor, considering tunable interactions. Mean-field results - condensate fraction, correlation length, superconducting gaps - are reported in crossover diagrams to locate the boundaries of the different pairing regimes. When the gap is of the order of the local chemical potential, superconductivity is in the crossover regime of the BCS-BEC crossover and the Fermi surface of the small band is completely smeared by the gap opening. In this situation, small and large Cooper pairs coexist in the total condensate, which is the optimal condition for high-T_c superconductivity [5]. The ratio between the gap and the Fermi energy in a given band results to be the best detection parameter for experiments to locate the system in the BCS-BEC crossover. Using available experimental data, our analysis shows that iron-based superconductors have the partial condensate of the small Fermi surface which is in the crossover regime of the BCS-BEC crossover [6], supporting in this way the recent ARPES findings [7, 8].

We also discuss different physical systems in which the multigap and multiband BCS-BEC crossover can be realized. Two examples are considered here: (i) superconducting stripes in which shape resonances and multigap physics at the band edge play a cooperative role in enhancing superconductivity in the crossover regime of pairing [2], and (ii) superfluidity in ultracold fermionic gases confined in quasi-1D traps [9]. In the case of superconducting stripes, we review the experimental state of the art and recent progresses in this field.

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Emergent phenomena in multigap superconductors



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Keywords:

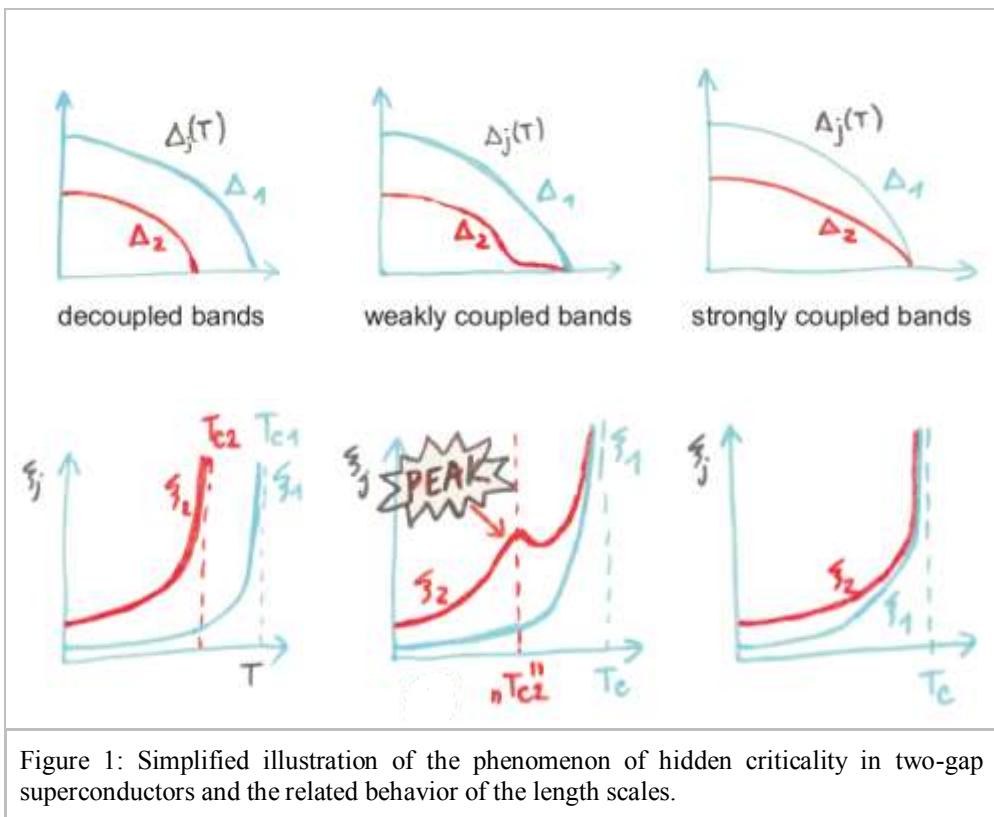
multiband/multigap/multicomponent superconductivity –
(fractional) vortex matter - magnetic phenomena

Multiband/gap superconductivity is emerging as a complex quantum coherent phenomenon with physical consequences which are different from or cannot be found at all in single-gap superconductors. This became particularly relevant after the recent discoveries of predominantly multi-band/gap superconducting materials, e. g. transition metal-borides, iron-pnictides and chalcogenides. In these materials the cross-pairing between bands is typically disfavored energetically, hence multiple coupled condensates coexist, hybridize and govern the overall superconducting behavior. The increased number of degrees of freedom allows for novel effects which are unattainable otherwise. For recent Special Issue of Superconductor Science and Technology devoted to this topic, please see [1].

In this talk, I will focus on few such effects, and discuss their theoretical predictions, simulations and experimental evidences. In particular, I will discuss the emergence and stabilization of fractional-flux vortices [2], their dynamics and observation in magnetic and transport measurements, then hidden criticality [3] where length scales of involved condensates can become radically disparate [4], unusual magnetic behavior that cannot be classified into standard types [5] and can lead to e. g. giant paramagnetic response [6], and first prediction of type-I behavior in known multigap compounds.

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Superconducting correlations in metallic nanograins coupled to an environment

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Conventional superconductivity is inevitably suppressed in ultra-small metallic grains for characteristic sizes smaller than the Anderson limit. Experiments have shown that above the Anderson limit the critical temperature may be either enhanced or reduced when decreasing the particle size, depending on the superconducting material. [1-5] In addition, there is experimental evidence that whether an enhancement or a reduction is found depends on the strength of the electron-phonon interaction in the bulk.

We present a study of the superconducting correlations in nanograins coupled to a dissipative environment. We have shown how environmental entanglement emerges in the ground state of grain systems and why it has a strong influence on the superconducting characteristics. We have accounted for the pair-breaking effect due to thermal phonons, which broadens the single electron levels, as well as for phonons that renormalize the band electron mass. In our theory, as corroborated by the experimental observations, quantum confinement can either increase or decrease the average superconducting critical temperature, depending on the material parameters. Our analysis conclusively shows that a slight decrease of T_c for smaller samples is expected for the strongly phonon-coupled nanoparticles of lead while an increase is typical for samples made of weakly phonon-coupled superconducting materials, both in accordance with experimental findings to date.

This work was supported by BELSPO Return to Belgium Grant (M. D. C.) and the Research Foundation – Flanders (FWO).

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SESSION 8

The Kerr effect in the chiral state of strontium ruthenate



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Keywords: spin triplet superconductor - strontium ruthenate, Kerr effect - chiral state

Strontium ruthenate is an interesting system with a Fermi liquid like normal state at low temperatures [1] and a very anomalous superconducting state [2]. It has been proposed as a spin triplet odd parity superconductor [3,4]. Unfortunately the proper interpretation of the experiments is challenging in many ways. The superconducting state of this tetragonal system breaks time reversal symmetry which points to the chiral state allowed by the group-theoretical analysis. Its thermodynamic properties, showing power low temperature dependence at low T , require a gap vanishing somewhere on the Fermi surface. The T independent spin susceptibilities measured with a magnetic field in the ab plane and along the c -axis are at odds with the theory which requires at least one of the components to change with temperature.

The possibility of using optical methods to detect time reversal symmetry breaking (TRSB) pairing states in unconventional superconductors was first suggested in the late 1980's. Recently, such dichroism was observed in polar Kerr effect measurements of the Sr_2RuO_4 [3], which showed a small Kerr rotation of light of wavelength $\lambda=1550$ nm, corresponding to a rotation of the plane of polarization by an amount approaching 90 nrad at $T=0$ and going to zero at T_c approximately linearly in (T_c-T) . The measurements provide clear evidence of the time reversal symmetry breaking below the superconducting transition temperature T_c .

The theoretical interpretation of the Kerr effect, however, is challenging in many ways. As it has been established [5,6] the effect vanishes in a clean system described by the one-band model. We will discuss the model [6] which takes into account all three relevant orbitals and three dimensionality of the system. The model has been shown to provide good description of the many thermodynamic and electrodynamic properties of the material. We shall show that it provides semi-quantitative description of the magnitude of the Kerr effect and its dependence on temperature in Sr_2RuO_4 . For most frequencies, it varies with temperature as $\Delta(T)^2$ near to T_c while for others, Hebel-Slichter like enhancement or decrease below T_c are observed.

Collaboration with B. L. Gyorffy, J. F. Annett, M. Gradhand and the financial support of NCN grant no. 2014/13/B/ST3/04451 is acknowledged.

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The Quantum Critical Phase of $\text{Sr}_3\text{Ru}_2\text{O}_7$ under Compressive and Tensile Strain



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Keywords: quantum criticality, metamagnetism, uniaxial pressure, strain, density waves, Ginzburg-Landau theory

$\text{Sr}_3\text{Ru}_2\text{O}_7$ is well-known to have a quantum critical phase around the critical endpoint of a metamagnetic transition. [1] The nature of this phase is not fully understood, although recently spin-density-wave order has been found in this phase. [2] In the phase, relatively weak in-plane magnetic fields induce strong transport anisotropy, suggesting that the phase is inherently anisotropic in nature. [3]

We have studied $\text{Sr}_3\text{Ru}_2\text{O}_7$ using new piezoelectric-based apparatus that can both compress and tension samples, and have shown that small anisotropic strains also induce a strongly anisotropic response. Modest compression (about 0.15%) increases the electrical resistivity by a factor of three. We discuss possible phase diagrams of the quantum critical phase against applied lattice distortion, and implications for the microscopic structure of the phase.

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Spin-orbit-induced orbital excitations in Sr_2RuO_4 and Ca_2RuO_4 : a resonant inelastic X-ray scattering study



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Keywords: Ruthenates – Spin-Orbit – d-Electrons – RIXS – XAS

Ruthenate-oxide materials attract much attention due to the interesting ground states they exhibit, such as unconventional superconductivity in Sr_2RuO_4 or Mott physics in Ca_2RuO_4 . The role of electron correlations, Hund's coupling and spin-orbit interactions is still being debated and explored [1,2].

In this talk [3] we present a study on the Ru 4d-orbital occupation and excitations in $(\text{Ca/Sr})_2\text{RuO}_4$, performed through a combination of X-ray Absorption Spectroscopy (XAS) and high resolution oxygen K-edge Resonant Inelastic X-ray Spectroscopy (RIXS). The ruthenium 4d orbital occupation and excitations were probed through their hybridization with the oxygen p-orbitals.

A minimal model, taking into account crystal field splitting and spin-orbit coupling, is presented to account for the observations. Implications on electronic structure, Mott physics and superconductivity are discussed.

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Quasiparticle dynamics and spin-orbit texture of Sr_2RuO_4



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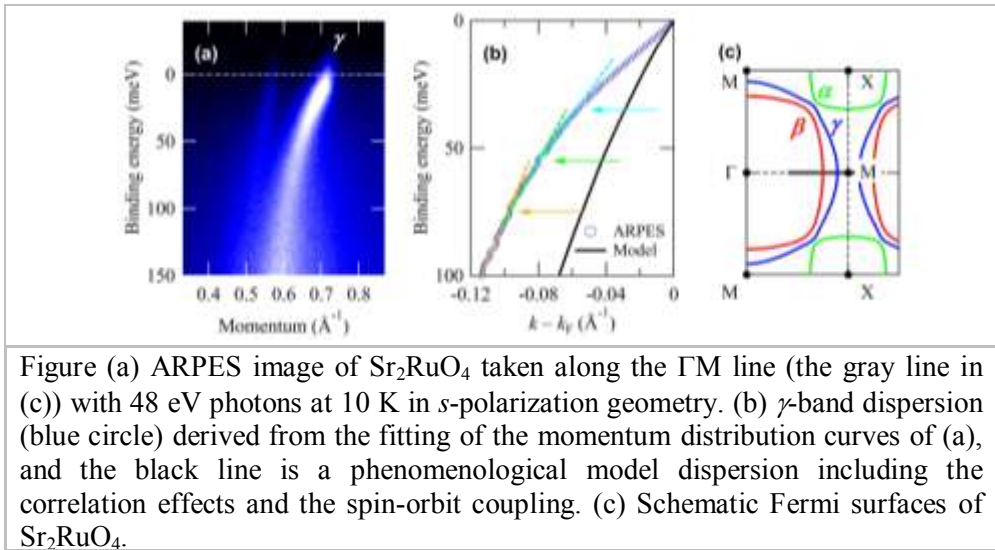
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Keywords: Ruthenate – ARPES – Oxygen isotope effect – Spin-resolved ARPES

Single-layered ruthenate (Sr_2RuO_4) is well-known as a typical spin-triplet superconductor, possibly associated with the chiral p-wave symmetry [1,2]. Clarifying quasiparticle dynamics and spin-orbit texture could be pivotal to understand the unconventional superconductivity of Sr_2RuO_4 . Here we investigated the oxygen isotope effects on the quasiparticle dynamics, especially on multiple kink structures at lower than 100 meV (Fig. 1) [3]. The results will be discussed in terms of the coupling against phonon modes, ferromagnetic fluctuations, and/or antiferromagnetic fluctuations as reported by inelastic neutron scattering experiments. We also studied the spin-orbit texture of Sr_2RuO_4 by high-resolution spin-resolved ARPES using high efficient VLEED-type polarimeters. We observed in-plane spin-polarization for all the three bulk bands in the vicinity of the Fermi level, which is hardly explained by the conventional spin-orbit coupling as recently proposed [4].

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SESSION 9

Interaction of electrons with the out-of-plane vibrational modes in graphene

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We investigated decoherence of an electron in graphene caused by electron-flexural phonon interaction. We found out that the flexural phonons can produce dephasing rate comparable to the electron-electron one. The problem appears to be quite special because there is a large interval of temperatures where dephasing rate cannot be obtained using the golden rule. We evaluated this rate for a wide range of density (n) and temperature (T) and determine several asymptotic regions with temperature dependence crossing over from $1/\tau_\phi \sim T^2$ to $1/\tau_\phi \sim T$ when temperature increases. We also found $1/\tau_\phi$ to be a non-monotonous function of n . These distinctive features of the new contribution can provide an effective way to identify flexural phonons in graphene through the electronic transport by measuring the weak localization corrections in magnetoresistance.

Graphene: the good, the bad, and the beauty

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Graphene is probably the most fascinating material ever discovered, but it has some drawbacks: it has no gap, it is not superconducting, and it has a weak spin-orbit coupling. The interesting electronic properties of graphene, such as the presence of charge carriers that behave as if they would have no mass, are rooted on the honeycomb lattice of the carbon atoms. A key question in this regard is: if we engineer a honeycomb lattice out of semiconducting nanocrystals, is it going to behave like graphene or like the semiconducting building blocks?

In the first part of the talk, I will show that these systems, which have been experimentally synthesized last year [1], combine the best of the two materials. Honeycomb lattices of semiconducting nanocrystals exhibit a gap at zero energy, as well as Dirac cones at finite energies. In addition, they display topological properties [2], characteristic of the so-called topological insulators, but at room temperature [3].

In the second part of the talk, I will discuss how to describe the full dynamical electromagnetic interaction in 2D systems like graphene, where the electrons are constrained to move in the 2D plane, whereas the photons move in 3D. By using the so-called pseudo-QED approach, I will show how quantized currents emerge at the edges of this system, while the bulk remains insulating [4].

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Graphene Superlattices

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Keywords: Graphene, hexagonal boron nitride, 2D materials, graphene heterostructures, superlattice

Recent advances in the fabrication of heterostructures based on 2D atomic crystals have opened up several new directions in graphene research [1]. It has recently been realised that hexagonal boron nitride (hBN) can be used not only as a defect free and atomically flat substrate that dramatically improves mobility of graphene devices, but also as a material that creates a smooth periodic potential for Dirac electrons in graphene. This potential arises due to the small lattice mismatch between the two materials resulting in the formation of a moiré pattern, as previously observed in STM measurements [2]. For aligned graphene and hBN crystals, the period of the superlattice potential is as large as 14 nm and leads to a dramatic reconstruction of the band structure with the formation of new Dirac points in the spectrum. In high magnetic fields up to 30 T we approach the regime of one flux quanta per superlattice unit cell where the transport and capacitance data clearly reveal features of the spectrum predicted in the seminal paper of Douglas Hofstadter [3] known as the Hofstadter butterfly.

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Figure 1: One of the possible scenarios for the reconstruction of graphene's spectrum. The band structure is plotted only for the first and second super Brillouin zone (SBZ), shown in brown and green, respectively. Secondary Dirac cones appear in both conduction and valence bands at the edges of the SBZ, shown by the black hexagon

Valley Hall effect in bilayer graphene



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Keywords : graphene – valleytronics – non-dissipative electronics

Certain specific crystal structures result in degenerate local minima (conduction band) or maxima (valence band) called “valleys” in the band structure. “Valleytronics” is a newly developed concept for electronics utilizing the occupation degree of freedom of valleys as an information carrier. Honeycomb lattice systems such as graphene and transitional metal dichalcogenides (TMDCs) are ideal materials for valleytronics. These systems have K and K' valleys that have opposite electron chiralities. When spatial inversion symmetry is broken in these systems, valley contrasting Berry curvature emerges. This results in valley Hall effect [1] and inverse valley Hall effect, which enable generation and detection of a pure valley current. Valley Hall effect was initially demonstrated with photo-generated valley polarized electrons in monolayer MoS₂ [2]. However, its short inter-valley scattering length prevents detection of the pure valley current. Compared to TMDCs, graphene has longer inter-valley scattering length due to its high crystal quality, but requires external potential to break the spatial inversion symmetry. Recently, valley Hall effect was demonstrated in aligned monolayer graphene on h-BN via nonlocal resistance measurement, using the superlattice potential imposed by h-BN to break the spatial inversion symmetry [3]. For the case of bilayer graphene, however, a perpendicular electric field called displacement field can be used to break spatial inversion symmetry. Therefore, the alignment to h-BN is not required. The tunable displacement field allows for further controllability of the valley Hall effect and unambiguous detection of the pure valley current.

We use dual-gated bilayer graphene in the Hall bar geometry to electrically control broken inversion symmetry or Berry curvature as well as the carrier density to generate and detect the pure valley current (Fig. 1). We measure both local and non-local transport at temperatures between 1.5 K and 200 K. We find enhancement of the nonlocal resistance near the charge neutrality point when we increase the perpendicular electric field. The observed non-local resistance is much larger than what is expected as the Ohmic

contribution of the classical current diffusion from van der Pauw formula with measured local resistivity. We also find a cubic scaling between the nonlocal resistance and the local resistivity at the charge neutrality point at zero-magnetic field in the insulating regime where the local resistivity increases with lowering the temperature, when the local resistivity is lower than $\sim h/4e^2$. These observations prove existence of the pure valley current in the bulk insulating state [4], providing a significant contribution to the advancement of non-dissipative electronics.

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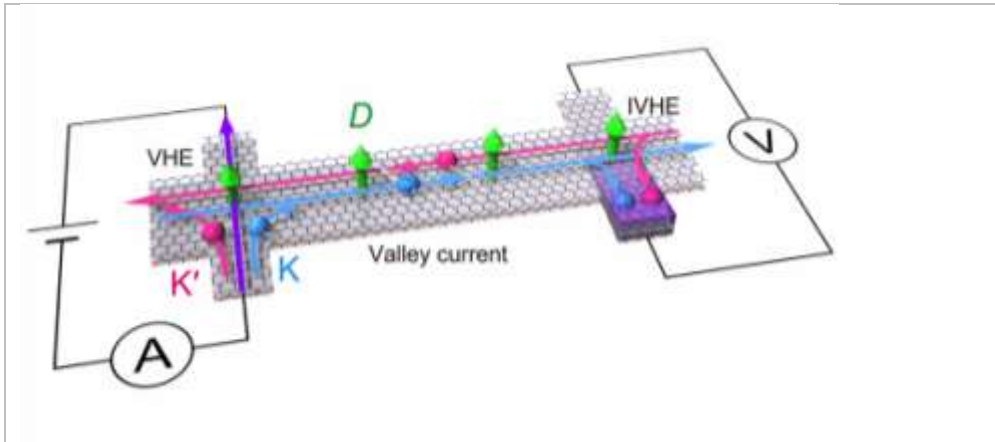


Figure 1: Schematic description of the nonlocal resistance measurement and the nonlocal transport mediated by pure valley current. Electric field driving the charge current in the left generates a pure valley current in the transverse direction via valley Hall effect. This valley current is converted into electric field or nonlocal voltage in the right via inverse valley Hall effect to generate the nonlocal resistance.

Magnetic Force Microscopy of spin reorientation of iron tin

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In this talk I will show the application of temperature-dependent magnetic force microscopy to study magnetic phase transitions in magnets. We applied this probe to study iron tin (Fe_3Sn_2), which is a layered ferromagnet, whose building blocks are Kagome planes, with a Curie temperature of 640 K. It has a spin reorientation, where the magnetic moments rotate from the transverse direction towards the planes on cooling, displays thermal hysteresis, and previously it has been reported to exhibit glass-like phenomena. As the spin reorients, the domain structure evolves from a branched dendritic high temperature state to a completely different domain structure at low temperatures. Our studies show that the spin reorientation is of first order and the system displays phase coexistence of magnetic easy axis perpendicular and parallel to the Kagome plane.

SESSION 10

Electronic and bosonic excitations in high temperature superconductors analyzed by time-resolved ARPES



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Keywords: bosonic excitations, time-resolved spectroscopy

Analysis of excitations in materials is of wide spread interest due to the coupling of electronic and bosonic degrees of freedom, in particular for high temperature superconductors. Typically the spectrum and dispersion of excitations is investigated by e. g. inelastic scattering and angle-resolved photoemission spectroscopy (ARPES). Here we report on femtosecond time-resolved ARPES results on the cuprates and the Fe-pnictides which were obtained by 1.5 eV pump and 6 eV probe photon energies with typically 100 fs time resolution. We discuss how such excitations are probed in tr-ARPES. On the cuprates we have identified a weakening of the well known kink in the electronic structure $E(k)$ near 70 meV below the Fermi level E_F , which represents a pump-induced reduction of the electron-boson coupling strength [1]. Coupling of electrons to that mode is also evident at an energy of 70 meV above E_F from a step in the energy-dependent electron relaxation times $\tau(E)$. A pronounced decrease of the step height in $\tau(E)$ with increasing pump fluence reflects that weakening of coupling also above E_F . Experiments on Fe-pnictides exhibit a similar step in the energy dependent electron relaxation times, although the effect is weaker and occurs at higher energies in agreement with e. g. inelastic neutron scattering experiments. Furthermore, electron redistribution upon pump laser excitation modifies the Fermi momentum k_F [1], which allows (a) to transiently change the effective doping level and (b) suggests a new way to probe the dynamic response of the Fermi surface of complex materials.

This work was conducted in collaboration with I. Avigo, S. Freutel, M. Ligges, L. Rettig, M. Sandhofer, J. D. Rameau, P. D. Johnson, P. Zhou, G. D. Gu, H. Eisaki, T. Wolf, P. Gegenwart, H. S. Jeevan, A. F. Kemper, and M. Sentef.

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Ultrafast laser control of the magnetic exchange interaction

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Keywords: Ultrafast dynamics of correlated materials

Femtosecond laser technology has opened the possibility to control complex condensed matter phases with intertwined spin, charge, and lattice order on microscopic timescales. An intriguing pathway to achieve this goal is to modify the emergent interactions in the material by light. In this talk we discuss two pathways to modify the magnetic exchange interaction J with ultra-short laser pulses in the prototype Mott-Hubbard insulator. First, we demonstrate an ultrafast reduction of J within a few electron hopping times after photo-doping (exciting nonequilibrium distribution of doublon and hole carriers in a Mott insulator) [1]. The value of J is obtained by simulating laser-induced spin precession in a canted antiferromagnet. Quantitatively, the effect of photo-doping on the value of J is comparable to the effect of chemical doping. The electronic dynamics in the Hubbard model is obtained from nonequilibrium dynamical mean-field theory (DMFT) [2]. Furthermore we demonstrate the possibility of a reversible modification of exchange interactions in systems that are driven by off-resonant laser fields [3], using both DMFT and analytical Floquet theory. In the regime of strong-driving, even the sign of the exchange coupling can be reversed under the influence strong driving.

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Dynamics of fluctuations in high temperature superconductors far from equilibrium conditions



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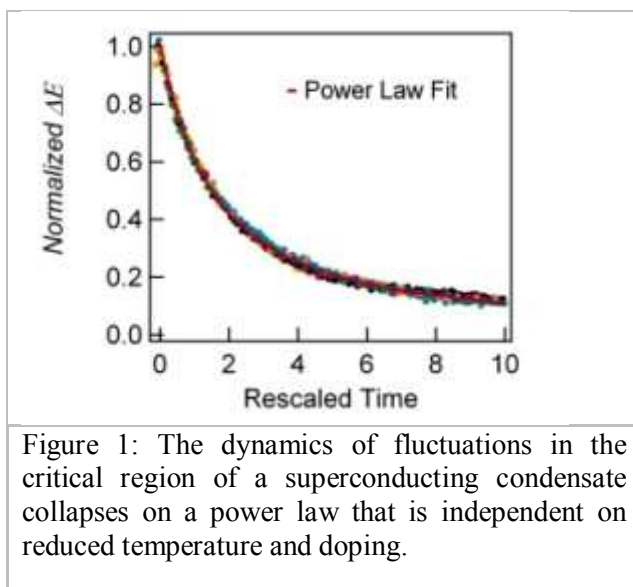
Keywords : cuprates – fluctuations – non-equilibrium

Despite the extensive literature on high temperature superconductors, the critical dynamics of an incipient condensate has so far been studied just in equilibrium conditions. Here, I show that resolved THz measurements of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+d}$ discriminate the temperature regimes where superconductivity is coherent, fluctuating or vanishingly small [1]. Above the transition temperature, the recovery to equilibrium conditions displays power law behavior and scaling properties. The experimental evidence that some of the exponents weakly depend on doping level provide hints of universality in systems far from equilibrium. We find partial agreement between the scaling law of the optimal doped sample and the Time Dependent Ginzburg-Landau (TDGL) model. Inherent limits of TDGL call for non-equilibrium field theories treating fast degrees of freedom and fluctuations on equal footing.

Our second experimental approach is time resolved photoelectron spectroscopy. I will show that inelastic scattering of nodal quasiparticles decreases when the temperature is lowered below the critical value of the superconducting phase transition. This drop of electronic dissipation is astonishingly robust and survives to photoexcitation densities much larger than the value sustained by long-range superconductivity.

The unconventional behaviour of quasiparticle scattering is ascribed to superconducting correlations extending on a length scale comparable to the inelastic mean-free path. According to this finding, a impulsively excited condensate enters in a regime without phase coherence but finite pairing amplitude. The latter vanishes near to the critical temperature and has no evident link with the pseudogap observed by Angle Resolved Photoelectron Spectroscopy. These results open a timely connection between superconductors and Bose-Einstein condensates of ultra-cold atoms.

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SESSION 11

Dynamic phase transitions in a honeycomb superconducting network



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Keywords : vortex matter – dynamic Mott transitions – tunable superconducting metamaterials – universality class

The magnetoresistance of an array of superconducting islands on top of a normal metal is investigated, where the islands are placed in a honeycomb lattice. This system is found to undergo a dynamic phase transition, as when the current is increased the magnetoresistance minima turn to maxima at rational values of the frustration factor. This observation was also done in a previous study on square lattices [1], and is identified as a vortex Mott insulator to metal transition, where the vortices play the role of electrons in an electronic Mott Insulator. On the magnetoresistance data, scaling analysis is done at integer frustration factors and the critical exponent is reported. The role played by the underlying hexagonal geometry in the nature of the dynamic phase transition is discussed.

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Vortex Mott insulator in nanoperforated TiN films



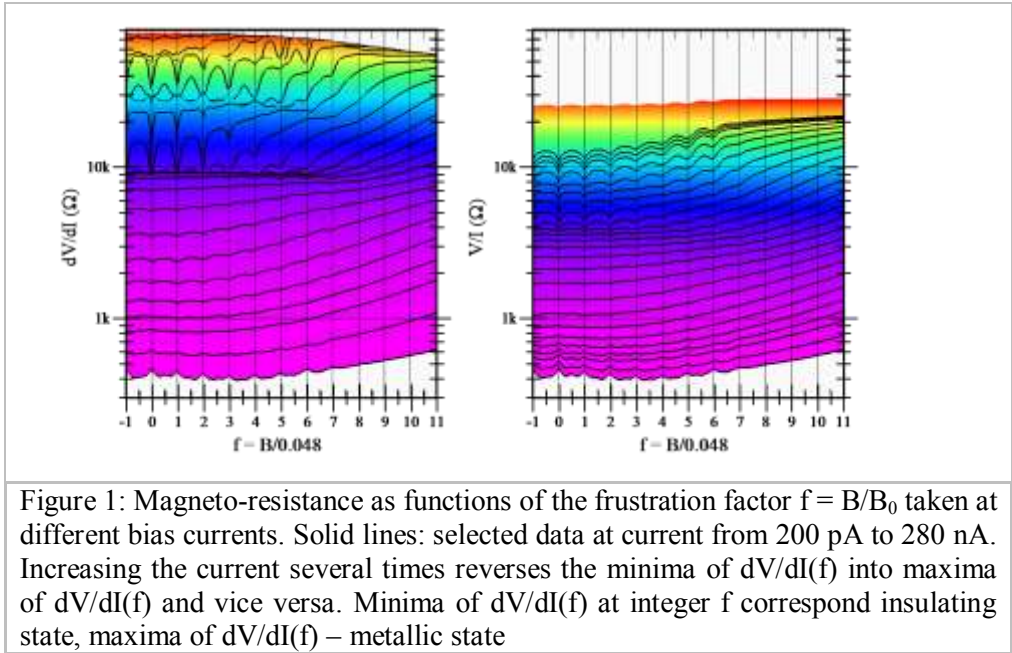
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Keywords : nanoperforated films – vortex – magnetic field

We present an experimental observation of the electric current induced vortex Mott transition in nanoperforated TiN films. Nanopatterning transforms a thin TiN film into an array of superconducting islands connected by weak links. Magnetic field-induced vortices are localized in the holes, which provide energetically favorable positions for them. A vortex Mott insulator forms at the fields where by filling number of vortices trapped by holes is integer. We find multiple insulator-to-metal transitions where minima of the differential resistance dV/dI at filling factors $f = B/B_0$ reverse into maxima, and metal-to-insulator transitions where maxima of $dV/dI(f)$ reverse into minima, upon increasing the current, see fig 1.



STS of vortex cores in superconductors: From Abrikosov to Josephson

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In this talk we will discuss the spectroscopic signatures of quantum vortex cores in superconductors recently revealed by Scanning Tunneling Spectroscopy. Starting from a well-known case of Abrikosov vortex lattice in bulk materials, we will present several cases emerging in nano-structured superconductors.

We will first focus on effects of lateral confinement in superconducting islands of a size close to the coherence length [1]. Then we will discuss the vortex phases observed in ultra-thin films such as single atomic layers of Pb grown on Si(111). We will show that in these ultimate superconductors two kinds of vortices, namely Abrikosov (Pearl) and mixed Abrikosov-Josephson vortices [2], coexist [3]. Finally, we will demonstrate that Josephson vortices inside S-N-S Josephson junctions are also characterized by cores, and can be measured by Scanning Tunneling Spectroscopy [4].

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Vortex dynamics at the sub-nanometer scale

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Superconducting Quantum Interference Devices (SQUID) are traditionally the most sensitive device for measuring magnetic field. However, because of their relatively large sizes ($> 1 \mu\text{m}^2$) and limitations on reducing the device-to-sample distance to submicron range, SQUIDS were not used so far for magnetic imaging at the nanoscale. We have developed nano-SQUIDS-on-tip (SOT) made of Pb with an effective diameter of down to 46 nm and flux noise of $\Phi_n = 50 \text{ n}\Phi_0/\text{Hz}^{1/2}$ at 4.2 K that are operational up to unprecedented high fields of 1 T [1]. The corresponding spin sensitivity of the device is $S_n = 0.38 \mu\text{B}/\text{Hz}^{1/2}$, which is about two orders of magnitude more sensitive than any other SQUID to date.

Using this novel technique, we have carried out study of dynamics of single vortices in superconductors subjected to ac and dc drive. The outstanding sensitivity of the SOT allows probing vortex displacements as low as 10 pm [2]. Thus we were able, for the first time, to measure the structure of disorder-induced vortex pinning potential as a function of the position with sub-nanometer resolution. The study finds rich internal structure of the pinning potential and of the restoring force, and reveals unexpected phenomena such as softening of the restoring force, nontrivial vortex trajectories within a single potential well, pronounced anisotropy, and abrupt depinning. The results shed new light on the importance of multi-scale random disorder on vortex dynamics and thermal fluctuations even at 4.2 K.

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SESSION 12

Electronic and magnetic states at cuprate/manganite interfaces

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Keywords : complex oxides – interfaces – manganites – cuprates

We have studied $(\text{CaCuO}_2)_m/(\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3)_n$ superlattices (SLs), a new system that can be considered as the parent compound for superconducting/magnetic heterostructures previously reported in literature[1,2]. In fact, CCO is the simplest undoped antiferromagnetic parent compound of cuprate superconductors. The results obtained by linear and circular dichroism in soft x-ray absorption (XAS-LD and XMCD) and hard x-ray photoemission spectroscopy (HAXPES) are compared with the case of LSMO thin films to elucidate the role of the interface reconstruction in cuprate/manganite systems. In particular, XAS-LD data show that in CCO/LSMO SLs grown in strongly oxidizing conditions, extra apical oxygen ions at the interface favors $3d_{z^2}-r^2$ orbital occupation of Cu and Mn valence electrons. Apical oxygen contributes to localize extra holes in the optimally doped LSMO block. This, in turn, favors the formation of the AF phase that is seen in the transport properties [3] and XMCD measurements, as in the case of the dead-layer in single layer LSMO films [4].

The interface reconstruction mediated by apical oxygen formation can also explain the Mn3s exchange splitting measured by HAXPES. While an increasing of the Mn3s splitting with the reduced valence and covalency is observed in LSMO thin films [5], the Mn3s splitting in CCO/LSMO SLs increases with the enhanced Mn^{4+} content and with the expected AF insulating phase in the dead-layer of LSMO. The effect of hole localization in the O 2p orbital was reported in literature to explain the exchange splitting in mixed valence manganites with different doping concentration [6].

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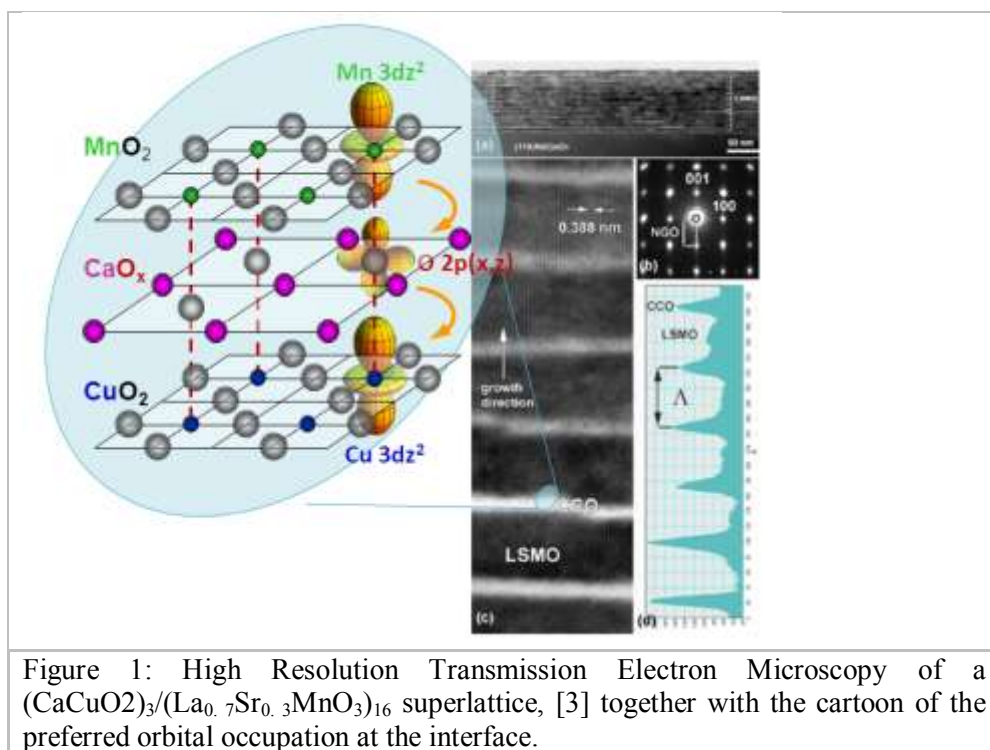


Figure 1: High Resolution Transmission Electron Microscopy of a $(\text{CaCuO}_2)_3/(\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3)_{16}$ superlattice, [3] together with the cartoon of the preferred orbital occupation at the interface.

Novel electronic state in n-type high- T_c cuprate superconductors observed by transport properties and muon spin relaxation]



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Keywords: electron-doped high- T_c T'-cuprate, transport properties, muon spin relaxation, Ce-free superconductivity

In order to investigate the electronic state relating to the Ce-free superconductivity in the parent compound of electron-doped high- T_c cuprates with the so-called T' structure [1,2], we have performed transport and muon-spin-relaxation (μ SR) measurements of T'-Pr_{1.3-x}La_{0.7}Ce_xCuO_{4+ δ} (PLCCO) single crystals and Ce-free T'-La_{1.8}Eu_{0.2}CuO_{4+ ψ} (LECO) polycrystals [3,4]. It has been found from the *ab*-plane electrical resistivity in PLCCO with $x = 0.10$ that a strongly localized state of carriers in the as-grown sample changes to a metallic state with a Kondo effect in the reduced superconducting (SC) sample. The Hall resistivity of the reduced SC sample of $x = 0.10$ has revealed the existence of both hole and electron carriers. The μ SR spectra of PLCCO with $x = 0.10$ and LECO have revealed that, in the ground state, a long-range magnetic order of Cu spins in the as-grown sample changes to a short-range one coexisting with the superconductivity in the reduced SC sample. The formation of the short-range magnetic order due to a tiny amount of excess oxygen in the reduced SC sample suggests that the T'-cuprate exhibiting the Ce-free superconductivity is regarded not as a simple band metal but as a strongly correlated electron system. These results can be explained in terms of a band picture based on the strong electron correlation [3]. That is, the collapse of the charge-transfer gap between the upper Hubbard band of the Cu3d_{*x-y*² orbital and O2*p* band due to the square planer coordination of oxygen in the T'-cuprate results in the generation of a finite density of states at the Fermi level due to O2*p* holes and Cu3d_{*x-y*² electrons without Ce substitution.}}

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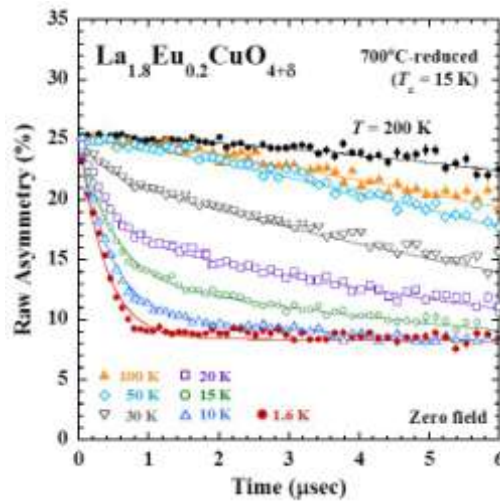


Figure 1: Zero-field μ SR time spectra of the 700°C-reduced superconducting samples of $\text{La}_{1.8}\text{Eu}_{0.2}\text{CuO}_{4+\delta}$. Solid lines indicate the best-fit results using the analysis function.

About superconductivity and magnetism in 2DEGs at oxide interfaces

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The nature of the ground state of the two dimensional electron gas (2DEG) at the interface between the LaAlO_3 and SrTiO_3 wide bandgap insulators, presumably as a consequence of polar discontinuity [1], has been for years highly controversial [2], due to the initially contrasting reports of magnetism [3] and superconductivity [4]. More recently, several reports have accredited the idea of a phase-separated ground state, where superconductivity and magnetism can coexist. .

In this work, the low temperature magnetic and magneto-transport properties of the widely celebrated $\text{LaAlO}_3/\text{SrTiO}_3$ interfaces in the proximity of the superconducting temperature are compared with the properties of three novel oxide-based polar-nonpolar interfaces, also hosting a 2DEG, i. e. $\text{LaGaO}_3/\text{SrTiO}_3$ [4], $\text{NdGaO}_3/\text{SrTiO}_3$ [5] and $\text{LaAlO}_3/\text{EuTiO}_3/\text{SrTiO}_3$ [6], all recently developed in Naples. Similarities and differences are discussed.

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The superconducting proximity effect in topological insulator/superconductor hybrid systems: theoretical exploration and experimental probes

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The exploration of Majorana physics in topological insulators (TIs) relies on the subtle interplay between the band structure of the materials and (induced) correlated phases with superconducting order or spin-polarization. While such effects are easily introduced into the Hamiltonian of a model system, the combination of materials with rather dissimilar properties imposes some challenges for the experimental realization. Exotic behavior may arise when combining superconductors with materials of nontrivial band structure. Here, I present three experiments which study different aspects of the proximity effect between topological insulator materials and conventional superconductors. Using conductance spectroscopy on quasi-ballistic S/TI/N structures as a tool, we explore the magnitude of the induced order parameter on the surface of a topological insulator. Although such spectra share many features with theoretical predictions for p-wave order parameter superconductivity, a closer examination of realistic material parameters for S/TI/N devices reveals a more complicated situation which makes it difficult to determine p-wave conductance features in such experiments reliably without extensions to presently available theory. Yet, an indicator of non-s-wave-type correlations in the induced superconductivity of TIs may be found by simultaneously probing the nonlocal conductance in multi-terminal devices. Here, quasiparticle transport is examined, and our experiments reveal an unusual, bias-odd component. Besides magnitude and shape of the induced gap, information about band topology is directly accessible if Josephson coupling between two superconducting electrodes is established. Experiments on gate-tunable TI Josephson devices show that the supercurrent decreases abruptly when the carrier density on the TI surface approaches a critical value. This value is estimated to lie well above the bottom of the conduction band. Using a simple model, the drop in supercurrent can be linked to a displacement of Andreev bound states which is driven by the band topology on the TI surface. The mechanism is related to the emergence of Majorana fermion states and exemplifies the importance of studying the connection between topology and correlation effects of superconductor-topological insulator structures in realistic geometries.

Shape resonance in a single slab for optimum T_c in 2DEG

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Keywords: shape resonance; multi-condensates superconductivity; heterostructures at atomic limit

The shape resonance in the superconducting gaps has been proposed as the mechanism behind high temperature superconductivity in cuprates [1-5], diborides [5-7] iron based heterostructures at atomic limit [8]. multi gap superconductor in the clean limit. We discuss here the two condensates scenario in the superconducting two-dimensional electron gas (2DEG) [9,10] at the interface between two insulating oxides. The prediction of the shape resonance scenario for high temperature superconductivity was proposed for cuprates [1,4] based on experimental evidence of two (or three) main electronic components. The key experimental data show the first component in the Fermi arc around (π, π) characterized by a pure $ml=2$ orbital symmetry, in the weak coupling limit $2\Delta/T_c \ll 3.5$ and a second component in the hot spot $(\pi, 0)$ in the k -space, characterized by pseudo-Jahn Teller polarons formation with mixing of $ml=0$ and $ml=2$ orbital symmetry, with a large superconducting gap ($2\Delta/T_c \gg 3.5$) in the strong coupling limit. In the diborides the critical temperature up to 40K is given by the hot spot in the strong coupling limit ($2\Delta/T_c = 4.5$) at the Γ point of the σ band near a “neck disrupting” Lifshitz transitions coexisting with π electrons in the weak coupling limit ($2\Delta/T_c = 1.5$). In the 2 DEG confined within at the oxide-oxide interface the formation of mini-bands are generated by quantum size effects in a slab of 5 nanometers thickness. The superconductivity appears at the BEC-BCS crossover in the upper subband with strong pairing strength in the shallow Fermi surface, pointing toward the best configurations for enhanced superconductivity in 2DEG. We show the Fano-like antiresonance with the critical temperature going to zero where the chemical potential is tuned at the band edge i.e at the Lifshitz transition for “appearing” of a new Fermi surface spot [10].

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SESSION 13

***In situ* observation of phase separation and hierarchical microstructure of $K_xFe_{2-y}Se_2$ single crystals**



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Keywords: phase separation, in situ SEM observation, FIB-SEM, 3D microstructure

As solid-state phase transformations occur, materials exhibit rich microstructures depending on the heat treatment conditions, for example quenching temperatures, heating and cooling rates, and pressure [1,2]. The mechanical [3], magnetic [4], transport and superconducting properties [5] of materials can be significantly changed by tuning microstructures upon heat treatment. The $K_xFe_{2-y}Se_2$ single crystals exhibit an iron vacancy order-disorder transition at $T_s \sim 270$ °C [6,7]. Below T_s two spatially separated phases, a minority/superconducting phase and a majority/iron vacancy-ordered phase, were observed through x-ray diffraction [8], transmission electron microscopy (TEM) [9], scanning electron microscopy (SEM) [5,10]. It was found that the superconductivity in the $K_xFe_{2-y}Se_2$ single crystals is strongly dependent on the heat treatment conditions [5]. However, the nature of this phase separation is not well understood. Here, temperature dependent SEM images provide compelling evidence that phase separation corresponds to a nucleation and growth process rather than a spinodal decomposition. The superconducting phase is the remnant of high temperature phase after iron vacancy order-disorder transition. Three-dimension (3D) spatial distribution of superconducting phase in the iron vacancy ordered matrix was revealed by using focused ion beam scanning electron microscopy (FIB-SEM). Our results clearly show that superconducting phase forms a hierarchical structure. Understanding the formation of this hierarchical structure not only can guide the synthesis of bulk superconductors in the future, but also greatly enrich our knowledge about the interplay between phase separation and solid-state phase transformations.

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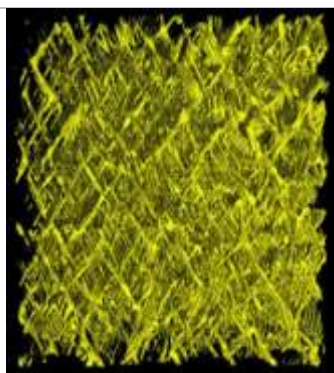


Figure 1: 3D reconstructed microstructure of superconducting phase in the $K_xFe_{2-y}Se_2$ single crystals, (100) plane view.

Disordered Fe vacancies and superconductivity in potassium-intercalated iron selenide ($\text{K}_{2-x}\text{Fe}_{4+y}\text{Se}_5$)



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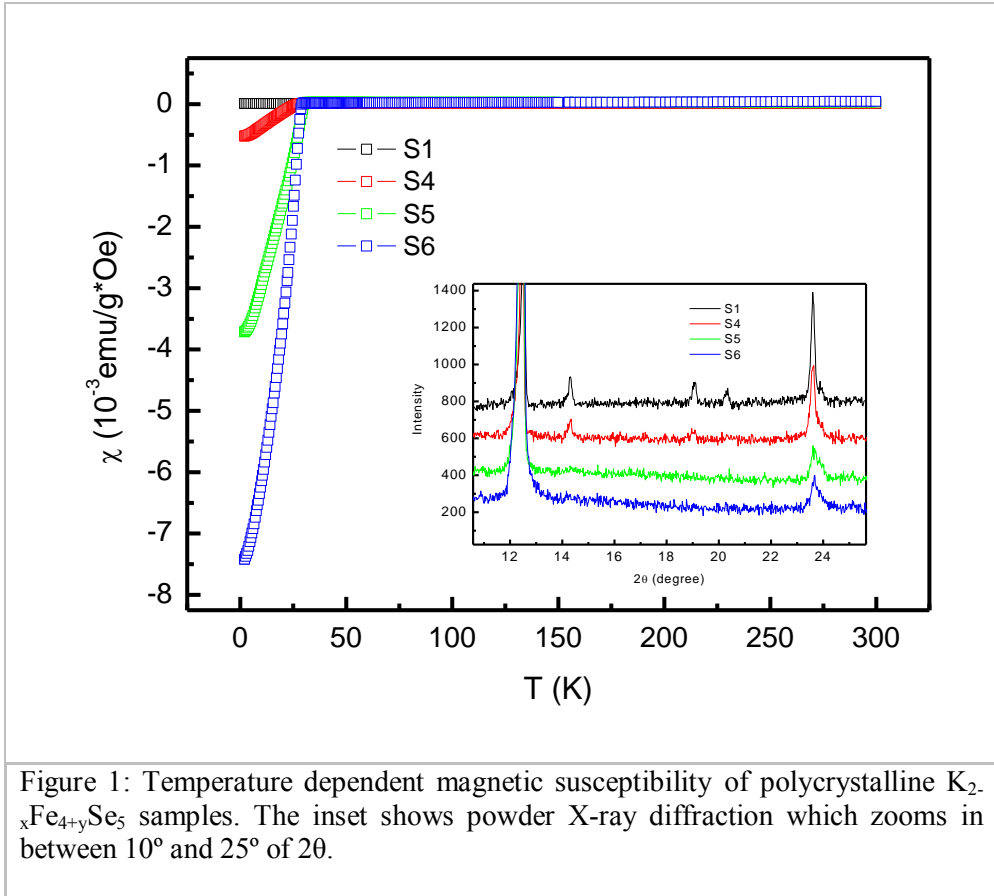
Keywords: mechanisms for high T_c – FeSe superconductors – disordered superconductors

The iron-based superconductors may contain many similarities to the cuprates, and the rapid rise in reported T_c s in the FeSe family is nearing the values of those in the cuprates. The Fe based superconductors contain layered structure and the superconducting dome borders a magnetic order in the parent compound, similar also to the cuprates. Similarly, the superconductivity appeared from the suppression of the magnetic order by doping [1, 2]. In the high- T_c potassium intercalated FeSe [3], there has been significant debate regarding what the exact parent compound is. A recent study on the non-superconducting Fe_4Se_5 [4], which exhibits the $\sqrt{5} \times \sqrt{5}$ Fe-vacancy order and is magnetic, shows that it becomes superconducting after high temperature annealing. Here we report a systematic study of $\text{K}_{2-x}\text{Fe}_{4+y}\text{Se}_5$ compounds with controlled stoichiometry. We find the superconductivity occurs when Fe-vacancy order is gradually suppressed. Our experiments lead us to believe Fe-vacancy order state is the non-superconducting parent phase in potassium intercalated FeSe, and possibly to the Fe-chalcogenide superconductors.

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Spectromicroscopy of phase-separated iron chalcogenide superconductors

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Keywords: Fe-based superconductors, phase separation, microscopy

Understanding the interplay between superconductivity and magnetism in iron-based superconductors is likely to provide significant insights into the elusive mechanisms responsible for high temperature superconductivity. The co-existence of magnetic order and superconductivity is a common feature of the iron-based superconductors, raising the question of whether these phases are spatially distinct or whether the same electrons are responsible for both phenomena.

In the case of the $A_x\text{Fe}_{2-y}\text{Se}_2$ compounds, with T_c values of about 30K [1], the intrinsic phase separation is very extreme, with significant chemical and structural differences associated with the spatially distinct electronic phases. Here we will present recent results on the microstructural development of $Rb_x\text{Fe}_{2-y}\text{Se}_2$ single crystals on annealing at temperatures above and below the phase separation temperature followed by cooling at different rates. SQUID magnetometry has been used to analyse the influence of the heat treatment protocol on the superconducting transition temperature.

Energy Dispersive X-ray mapping has been carried out at low voltage in a Scanning Electron Microscope to examine the chemical composition of the individual phases in the crystals. This chemical variation has been linked to structural variations using our novel high resolution Electron Backscatter Diffraction technique, confirming that the minority phase in the crystal is Fe-rich and has a larger unit cell c/a ratio [2].

In addition, Scanning Photoemission Microscopy (SPEM) has been carried out on the SpectroMicroscopy beamline at Elettra synchrotron to investigate the differences electronic structure between the two phases, enabling direct correlation between the electronic properties and chemistry/structure of each phase. Near-Fermi-level maps clearly show the same microstructural features as the SEM studies, with the lowest binding energy Fe 3d peak being enhanced in the Fe-rich minority phase, providing evidence that this minority phase is the metallic phase that becomes superconducting at low temperature [2].

Our recent work using Photoemission Electron Microscopy (PEEM) at Diamond Light Source to carry out spatially resolved core level X-ray Absorption Spectroscopy and linear dichroism experiments will also be reported.

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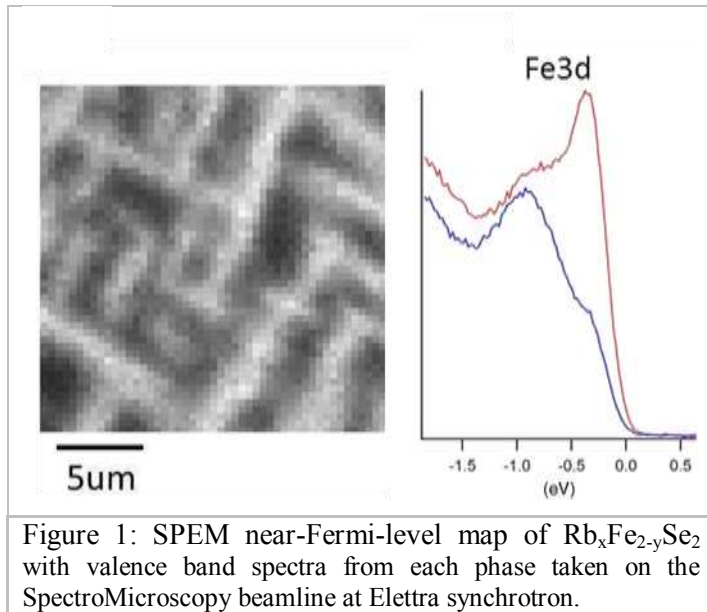


Figure 1: SPEM near-Fermi-level map of $\text{Rb}_x\text{Fe}_{2-y}\text{Se}_2$ with valence band spectra from each phase taken on the SpectroMicroscopy beamline at Elettra synchrotron.

SESSIONE 14

Local Fe modes and superconductivity in $K_{0.8}Fe_{2-y}Se_2$



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Keywords: mechanisms for high T_c – local Fe modes – phase separation

The coexistence of insulating and superconducting phases in the $K_xFe_{2-y}Se_2$ family of Fe-based superconductors is investigated using neutron scattering on samples grown under different conditions. In the $K_xFe_{2-y}Se_2$ family, three scenarios have so far been proposed regarding the superconducting phase. In the first, a superconducting minority phase with the 122 composition is separated from the insulating and majority 245 phase. Under this scenario several phase diagrams have been developed in which the superconducting phase is sandwiched between a semiconducting and insulating, antiferromagnetic phase. In the second, the superconducting and insulating phases coexist as part of an inhomogeneous structure, hence no phase separation. And in the third, a purely superconducting phase of the alkali intercalated FeSe can be made with the 122 structure that has no other phases. By probing the local structure, we observe that superconductivity emerges in a locally distorted Fe sublattice that accommodates two kinds of bonding environments, forming a double-well distribution that changes with the concentration of K. In addition, the Fe bond distribution is very sensitive to sample preparation and is directly related to the superconducting transition. Implications to the coexistence of the insulating and superconducting phases will be discussed.

Superconductivity of Single-Layer Films of FeSe with T_c above 100 K



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Keywords: Interface enhanced superconductivity, four-point probe transport measurement

Recently, interface has been employed to enhance superconductivity in the single-layer FeSe films grown on $\text{SrTiO}_3(001)$ (STO) with a possible T_c of ~ 80 K [1], which is nearly ten times of the T_c of bulk FeSe and is above the T_c record of 56 K for the bulk Fe-based superconductors. This work together with those on superconducting oxides interfaces [2] revives the long-standing idea that electron pairing at a two-dimensional interface between two different materials is a potential path to high transition temperature (T_c) superconductivity [3-5]. Subsequent angle-resolved photoemission spectroscopy measurements reveal different electronic structure from those of bulk FeSe [6-8] and superconducting gap ~ 65 K, supporting the interface effect proposed in Ref. 1. Here I will introduce the observation of high T_c superconductivity in the FeSe/STO system by using in situ 4-point probe electrical transport measurement that can be conducted at an arbitrary position of the FeSe film on STO. The main result is that the superconducting behavior is detected at a temperature above 100 K, which makes FeSe/STO the exciting and ideal research platform for higher T_c superconductivity [9].

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Pairing Symmetry and Fermi-Surface Topology in Fe-Based-122 Superconductors

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Keywords: $s\pm$ - and d-wave pairing symmetries, heavily electron-doped compounds, Fermi-surfaces, disordered scatterings, local density states and Andreev bound states.

The pairing symmetry of superconductivity in highly electron doped $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x\text{As})_2$ and $\text{A}_y(\text{FeSe})_2$ (with $\text{A}=\text{K}, \text{Cs}$) compounds which have similar crystal and band structures [1, 2], are examined. Based on our previous approach [3,4] and using nearest-neighboring (NN) and next-nearest-neighboring (NNN) intra-orbital pairing interactions on a square lattice which representing the Fe-sites, we find that the pairing symmetry changes from the $s\pm$ -wave to d-wave like without nodes as the doped electrons filled up the hole pockets of the Fermi surface near the Γ -point. For these electron-doped compounds, the $s\pm$ -pairing symmetry is shown to persist from under- to over-doped samples ($x < 0.4$ and $y < 0.8$). In the heavily electron-doped region, the d-wave pairing symmetry are predicted for both of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x\text{As})_2$ (with $x > 0.4$) and $\text{A}_y(\text{FeSe})_2$ with ($y \sim 0.8$ to 1). However, it is well known that the superconductivity has never been observed experimentally [1] in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x\text{As})_2$ with $x > 0.4$, here we show numerically that the d-wave superconductivity in this material could be completely suppressed by disordered scatterings due to the randomly distributed Co atoms in the Fe-plane. This result is consistent with experimental measurements. Local density of states spectra near a strong impurity to distinguish $s\pm$ -wave and d-wave scenarios are calculated for highly electron-doped $\text{A}_y(\text{FeSe})_2$ superconductors with $y = 0.8$ to 1. We also demonstrate that for d-wave pairing symmetry, there exist Andreev's bound states inside the gap near the impurity, while there are no such in-gap states for $s\pm$ - pairing symmetry. Hopefully the signature of the d-wave pairing symmetry in this compound can be tested by future STM experiments.

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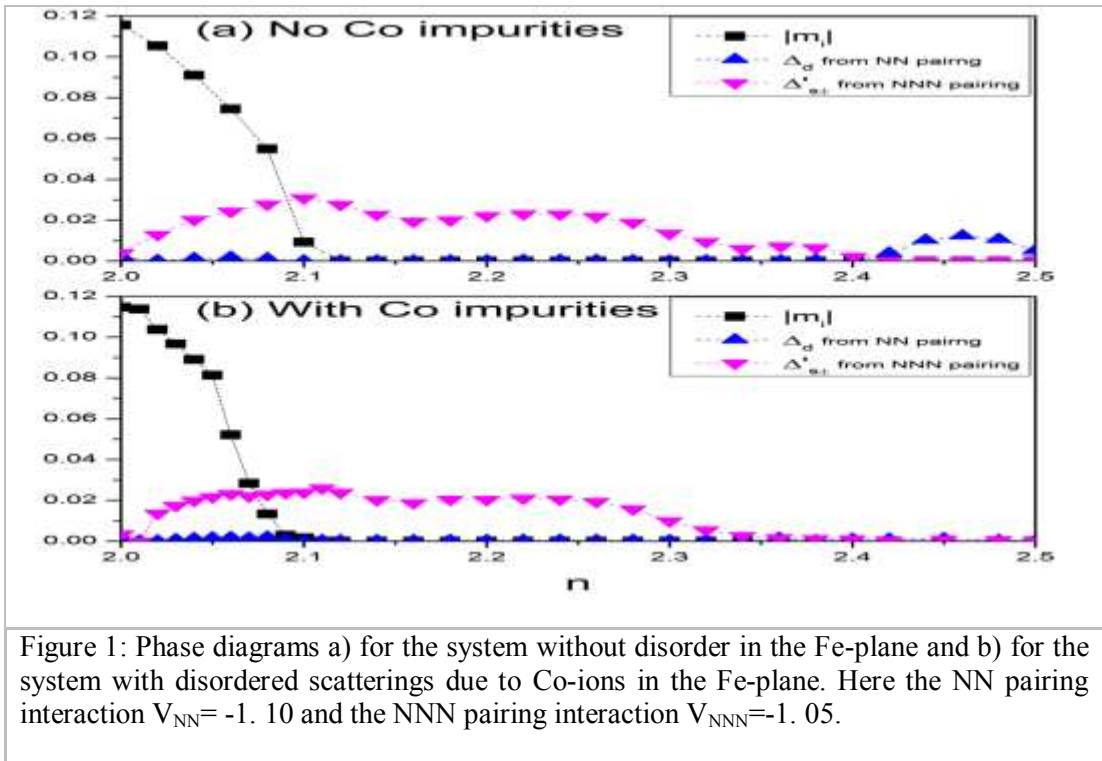


Figure 1: Phase diagrams a) for the system without disorder in the Fe-plane and b) for the system with disordered scatterings due to Co-ions in the Fe-plane. Here the NN pairing interaction $V_{NN} = -1.10$ and the NNN pairing interaction $V_{NNN} = -1.05$.

SESSION 15

Electrochemical charge doping in conventional and unconventional superconductors: the cases of NbN and Ba-122



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Keywords: Field effect, Iron-based superconductors,

The use of polymer electrolyte solutions (PES) for electrochemical gating [1] in order to produce electric-double-layer field-effect devices for fundamental physics investigations is becoming increasingly popular. By using this technique, ultrahigh electric fields of the order of 10-100 MV/cm can be obtained at the interface between the sample and the PES, which in turn give rise to record modifications of the surface charge density of the material (up to more than 10^{14} charges/cm²). This defect-free, purely electrostatic induction of high surface charge densities can even lead to a superconducting phase transition in insulating or semiconducting materials [1, 2].

By using a novel PES and a standard electrochemical-gating field-effect technique we recently succeeded in inducing surface charge densities up to more than 4×10^{15} charges/cm² in metallic thin films of Au, Ag and Cu [3,4] resulting in a considerable reversible variation of resistance (about 10% at 4 K in Au) [3]. The induced surface charge was determined by a suitable modification of a classic method of electrochemistry called double-step chronocoulometry and the results were also confirmed by standard Hall-effect measurements.

Here we present the results we obtained with the same technique in thin films of superconductors, either conventional (namely NbN) and unconventional (Fe-based 122 compounds). In NbN the intense charge doping induces a small shift in the critical temperature, whose amplitude depends on the film thickness and whose sign is reversed at the change of gate-voltage polarity. These two facts strongly indicate that the induced charge is actually distributed in a region much larger than the screening length. Indeed, the dependence of T_c on the induced surface charge density, predicted by means of ab-initio DFT and strong-coupling Eliashberg calculations, can be reconciled with the experimental

findings only if the thickness of the charge induction layer is comparable to that of the whole film.

Analogous experiments have been carried out in thin films of Ba-122 (either undoped or optimally P-doped, on different substrates). The results are here discussed with particular reference to the thickness of the charge injection layer (which also in this case seems to be larger than the electronic screening length) and to the role of pure charge doping versus chemical doping.

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Tuning the quantum critical point by Mn impurities and chemical pressure in $\text{LaFeAsO}_{0.89}\text{F}_{0.11}$



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Keywords: interplay of Magnetism and Superconductivity, effect of magnetic impurities, effect of chemical pressure

The interplay between magnetism and superconductivity has been studied in optimally F doped $\text{LaFeAsO}_{0.89}\text{F}_{0.11}$ (La1111F) compound by combining the poisoning effect of magnetic Mn impurities in the Fe site and the beneficial effect of the chemical pressure, by Y/La substitution, on the superconducting transition T_c .

Detailed muon spin spectroscopy studies evidence that a very tiny amount of Mn/Fe substitution (around 0. 2% !) quenches superconductivity in pure optimally doped La1111F system and creates the recovery of a static magnetic phase [1].

Nuclear quadrupolar and magnetic resonance measurements display a progressive increase of the low-energy spin fluctuations upon Mn substitution with the typical behaviour expected nearby an antiferromagnetic Quantum Critical Point [1].

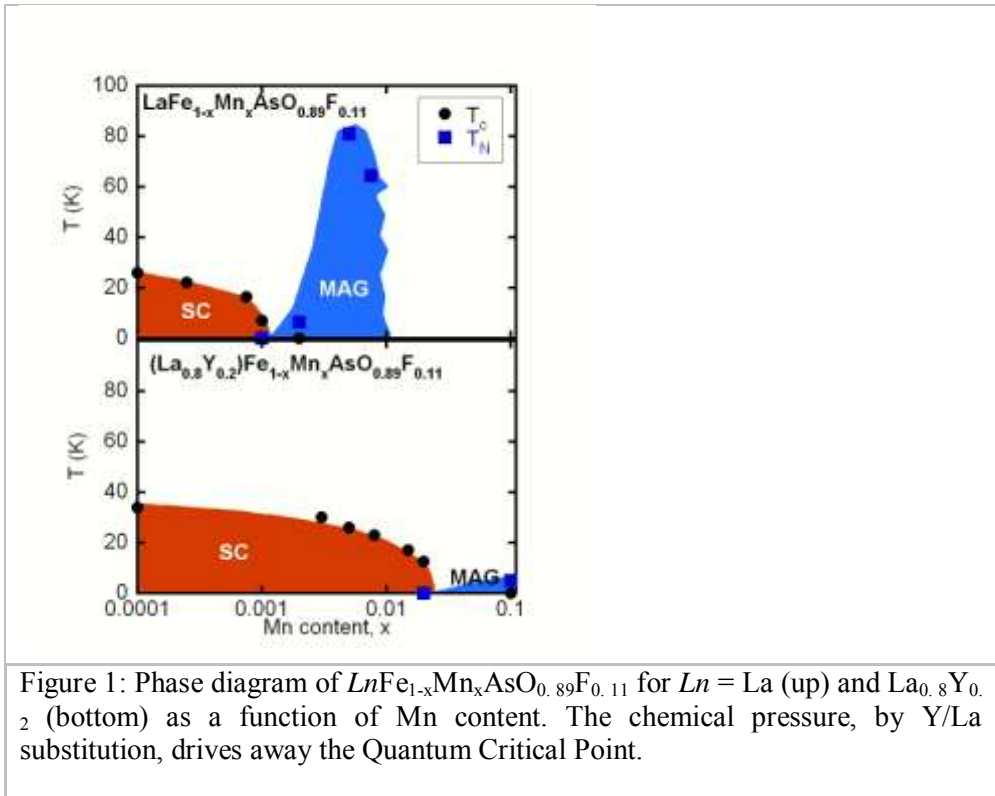
On the other hand, when 20% of La is substituted with the smaller Y, the Mn threshold for the disruption of superconductivity is significantly increased by more than one order of magnitude (see Fig. 1), indicating a huge effect of the chemical pressure on the system [2]. In particular, the gradual addition of Y at constant Mn content of 0. 5% in $\text{LaFeAsO}_{0.89}\text{F}_{0.11}$ progressively increases the superconducting transition T_c from zero to 30 K, with a much greater rate than observed in the Mn free compound [3].

The results indicate that La1111F is nearby a QCP and that the internal pressure gradually drives the system away from it. The disruption of the superconducting phase is associated

with the enhancement of low-frequency fluctuations possibly competing with the ones driving superconductivity.

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Structural complexity in $\text{RE}_2\text{MO}_{4+\delta}$: where are the limits?



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Keywords: non-stoichiometric oxides, oxygen ordering, charge ordering, DFT Molecular Dynamics, neutron scattering, synchrotron diffraction, oxygen diffusion,

Hole doping in RE_2MO_4 type oxides is generally achieved by substituting trivalent rare earth cations by cations as Sr or K. Another elegant way to oxidize the transition metal M is oxygen intercalation via an electrochemically controlled reaction. The main difference between these two methods is that oxygen intercalation proceeds at already ambient temperature, while cation substitution requires high reaction temperatures.

While the latter method consequently results in thermodynamically controlled reaction products, oxygen intercalation proceeding at ambient temperature allows to obtain kinetically stabilized phases which might not be available by high temperature synthesis. The degree of structural and electronic complexity induced is therefore supposed to attain a superior level compared to phases obtained at high temperature.

We have investigated a series of oxides, comparing the influence of oxygen intercalation and Sr-doping on oxygen ordering and electronic properties. In this context $\text{La}_{1.6}\text{Sr}_{0.4}\text{CoO}_4$ shows AF-ordering with a $T_N = 46\text{K}$, while the equivalent $\text{La}_2\text{CoO}_{4.25}$ shows a T_N of 36 K. A similar behavior is observed comparing $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ with $\text{SrCoO}_{2.5+\delta}$, where Sr-doping or oxygen intercalation continuously increases the amount of Co^{4+} and which results in ferromagnetic ordering, correlating the increase of T_C with the formation of Co^{4+} [1-3]. Long range oxygen ordered intermediates have been identified in both cases by synchrotron/neutron diffraction for different oxygen doping.

We will present here the installation of long range oxygen ordering achieved at ambient temperature in different oxides via oxygen intercalation. The degree of structural complexity yields in certain cases giant superstructures especially found for the $(\text{Nd/Pr})_2\text{NiO}_{4+\delta}$ systems. Exploring structural changes as a function of the charge transfer obtained *in situ* by synchrotron diffraction on single crystals during electrochemical oxidation, allowed to explore the complete phase diagram of $\text{Pr}_2\text{NiO}_{4+\delta}$. From MD simulations we recently explored the oxygen diffusion pathways down to ambient temperature, confirming the strong structural correlations to be induced by high oxygen mobility at low T [4]. The evolution of structural complexity as a function of δ and T will be discussed.

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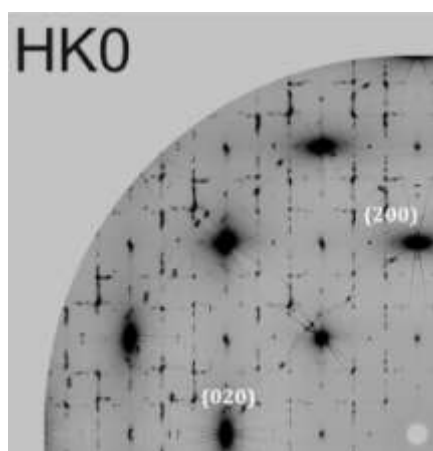


Figure 1:

(hk0)-plane of $\text{Pr}_2\text{NiO}_{4+\delta}$ showing strong basic reflections and weak reflections related to oxygen. The very weak reflections in case of $\text{Pr}_2\text{NiO}_{4+\delta}$ are related to charge ordering.

Towards Critical Current by Design



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Keywords: Vortex dynamics, Large-scale TDGL simulations, critical current, magnetoresistance

Understanding the dynamic behaviour of vortex matter in complicated pinning landscapes is a major challenge for both fundamental science and energy applications. In particular, optimizing type, size and density of pinning centers can significantly enhance the critical current. Based on the time-dependent Ginzburg-Landau equation, we developed a numerical approach towards finding these optimal pinning configurations.

Performing large-scale simulations of the vortex dynamics [1,2], we analyzed a number of different inclusion types and found optimal pinning configurations corresponding to the largest critical current in the geometries under consideration. In particular, we studied the interplay between vortex-vortex and vortex-inclusion interactions in a system including nanorod and columnar defects. This system represents a superconducting tape irradiated by heavy ions at an angle (see Fig. 1). Our simulation results agree with several experimental results and predict how the observed critical current could be further increased.

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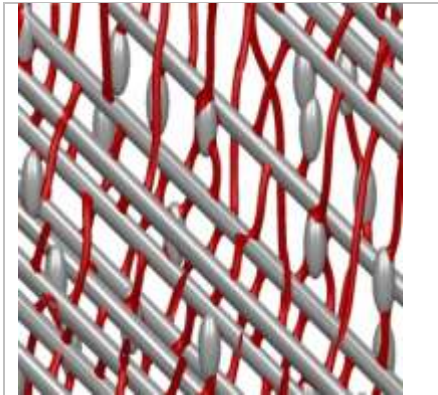


Figure 1: Vortex lines (red) pinned on an array of nanorods and columnar defects oriented at 45° with respect to the nanorod orientation.

CHAPTER 3

SESSION 16

Orbitronics - optical control and electrical readout of coherent orbital states in a solid

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Recent experiments [1,2] to examine the optical (THz) control and electrical readout of coherent orbital superpositions for phosphorous defects in both bulk silicon and silicon-based metal-oxide field effect transistors are described.

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Pinning Stripes in $\text{La}_{2-x}(\text{Ba,Sr})_x\text{CuO}_4$



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Keywords : stripes, cuprates, superconductivity, pinning

Studies of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ (LBCO) have provided evidence for the intertwining of antiferromagnetic, charge, and superconducting orders, especially in the form of the pair-density-wave (PDW) state [1]. For example, inelastic neutron scattering (INS) measurements on LBCO with $x = 0.095$ with $T_c = 32$ K have demonstrated the absence of the spin gap or spin resonance common to the cuprates with uniform d-wave superconductivity, thus suggesting, instead, the presence of PDW superconductivity [2]. The stripe order in LBCO is generally detected only in the structural phases in which there are two inequivalent oxygen sites within the CuO_2 planes. Hence it is of interest to better understand the features that lead to this inequivalency. Recently, an INS study has detected the fluctuations of CuO_6 octahedral tilts directly associated with the inequivalent oxygen sites [3]. At higher temperatures, the entropy associated with these octahedral tilts favors a state in which the tilts remain dynamic, resulting in a structure with equivalent in-plane oxygen sites. When the tilts develop a static component, stripes can be pinned.

The observation of charge stripe order in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) [4,5] has seemed to challenge this scenario, as the average structure presumably has no distinct in-plane O sites. This has motivated a new study of the structure and dynamics of LSCO. INS measurements on a crystal with $x = 0.07$ and $T_c = 20$ K have detected, for the first time, octahedral tilt fluctuations associated with inequivalent oxygen sites [6]. From the temperature dependence of the intensity of the tilt fluctuations, it is possible to infer that there is some freezing in of inequivalent oxygen sites below ~ 100 K. Freezing of incommensurate antiferromagnetic spin correlations is observed below T_c . These results indicate that there is some consistency in the occurrence of stripe order in LSCO and LBCO.

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Electron and hole pockets in charge-ordered phase of underdoped $\text{YBa}_2\text{Cu}_3\text{O}_y$

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Keywords: cuprates – energy spectrum – charge ordering

The energy spectrum of underdoped cuprates consists of the hole-like excitations seen by ARPES on the so-called “Fermi arcs” (FAs) and of the small electronic pocket (*e*-pocket) first visualized via observation of quantum oscillations (QOs) in the underdoped YBCO [1]. The X-rays experiments [2] revealed recently the tendency there to charge ordering (CO). As the *e*-pocket is directly accessible only via the low-temperature QOs, the popular view is that the latter emerges in the process of reconstruction of Fermi surface (FS) in some CO transition with a bi-directional structural vector $Q=(Q_x, Q_y)$.

Another slow QOs branch was found in the CO phase of YBCO in more recent experiments [3] and was attributed to small pockets of holes (*h*-pockets). The disappearance of QOs in the *c*-axis magneto-resistance upon increase of temperature towards the CO transition indicates that the *h*-pockets are indeed inherent in the CO state [3].

We argue that FS reconstruction scenario can be applicable only with regard to formation of small *h*-pockets. The QOs leave undefined positions of all pockets in the Brillouin zone (BZ). However below temperature T_{CO} of the CO transition with a bi-directional structural vector $Q=(Q_x, Q_y)$ the *e*-pocket is expected to form on FS in the vicinity of nodal point. As onset of superconductivity (SC) is known to remove CO, such pocket would not persist down to low temperatures, in the direct contradiction with observation of the residual linear in temperature electronic contribution into the specific heat in the SC phase [4].

Whether the charge density wave (CDW) structural vector in YBCO is uniaxial or biaxial remains unresolved experimentally. We argue that appearance of new QOs [3] in the CO phase is consistent with the uniaxial CDW vector Q_0 rotating between the neighboring CuO_2 -planes by ninety degrees.

Origination of *h*-pockets at CO onset is shown in Fig. 1. Four FAs in the tetragonal BZ are shown by thick red lines. The left arcs are also drawn being shifted to the right at interaction with a CDW potential with the uniaxial vector $Q=(Q_x, 0)$. *A*, *A'* and *A*, *A'* are the ending points of arcs; dashed lines show locus of the ‘bare’ FS “buried” under the pseudogaps seen in ARPES along the antinodal direction. The points *B* and *B* corresponding to FAs crossing are singular: in their vicinity two branches of the initial spectrum become split in the CO transition. Below T_{CO} the nearby spectrum becomes gapped and *h*-pockets (pink color) may form in two areas of a triangular shape each via

potentials owed to the new gaps at B , B and that of the large pseudogaps along the ‘bare’ FS at A , A' and A , A' . (Outside that region scattering of the FAs excitations on CDW fluctuations is strong smearing this branch of spectrum at low temperatures [5, 6]. The e -pocket is at the Γ -point and is shown as a grey circle).

In summary, we conclude that the CO parameter with the uniaxial vector Q alternating between the adjusting CuO_2 -planes suggests a plausible interpretation of the low frequency QOs in terms of h -pockets in the CO phase of YBCO [3].

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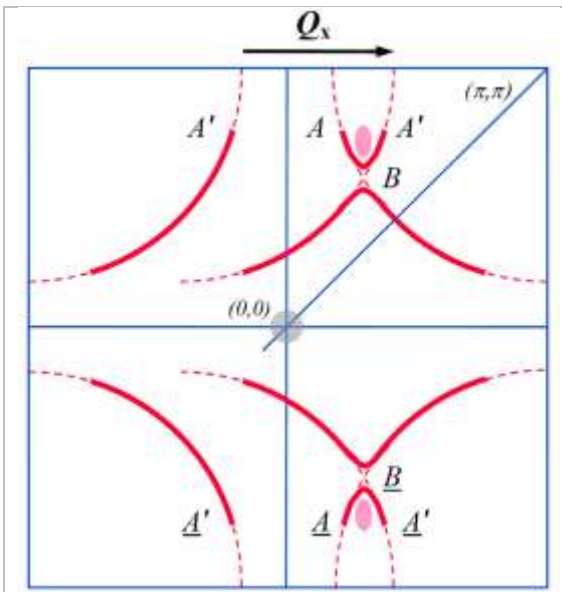


Figure 1. Origination of h -pockets at CO onset. See text for the details.

Understanding the evolution of spin and charge excitations in the cuprates



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Keywords : mechanisms for high T_c ; charge and spin excitations; resonant inelastic x-ray scattering

How coherent quasiparticles emerge by doping quantum antiferromagnets is a key question in correlated electron systems, whose resolution is needed to elucidate the phase diagram of copper oxides. Recent resonant inelastic X-ray scattering (RIXS) experiments in hole-doped cuprates have purported to measure high-energy collective spin excitations that persist well into the overdoped regime and bear a striking resemblance to those found in the parent compound, challenging the perception that spin excitations should weaken with doping and have a diminishing effect on superconductivity. Here we show that RIXS at the Cu L3-edge indeed provides access to the spin dynamical structure factor once one considers the full influence of light polarization. Further we demonstrate that high-energy spin excitations do not correlate with the doping dependence of T_c , while low-energy excitations depend sensitively on doping and show ferromagnetic correlations. This suggests that high-energy spin excitations are marginal to pairing in cuprate superconductors.

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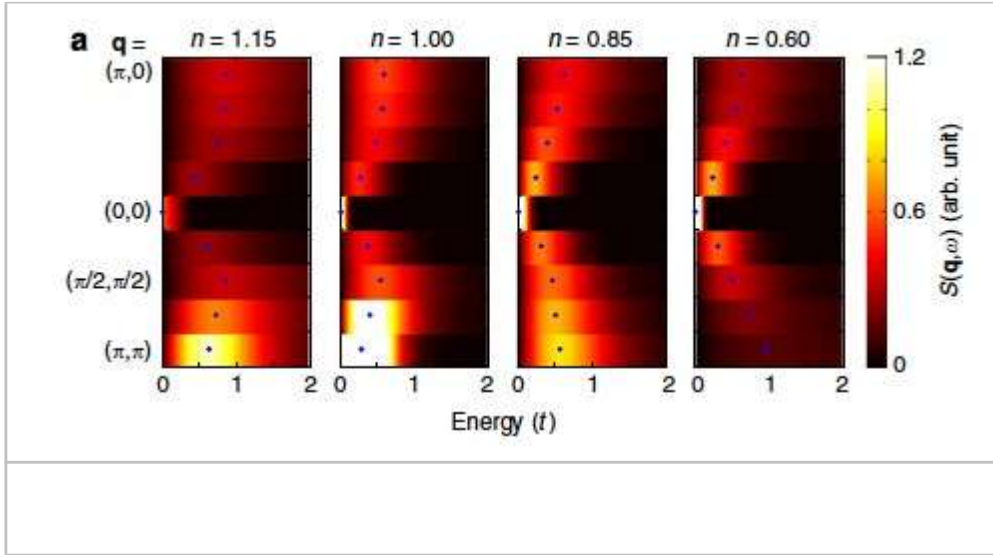


Figure 1: The spin dynamical structure factor $S(q, \omega)$ calculated using DQMC for the Hubbard model. False colour plots of the spectra along high symmetry directions in the Brillouin zone for different electron concentrations n .

Shape resonance near neck disrupting Lifshitz transitions in iron-based superconductors



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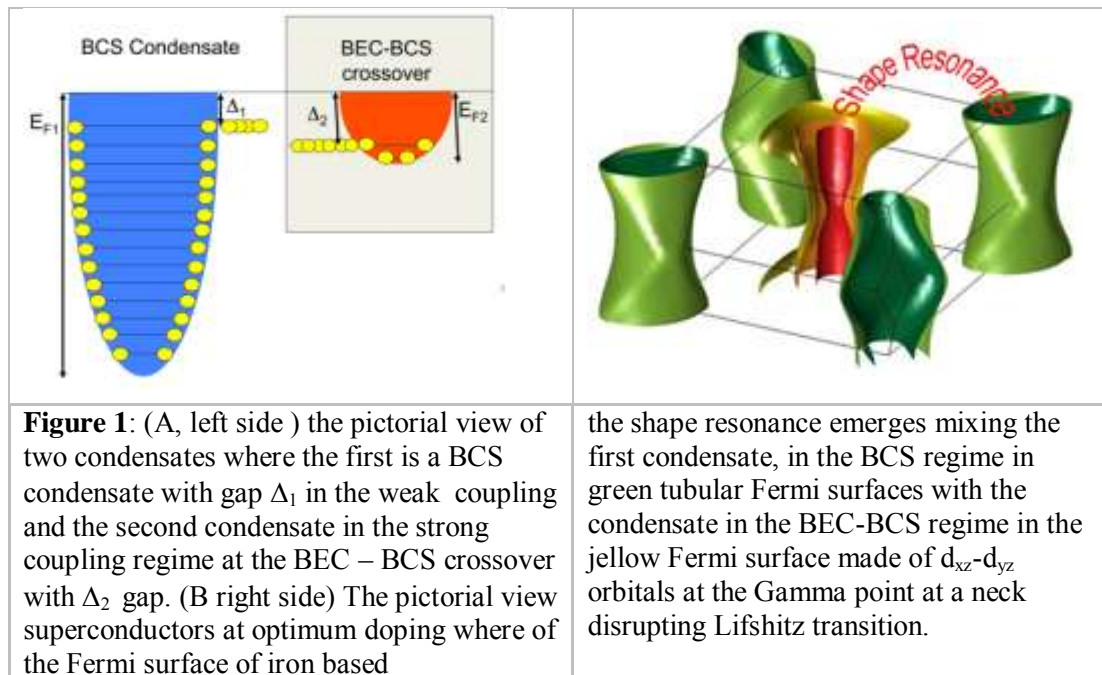
Keywords: shape resonance between superconducting condensates; neck disrupting Lifshitz transitions;

The *superstripes* phase [1,2] is defined as a particular phase of a many body quantum system where the spontaneous breaking of translational symmetry takes place below a critical temperature T^* and coexists with the spontaneous breaking of gauge symmetry breaking below T_c [1-3]. The search for high temperature superconductivity in particular *superstripes* phases has opened a new paradigm alternative the common accepted paradigm where the spontaneous breaking of translational symmetry suppresses the spontaneous breaking of gauge symmetry. In 2000 the *superstripes* name was coined to indicate that high temperature superconductivity with a nanoscale coherence length emerges in superstripes phases characterized by nanoscale phase separation. In this complex phase: lattice, charge, orbital striped CDW due to extrinsic effects (like misfit strain [4,5] and/or dopants self organization [6]), CDW nano-puddles due to intrinsic effects [6,7] (due to electron-electron and/or electron-phonon interactions) and SDW due to magnetic interactions form complex networks of multiple components where nano-puddles coexist with percolating networks of superconducting domains with a scale free distribution ranging from a smaller size as short as the superconducting coherence length [8].

The complex percolating network of superconducting units [8] is made of a low dimensional superconducting phase where two superconducting condensates coexist and are interacting via the pair transfer exchange-like interaction. In this talk we show that high temperature superconductors discovered so far are in a the universal regime described in Fig. 1 where multiple Fermi surface spots host a Fermi liquid condensing in a BCS regime while there is a hot spot in the k -space with a minority of charges in the strong coupling regime forming a condensate in the BEC-BCS regime. We show that in iron based superconductors the hot spot is made by a band of d_{xz} , d_{yz} orbital symmetry at a neck disrupting Lifshitz phase transition [9-15] as in cuprates and diborides [16]

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SESSION 17

Evidence for *s*- and *d*-wave pairing instabilities in Fe-based superconductors



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Keywords: coupling mechanisms in Fe-based superconductors – light scattering – spin fluctuations

In the iron-based systems spin, orbital or charge fluctuations may contribute to Cooper pairing. For clarification the electronic Raman effect of optimally doped $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ was studied in detail. Experimental results and an analysis of the spectra will be presented. [1,2] The analysis is based on LDA band structure calculations and the subsequent derivation of effective non-resonant Raman vertices. Experimentally a narrow, emergent mode appears in the B_{1g} ($d_{x^2-y^2}$) Raman spectra only below T_c , well into the superconducting state and at an energy below twice the energy gap on the electron Fermi surface sheets. The Raman spectra can be reproduced quantitatively with estimates for the magnitude and momentum space structure of the *s* pairing gap on different Fermi surface sheets, as well as the identification of the emergent sharp feature as a Bardasis-Schrieffer exciton, formed as a Cooper pair bound state in a subdominant $d_{x^2-y^2}$ channel. The physics is similar to that of an exciton in a semiconductor and is shown schematically in Fig. 1. The binding energy of the exciton relative to the gap edge shows that the coupling strength in this subdominant $d_{x^2-y^2}$ channel is as strong as 60% of that in the dominant *s* channel. This result suggests that the transition temperature in $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ is reduced since the $d_{x^2-y^2}$ potential breaks pairs in the *s* ground state. This effect may explain the further reduction of T_c on the overdoped side if, as expected theoretically, the relative strength of

the s channel continues to decrease. In Fe-based superconductors which lack central hole bands $d_{x^2-y^2}$ would then become the dominant pairing symmetry and, since a competing state is missing, T_c may increase again as indeed observed in the chalcogenides. This scenario is a strong case for spin-fluctuation induced superconductivity in the Fe-based superconductors. In addition, this experiment and the analysis mark the first clear manifestation of the Bardasis-Schrieffer mode predicted in 1961 [3].

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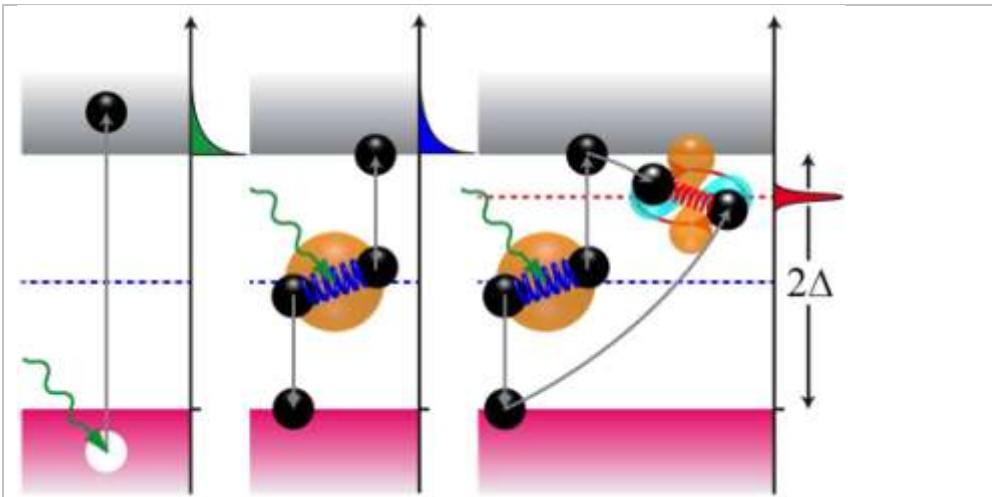


Figure 1: Schematic view of (left) gap excitations, (middle) pair breaking and (right) final state interaction in superconductors. In a light (green wiggly line) scattering experiment excitations across the gap and Cooper pair breaking add constructively leading to a square-root singularity at the gap edge in clean weakly coupled systems. The two partners of a Cooper pair can reform and build an exciton-like state with internal angular momentum. The binding energy of the exciton (red spring) is usually weaker than that in the ground state (blue spring).

Electrodynamic response in the electronic nematic phase of BaFe_2As_2



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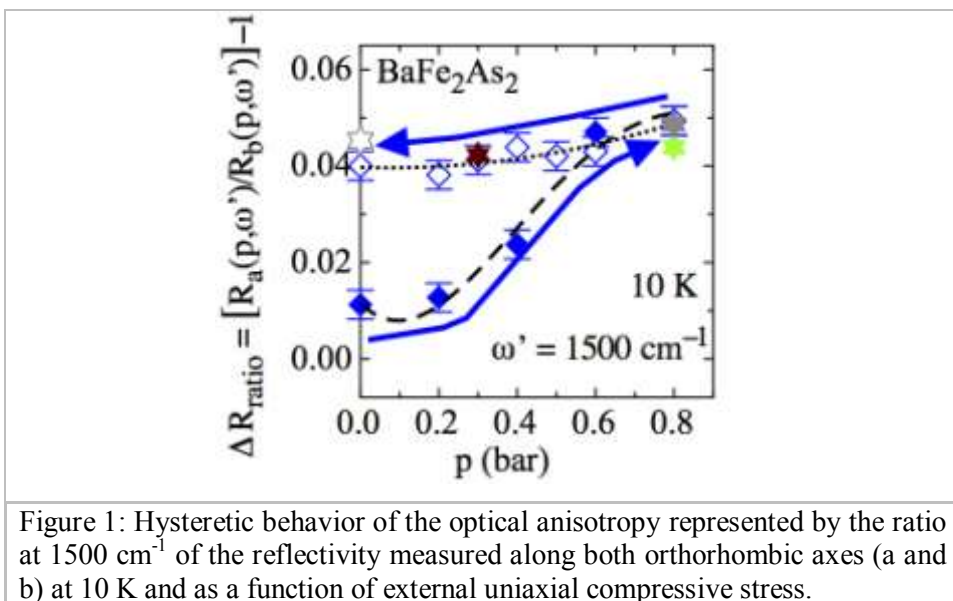
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Keywords: iron-pnictides, nematic phase, optical properties

We measure the in-plane optical reflectivity of BaFe_2As_2 beyond the MIR interval, studied so far, covering the spectral range from the far infrared (FIR) to the ultraviolet (UV), at several combinations of pressure, used to detwin the specimen, and temperature. Our goal is to probe the anisotropic response in the real part of the optical conductivity $\sigma_1(\omega)$, extracted from the reflectivity data via Kramers-Kronig transformations. We thus elucidate how the anisotropic optical metallic response evolves as a function of pressure, considered as an external symmetry breaking field, and across the ferro-elastic structural transition. At the center of our attention we then place the analysis of the spectral weight reshuffling over a large energy interval. We provide relevant information about the evolution of the effective metallic charge dynamics, upon tuning the degree of detwinning, in terms of scattering rate and plasma frequency of the itinerant charge carriers, which allows a direct link to the yet astonishing dc transport properties. We also reveal the pertinent energy scales of the title compound and we emphasize their implications with respect to the correlation effects shaping the nematic phase of BaFe_2As_2 [1,2].

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μ SR and infrared study of the spin reorientation transition and its reentrance below T_c in underdoped $\text{Ba}_{0.75}\text{K}_{0.25}\text{Fe}_2\text{As}_2$

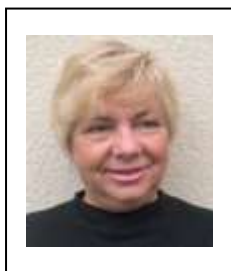
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In my talk, I will present a combined muon-spin-rotation (μ SR) and infrared spectroscopy study of the magnetic, electronic and structural properties of the pnictide superconductor $\text{Ba}_{0.75}\text{K}_{0.25}\text{Fe}_2\text{As}_2$. This underdoped sample exhibits a series of structural and magnetic transitions at $T^{\text{N1}} \approx 72\text{K}$, $T^{\text{N2}} \approx 32\text{K}$ and $T^{\text{N3}} \approx 18\text{K}$ and a superconducting onset at $T_c^{\text{ons}} \approx 28\text{K}$. Previous studies have shown that the first and the third structural and magnetic transitions yield into an orthorhombic and antiferromagnetic (o-AF) state with a stripe-like order and in-plane oriented spins. The second transition, however, involves a tetragonal structure and an antiferromagnetic (t-AF) state with the spins oriented along the c-axis. Our (μ SR) data establish the bulk nature of these transitions and they reveal characteristic changes of the magnitude and the orientation of the local field. I will show that these provide important clues about the so far unknown magnetic order of the t-AF state. The infrared data reveal that the spin density wave (SDW) in the t-AF state occupies a significantly larger part of the Fermi-surface than in the o-AF. The competition with superconductivity is therefore much more severe in the t-AF state. The reentrant transition into the o-AF at $T^{\text{N3}} \approx 18\text{K}$ is therefore most likely induced by superconductivity.

SESSION 18

Dynamical patterns of phase transformations from self-trapping of quantum excitons.



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Keywords: Pump induced phase transition, dynamical phase transition, neutral - ionic, excitons, charge transfer, dimerization

Phase transformations induced by short optical pulses is a new mainstream in studies of cooperative electronic states. We present a semi-phenomenological modelling of spacio-temporal effects expected when optical excitons are coupled to a symmetry breaking order parameter as it happens in organic compounds with neutral-ionic phase transitions. In our scenario, after a short initial pulse of photons, a quasi-condensate of excitons appears as a macroscopic quantum state which then evolves interacting with other degrees of freedom prone to instability. This coupling leads to self-trapping of excitons akin to self-focusing in optics. The locally enhanced density of excitons can surpass a critical value to trigger the phase transformation, even if the mean density is below the required threshold. The system is stratified in domains which evolve through dynamical phase transitions and may persist even after the initiating excitons have recombined. We recover dynamic interplays of fields such as the excitons' wave function, electronic charge transfer and polarization, spontaneous lattice dimerization [1,2].

A conceptual complication appears when both the excitation and the long range ordering are built from the intermolecular electronic transfer, like for the charge-transfer exciton in neutral-ionic systems [3, 4]. To describe both thermodynamic and dynamic effects on the same root we adopt for the phase transition a view of the Excitonic Insulator. This concept was put forward in 1960's as a hypothetical phase of a semiconductor which appears if the total energy of an exciton becomes negative. We call for the possible dynamic realization of this once exotic conjecture in circumstances of fast optical pumping.

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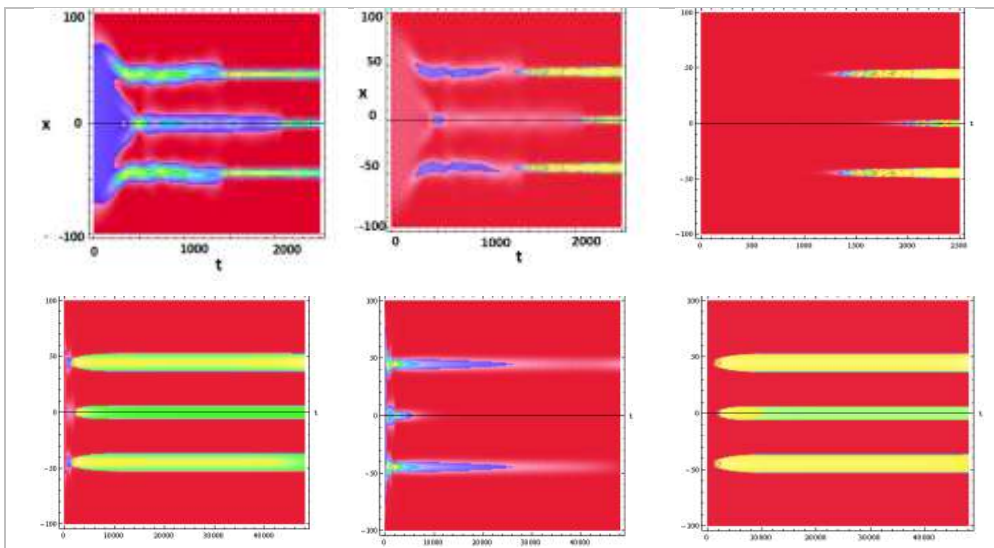


Figure 1: Emergence and subsequent time evolution of three domains of the ionic phase after a subcritical pumping. Upper and lower rows of panels show the processes at short and long times correspondingly. The columns show: the electron charge transfer (left), the excitons' wave function density (center), the spontaneous lattice dimerizations (right).

Nonlinear response of CDW ordered materials

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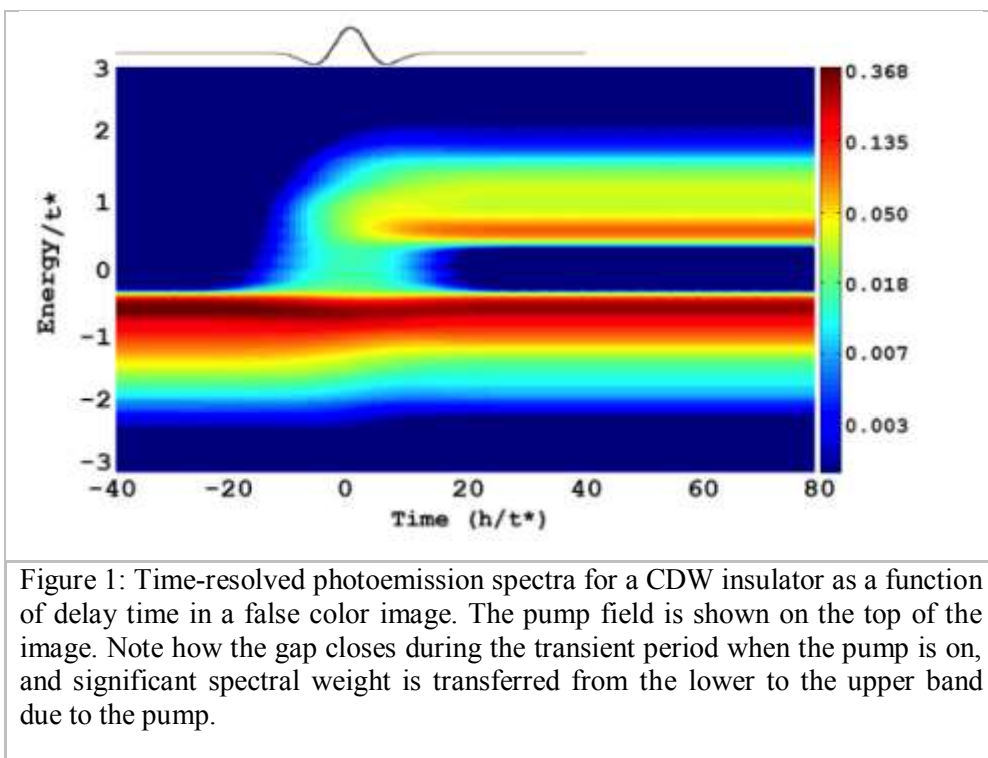
Keywords: Pump-probe photoemission, quantum excitation, charge density wave

In this work, we solve the simplest model for a CDW insulator placed into a time-dependent electric field. We examine the time-resolved photoemission spectroscopy which shows the transient closing of a gap (Figure 1.) during the time when the pump is present. We compare the results for this simple model with experiment, and discuss some modifications one expects to see as the model is made more complex to include electron-electron interactions and to include phonons. This work has been published in Ref. [1].

We also discuss the quantum excitation process, where electrons are excited from the lower to the upper band, as a function of the pump pulse amplitude and frequency. Summarizing the results as an excitation spectroscopy plot, we can see complex behavior which evolves from the quantum excitation depending primarily on the frequency of the driving pulse, to a process where nonlinear multiphoton excitations can be seen, to depending solely on the amplitude of the pulse, and then finally going into a new high amplitude regime, which has complex quantum oscillations. The physics behind this shows the evolution from energy-dependent quantum absorption to amplitude-dependent quantum absorption, the latter being a truly nonlinear quantum process. This work has been published in Ref. [2].

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Snapshots of the retarded interaction of charge carriers with ultrafast fluctuations in cuprates



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Keywords: electron-boson coupling, cuprates, non-equilibrium spectroscopy

One of the pivotal questions in the physics of high-temperature superconductors is whether the low-energy dynamics of the charge carriers is mediated by bosons with a characteristic timescale. This issue has remained elusive as electronic correlations are expected to greatly accelerate the electron–boson scattering processes, confining them to the very femtosecond timescale that is hard to access even with state-of-the-art ultrafast techniques. Here we simultaneously push the time resolution and frequency range of transient reflectivity measurements up to an unprecedented level, enabling us to directly observe the ~ 16 fs build-up of the effective electron–boson interaction in hole-doped copper oxides. This extremely fast timescale is in agreement with numerical calculations based on the t – J model and the repulsive Hubbard model, in which the relaxation of the photo-excited charges is achieved via inelastic scattering with short-range antiferromagnetic excitations.

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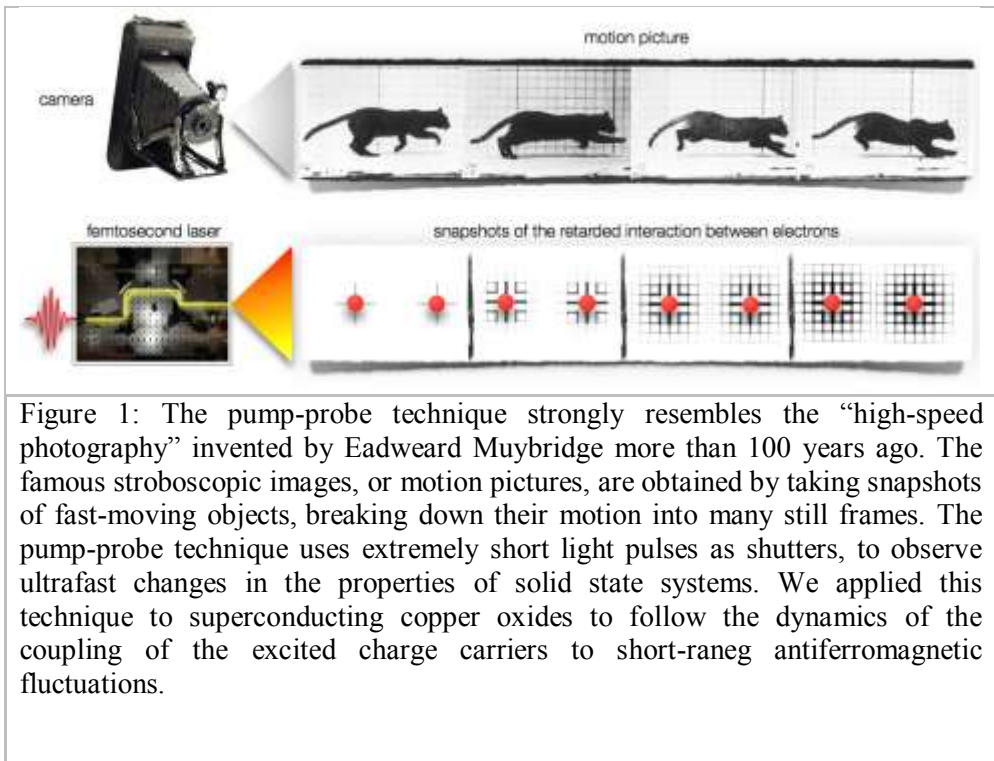


Figure 1: The pump-probe technique strongly resembles the “high-speed photography” invented by Eadweard Muybridge more than 100 years ago. The famous stroboscopic images, or motion pictures, are obtained by taking snapshots of fast-moving objects, breaking down their motion into many still frames. The pump-probe technique uses extremely short light pulses as shutters, to observe ultrafast changes in the properties of solid state systems. We applied this technique to superconducting copper oxides to follow the dynamics of the coupling of the excited charge carriers to short-range antiferromagnetic fluctuations.

Photo-induced charge ordering in strongly correlated oxydes



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Keywords: Charge ordering, orbital ordering, magnetism

Strong on-site Coulomb repulsions govern the physics of several complex oxydes. In particular, multiferroic materials, high-temperature superconductors, charge and orbitally ordered insulators among others, belong this family of compounds. Spectroscopically, valuable information comes from the quantification of the coupling parameters between low-energy excitations, such as phonons or spin-waves, and the high energy charge-transfer or Mott-Hubbard electronic states. Here we will present the results of our recent studies on high-temperature superconductors and insulating magnetic oxydes in which information on such a coupling is obtained via the Impulsive Stimulated Raman Scattering mechanism. The resonance between the many-body ground state responsible for the electronic properties of these materials, and the Charge-Transfer or Mott gap will be discussed. Furthermore, evidence for an out of equilibrium charge ordered state will be presented in few prototypical materials.

SESSION 19

Femtosecond dynamics of quantum many-body systems coupled to bosonic degrees of freedom



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Keywords: ultrafast dynamics – relaxation channels – antiferromagnetic spin excitations – phonon excitations

The substantial increase of the time-resolution and versatility of ultrafast techniques is paving the way to directly access the timescale of the fastest electron scattering processes in correlated materials. We made a joint experimental/theoretical effort to measure and model the ultrafast dynamics of photo-excited holes with the surrounding short-range antiferromagnetic background in doped cuprates on their relevant timescale (≈ 10 fs), that has been hitherto inaccessible [1]. This allows us to address one of the pivotal questions in the physics of high-temperature superconductors, i.e., whether the low-energy dynamics of the charge carriers is mediated by bosons with a characteristic timescale.

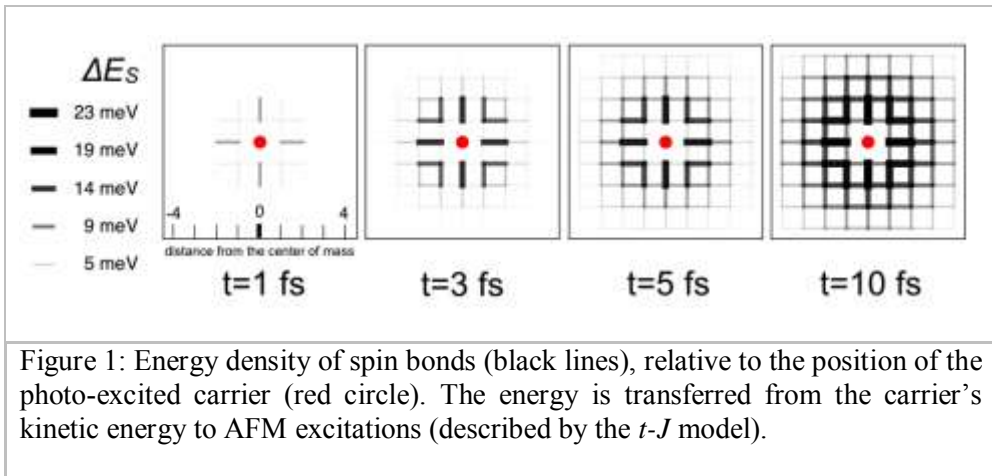
Our aim is to gain fundamental insight into the microscopic processes responsible for the ultrafast relaxation process of the photo-excited charge carriers. We apply state of the art numerical simulations within the out-of-equilibrium t-J model [2] and the Holstein model [3], which allow us to describe relaxation of the excess energy (stored initially in the form of highly-excited carriers) to antiferromagnetic (AFM) spin excitations and phonon excitations, respectively.

To understand the role of phonons and AFM excitations in non-equilibrium systems in more detail [4], the main theoretical questions that motivate our investigation are: (i) How efficient is the energy transfer to phonons/AFM excitations, depending on the characteristic energy scales of the electrons and phonons and the electron-phonon coupling strength? (ii) What is the relevant time scale for the energy transfer to phonons/AFM excitations? (iii) To which extent is the knowledge of the unitary time evolution required to describe the dynamics of a quantum many-body system, or in which cases are semi-classical approaches sufficient?

In the context of optimally doped cuprates, we show that the key relaxation mechanism at very short times corresponds to the creation of high-energy antiferromagnetic excitations in the close proximity of the photo-excited holes [1]. Such a mechanism enables an energy transfer of more than 1 eV on a 10 femtosecond time scale, see Fig. 1.

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Ultra-fast magnetic dynamics in Sr_2IrO_4



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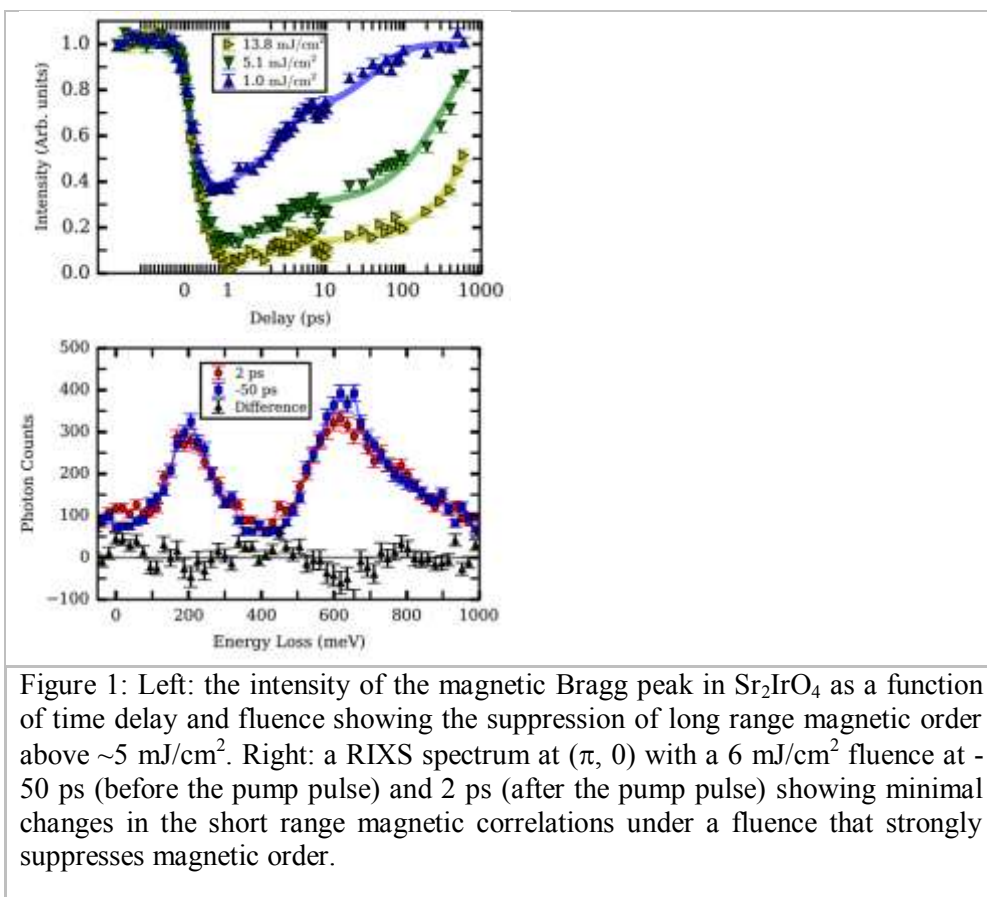
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Keywords : Iridates, ultra-fast, magnetic correlations, x-rays, resonant scattering

Despite growing interest in ultra-fast science, our ability to probe non-equilibrium magnetic states is typically limited to observing the presence or absence of long-range magnetic order. In the case where long-range magnetic order has been destroyed, it is usually impossible to determine whether the state one has created has a random spin configuration or whether short-range magnetic correlations persist. Here we study magnetism in Sr_2IrO_4 using a mid infrared ultrafast pump to excite carriers across the Mott gap. Ir L_3 edge resonant elastic x-ray scattering results, plotted in Figure 1, demonstrate that long-range magnetic order is destroyed in less than 300 fs and that long-range magnetic order only recovers on a timescale of several hundred ps. We then performed the first ever Ir L_3 edge time resolved resonant inelastic x-ray scattering experiment to probe the magnetic correlations after long-range magnetic order has been destroyed. Measurements at the Brillouin zone boundary $(\pi,0)$, plotted in Figure 1, show that the nearest neighbor magnetic correlations persist, despite the lack of long-range magnetic order. In contrast the magnetic correlations at (π,π) near the in-plane antiferromagnetic ordering wavevector, are modified in the magnetically melted state.

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The temporal evolution of carrier localisation, metastable state relaxation and symmetry breaking in complex materials.



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Keywords: time-resolved dynamics of complex materials -nanoscale phase separation - mechanisms for high T_c – quenched disorder – quantum devices - CDW

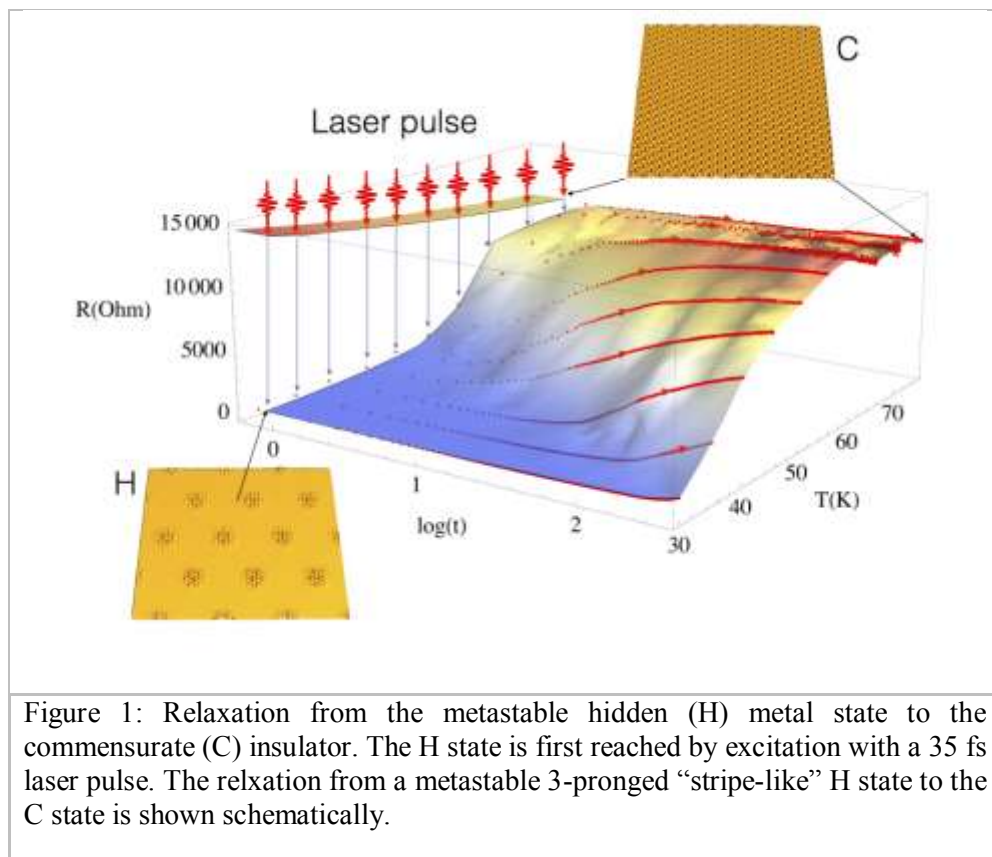
In complex materials where competing orders are present, non-equilibrium experiments can reveal the hierarchy of interactions that eventually determine the dominant order[1]. The pursuit of such non-equilibrium phenomena also reveals new states of matter[2], which cannot be reached under equilibrium conditions. In complex systems, such as cuprate superconductors and the currently fashionable layered chalcogenide systems, particularly strain and Coulomb interactions conspire to give different kinds of broken symmetry states. Here we compare the metastable polaronic states in TaS₂ [2,3] with cuprate superconductors[1], to find remarkable similarities in stripe formation and metastability phenomena associated with glassy relaxation dynamics[4] (Fig.1). Considering how superficially different these materials are, the similarity in their respective phenomenologies reveals an unexpected universality of the underlying mechanism for the formation of broken symmetry states in these materials.

Apart from fundamental significance, electrical pulse[3] and strain control[5] of the insulator-metal transition in these materials promises practical applications for ultrafast nonvolatile memories, offering superior performance to current memristors and chalcogenide phase change devices.

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Light induced meltdown of quasiparticles in high temperature superconductors

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By using high resolution *time*- and angle- resolved photoemission spectroscopy (tr-ARPES) we directly probe collective dynamics after optical excitation of an high temperature superconductor and study their influence on quasiparticles dynamics, electron-boson interaction, Cooper pair formation, superconducting gap and other competing orders. We observed that only quasiparticles beyond a particular boson mode respond to the pump laser excitations, while the others remain untouched and that the entire decay is governed by two different time scale. These processes are strongly momentum dependent with a sharp transition inside and outside the Fermi arc. These results point to a new dichotomy between the ultrafast gap and quasiparticles response within and beyond the Fermi arc and reveal a new window into the nature of the pairing interaction in high T_c superconductors.

Complex gap structures determined by time resolved spontaneous Raman scattering

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Keywords : mechanisms for high T_c – time resolved spontaneous Raman – 2 gaps

Raman scattering is sensitive to the so-called pair-breaking peak. In this process cooper pairs of the superconducting condensate are being broken up with a characteristic energy scale of 2Δ , where Δ represents the superconducting order parameter.[1] Since Raman scattering allows to probe different regions of the Brillouin Zone, it was being utilized as quasi phase-sensitive measurement technique in order to address the d-wave symmetry of the gap in superconductors. In steady-state measurements a couple of studies did show unusual behavior with doping and temperature revealing pseudo gap phases and information on a critical crossover for slightly overdoped materials.[1] By performing resonance Raman studies we did reveal the complex structure of the gap feature by tuning the incidence photon energy into different bands.[2] This was later confirmed by stimulated Raman scattering techniques.[3] However, in these measurements it is difficult to discriminate simple matrix element related resonance effects that occur upon tuning the incident photon energies from an intrinsic multi-gap feature as part of the electronic susceptibility.

In order to address this question we have performed time resolved spontaneous Raman scattering experiments.[4] Upon pumping the superconductor with a pump beam, the superfluid density will be reduced due to an increased temperature after thermalization ($dt > 2$ ps). The superfluid density will be then reduced and is then compensated by an increase of single particle in-gap states. If there is more than one dominant coupling channel one would expect the recovery of the superfluid density on more than one time scale. If there is more then one gap in the superconducting state one might see the reaction of the superfluid density on two different time scales. Indeed Fig. 1 (a) shows the transient response of the superconducting pair breaking peak. After 1.65 ps a contribution to the pair-breaking peak with larger spectral moments at higher energies is suppressed. After 6.6 ps there is a stronger suppression below 400 cm^{-1} (50 meV) visible. Furthermore, there is a visible pile up of spectral weight in the in-gap region. After 16.5 ps the transient is mostly suppressed and the superconducting state has been nearly fully recovered. Fig. 1(b) shows the transient with high time resolution. The intensity changes in the gap region are color-coded as indicated. It becomes quite apparent that the superconducting response is dominated by two nearly independent responses. Firstly, at higher energies a fast suppression within the first 3 ps of the pair-breaking excitation with a dominant spectral response $> 50\text{ meV}$ is evident that is followed by a pile up of in gap states. And secondly a

more robust and delayed suppression at lower energies (< 50 meV) after 5-6 ps is visible that also contributes to the pile up of in-gap states. These decoupled responses are strongly suggesting two contributions to the gap. However, for an understanding of the second, delayed Raman response one would need to account explicitly for hole-spin interactions and for the inhomogeneous nature of the charge distribution.

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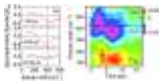


Figure 1: Time resolved spontaneous Raman scattering of B_{1g} (d-wave) symmetry of the gap and in-gap states. The pair-breaking excitation is suppressed by the pump, while in-gap states are being recovered as a result of a reduction of the superfluid density. Please note, that there are two distinct reactions of the pair breaking peak and two corresponding recoveries of in gap states strongly suggesting the presence of two distinct components to the pair breaking excitation.

SESSION 20

Charge ordered normal ground state and its interplay with superconductivity in the underdoped cuprates

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Keywords: quantum oscillations, high temperature superconductors, cuprate superconductors

Over the last few years, evidence has gradually built for a charge ordered normal ground state in the underdoped region of the cuprate high temperature superconductors. I will address the electronic structure of the normal ground state of the underdoped cuprates as accessed by quantum oscillations, and relate it to complementary measurements by other experimental techniques. The interplay of the charge ordered ground state with the antinodal gapped pseudogap state, and overarching magnetic and superconducting correlations will be further explored.

Anomalous Phonons and High Temperature Superconductivity in Copper Oxides



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Keywords : electron-phonon coupling – cuprates – charge fluctuations

It is well known that electron-phonon coupling is responsible for superconductivity in conventional superconductors, but the prevailing view is that it is not important in high temperature superconductivity. Yet, evidence that electron-phonon coupling is very strong for certain phonons in the copper oxides has been building. In particular, Cu-O bond-stretching phonons at 65-85 meV in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ are known to show anomalously large broadening and softening near the reduced wavevector $q=(0.3,0,0)$. [1]

Recently we systematically investigated spectral functions of these phonons by inelastic neutron and x-ray scattering and measured dispersions of electrons to which these phonons should be coupled by angle resolved photoemission (ARPES). [2] These electronic dispersions have kinks around 70 meV that are typically attributed to coupling of electrons to a bosonic mode (which could be a phonon) that mediates superconductivity. Remarkably, we found that the kinks remain strong in the heavily overdoped region of the doping phase diagram of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, even when the superconductivity completely disappears. [2]

We also found that doping dependence of the magnitude of the giant phonon anomaly is very different from that of the ARPES kink, i.e., the two phenomena are not connected. [3] In fact while the Cu-O bond stretching phonons show giant electron-phonon effects, there are no features in the electronic dispersions in the same samples that can be attributed to these phonons.

We show that these results provide indirect evidence that the phonon anomaly originates from novel collective charge excitations as opposed to interactions with electron-hole pairs. Their amplitude follows the superconducting dome so these charge modes may be important for superconductivity. The mechanism of the relationship to superconductivity is unclear, but a similar phonon anomaly in $\text{YBa}_2\text{Cu}_3\text{O}_7$, becomes greatly enhanced in the superconducting state. I will also discuss a possible relationship of phonon anomalies to dynamic charge stripes, whose spectrum we observed for the first time in nickelates. [4]

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Charge Order from Orbital-dependent Coupling Evidenced by NbSe₂



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Keywords : CDW – electron-phonon coupling – orbital dependence

Niobium diselenide has long served as a prototype of two-dimensional charge ordering, believed to arise from an instability of the electronic structure analogous to the one-dimensional Peierls mechanism. Despite this, various anomalous properties have recently been identified experimentally which cannot be explained by Peierls-like weak-coupling theories. Here, we consider instead a model with strong electron-phonon coupling, taking into account both the full momentum and orbital dependence of the coupling matrix elements [1]. We show that both are necessary for a consistent description of the full range of experimental observations. We argue that NbSe₂ is typical in this sense, and that any charge-ordered material in more than one dimension will generically be shaped by the momentum and orbital dependence of its electron-phonon coupling as well as its electronic structure. The consequences will be observable in many charge-ordered materials, including cuprate superconductors.

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SESSION 21

Superconductivity and Unusual Magnetic Behavior in Amorphous Carbon



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Keynotes: High T_c , amorphous carbon, peculiar magnetic behavior

Traces of superconductivity (SC) at elevated temperatures (up to 65 K) were observed by magnetic measurements in three different inhomogeneous sulfur doped amorphous carbon (a-C) systems: (a) in commercial and (b) synthesized powders and (c) in a-C thin films. (a) Studies performed on commercial (a-C) powder which contains 0.21% of sulfur, revealed traces of non-percolated superconducting phases below $T_c = 65$ K (Fig. 1). The SC volume fraction is enhanced by the sulfur doping. (b) a-C powder obtained by pyrolytic decomposition of sucrose did not show any sign for SC above 5 K. This powder was mixed with sulfur and synthesized at 400 °C (a-CS). The inhomogeneous products obtained, show traces of SC phases at $T_c = 17$ and 42 K. (c) Non-superconducting composite a-C-W thin films were grown by electron-beam induced deposition. SC emerged at $T_c = 34.4$ K only after heat treatment with sulfur. Other parts of the pyrolytic a-CS powder, show unusual magnetic features. (i) Pronounced irreversible peaks around 55-75 K appear in the first zero-field-cooled (ZFC) sweep only. Their origin is not known. (ii) Unexpectedly these peaks are totally suppressed in the second ZFC runs measured a few minutes later. (iii) Around the peak position the field-cooled (FC) curves cross the ZFC plots (ZFC > FC). These peculiar magnetic observations also ascribed to a-CS powder prepared from the commercial a-C powder and are connected to each other. All SC and magnetic phenomena observed are intrinsic properties of the sulfur doped a-C materials. It is proposed that the a-CS systems behave similarly to well-known high T_c cuprates and/or pnictides in which SC emerges from magnetic states.

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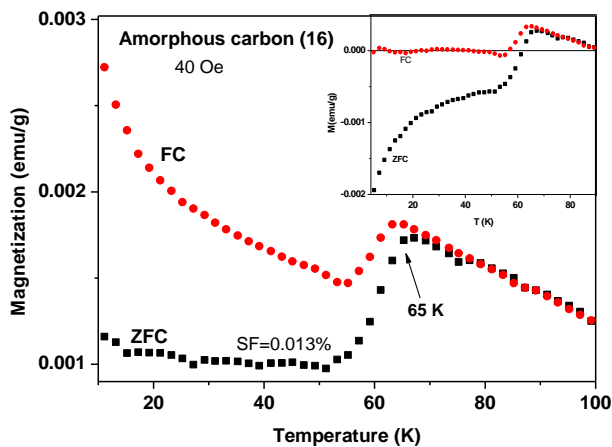


Fig. 1 : ZFC and FC magnetization plots of a-C. The inset shows the two curves after subtraction paramagnetic contributions.

Enhancement of Pressure on Novel Superconductivity

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High Pressure plays significant role in tuning superconductivity. Pressure can effectively modify spin, charge or orbital that in turn generate or optimize unconventional superconductivity. We will introduce our recent works of effects of pressures on variant of superconductors.

We thank our collaborators for their significant contributions.

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First-principles study on high T_c superconductivity in sulfur hydrides under high pressure



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Keywords: sulfur hydrides–density functional theory for superconductors–high pressure

The recent report of high superconducting transition temperature (T_c) up to 190K in H_2S under extremely high pressure ~ 200 GPa by Drozdov *et al.*[1] has stimulated a renewed interest in superconductivity in compounds comprising light elements. In fact, a variety of light-element systems have been studied as promising candidates for room-temperature superconductivity.

Especially, there are several theoretical predictions for high T_c superconductivity in sulfur hydrides. Li *et al.* [2] have performed a comprehensive study for H_2S and determined the most stable crystal structure for pressure up to 220GPa. They calculated T_c for the $P-1$ and $Cmca$ phase using the Allen-Dynes modified McMillan equation with the empirical Coulomb parameter $\mu^*=0.13$. They found that the maximum T_c is ~ 80 K at 160GPa. On the other hand, Duan *et al.* [3] studied metallization and superconductivity in $(H_2S)_2H_2$. They predicted that two metallic structures of H_3S with the $R3m$ and $Im-3m$ symmetries appear at 111 and 180 GPa, respectively. For these structures, T_c is evaluated to be 191K and 204K.

Since the band width of sulfur hydrides is generally very large [2,3,4], the Migdal approximation is expected to be valid. However, the validity of the choice of $\mu^*=0.13$ has not been examined. In Ref.[5], we recently performed a calculation based on density functional theory for superconductors [6,7] which is free from any empirical parameters such as μ^* .

The calculated T_c is plotted in Fig.1. We see that T_c s for H_3S with the $Im3m$ crystal structure are systematically higher than the experimental value. On the other hand, the experimental T_c s for the intermediate (high) pressure regime is similar to those for H_2S ($R3m$ - H_3S). This result suggests that there is another higher- T_c phase under higher pressure. We also performed a calculation with deuterium to estimate the isotope effect coefficient α . While large α remains a mystery in this system [8], we found that α can be larger than the conventional value (0.5) when multiple structural phases energetically compete and coexist.

This work was done in collaboration with R. Akashi (Univ. Tokyo), M. Kawamura (Univ. Tokyo), S. Tsuneyuki (Univ. Tokyo and ISSP) and Y. Nomura (Univ. Tokyo and RIKEN).

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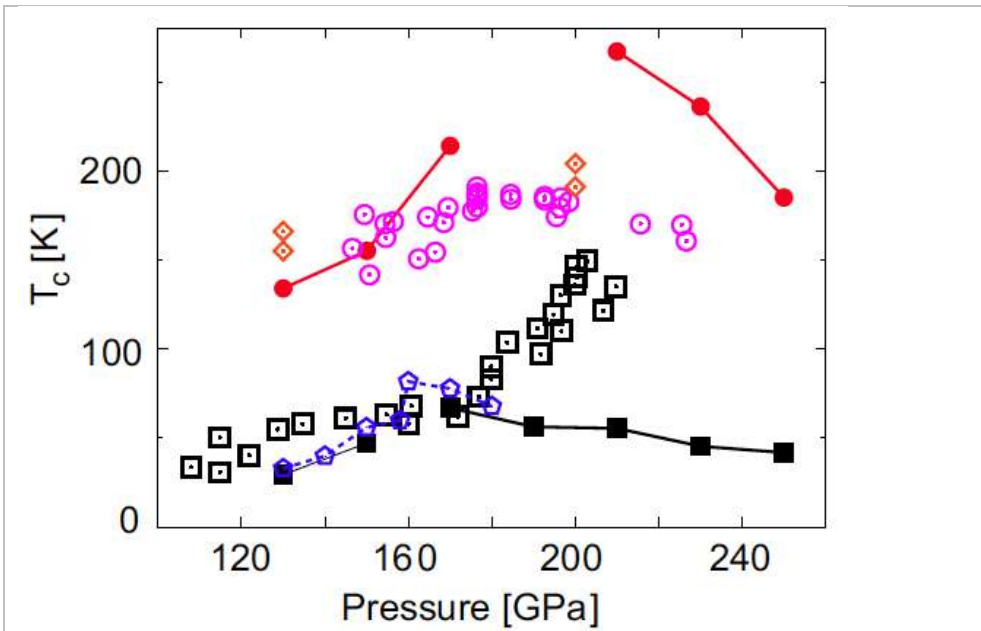


Figure 1: T_c obtained by the present SCDFT calculation for H_2S (solid circle) and H_3S (solid circle), together with the experimental values (open circle and square). Open pentagon and diamond denote the results based on the modified McMillan formula in Ref.2 and 3.

Emergence of high- T_c superconducting phase in $(\text{NH}_3)_y\text{M}_x\text{FeSe}$ and carbon-based superconductors under high pressure



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Keywords: iron chalcogenides, metal intercalation, pressure dependence of superconductivity, double-dome superconductivity, carbon-based materials, aromatic superconductors

The pressure dependence of the superconducting transition temperature (T_c) and unit-cell volume of $(\text{NH}_3)_y\text{Cs}_{0.4}\text{FeSe}$ was investigated in a wide pressure range of 0 to 41 GPa. The T_c decreases with increasing pressure up to 13 GPa, which can be related to the decreased c (or the decreased FeSe layer spacing), implying that a decrease in two-dimensionality lowers the T_c . In other words, an increase in Fermi nesting caused by the increase in two-dimensionality leads to the increase in spin fluctuation to strengthen the pairing interaction. The superconductivity was never observed down to 4.3 K at 11 GPa. When further increasing pressure, the superconductivity re-emerged above 13 GPa, with the T_c reaching 49 K at 21 GPa. The emergence of a new superconducting phase is not accompanied by a structural transition, as verified by pressure-dependent XRD. The T_c slowly decreased with increasing pressure above 21 GPa, and no superconductivity was observed at temperatures above 4.9 K at 41 GPa. The observation of a double-dome superconducting phase may provide a hint for clarifying the superconducting mechanism.

Metal intercalation to graphite provided various types of superconductors. The highest onset superconducting transition temperature, T_c^{onset} ($= 11.5$ K), was found in Ca intercalated graphite, which is expressed as 'CaC₆'. The T_c^{onset} increases up to 15.1 K at 7.5 GPa, implying a positive pressure dependence of superconductivity. However, no new metal intercalated graphite superconductors have recently been reported. In this study,

$\text{Ca}_x\text{K}_{1-x}\text{C}_y$'s have been successfully synthesized, and its structure was assigned to 'KC₈' type. The T_c increased continuously with increasing x . Furthermore, the pressure dependence of T_c in $\text{Ca}_{0.6}\text{K}_{0.4}\text{C}_8$ was investigated in a wide pressure range of 0 to 41 GPa. The superconducting phase of potassium (K) doped picene ($\text{K}_{3.0}\text{picene}$) solid has been prepared using an annealing technique, showing the T_c as high as 14 K at 0 GPa. The shielding fraction of the sample was 5.4%. We investigated the pressure dependence of T_c of the 14 K phases in $\text{K}_{3.0}\text{picene}$. The T_c of 14 K phase showed the positive pressure dependence, *i.e.*, the T_c linearly increased up to 1.1 GPa, and the dT_c / dp was evaluated to be 4.9 K GPa⁻¹. The maximum T_c realized was 18 K at 1.1 GPa. The maximum value of shielding fraction reached 18% at ~1 GPa. The positive pressure dependence of T_c in the 14 K phase of K_3picene suggests the unconventional superconductivity.

SESSION 22

Extremely high upper-critical fields in Pd based chalcogenide superconductors



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Keywords: multi-band superconductivity – galvanometric effects – penetration depth

Here, we will discuss the overall physical properties of the new Pd based chalcogenide superconductors. Recently, we reported the discovery of superconductivity in a new transition metal-chalcogenide compound, i.e. Nb₂Pd_{0.81}S₅, [1] with a transition temperature $T_c > 6.6$ K. Despite its relatively low T_c , Nb₂Pd_{0.81}S₅ is found to display remarkably high and anisotropic superconducting upper critical fields, e.g. $\mu_0 H_{c2}(T \rightarrow 0 \text{ K}) \cong 37 \text{ T}$ for fields applied along the crystallographic b -axis. For a field applied perpendicularly to the b -axis, $\mu_0 H_{c2}$ shows a linear dependence in temperature which coupled to a temperature-dependent anisotropy of the upper critical fields, suggests that Nb₂Pd_{0.81}S₅ is a multi-band superconductor. This is consistent with band structure calculations which reveal nearly cylindrical and quasi-one-dimensional Fermi surface sheets having hole and electron character, respectively. The static spin susceptibility, as calculated through the random phase approximation, reveals strong peaks suggesting proximity to a magnetic state and therefore the possibility of unconventional superconductivity. Subsequently, we reported the discovery of superconductivity in Nb₃Pd_xSe₇ [2] whose upper critical-field H_{c2}^b along the needle axis is observed to saturate at $H_{c2}^b(T \rightarrow 0 \text{ K}) \cong 14.1 \text{ T}$ which is $4.26 \times H_p$ with H_p being the Pauli-limiting field in the weak-coupling regime. The synthesis procedure also yields crystals belonging to the superconducting Nb₂Pd_xSe₅ phase. For both phases we find that superconductivity condenses out of an anomalous metallic state, i.e., displaying $\partial \rho / \partial T < 0$ above T_c , similarly to what is observed in the pseudogap phase of the underdoped cuprates. An anomalous metallic state, low-dimensionality, multiband character, extremely high and anisotropic H_{c2} 's would point to unconventional superconductivity. However after our initial publications Y. Lu et al. [3] reported the discovery of superconductivity in Ta₂Pd_xS₅, and attributed the very high upper critical fields to the absence of the paramagnetic pair-breaking effect due to the strong spin-orbit scattering associated with the Pd deficiencies embedded in the periodic lattice of heavy $5d$ Ta and $4d$ Pd. But a comparison [5] between the subsequently reported Ta₄Pd₃Te₁₆ [4] which is characterized by excess Pd, and Nb₃Pd_xSe₇ with $x \sim 0.75$ (see Fig. 1 below) suggests that instead t the

electronic anisotropy is the main parameter correlating with the extreme high upper critical fields observed in these materials, i.e. the higher the electronic anisotropy the higher the upper critical fields.

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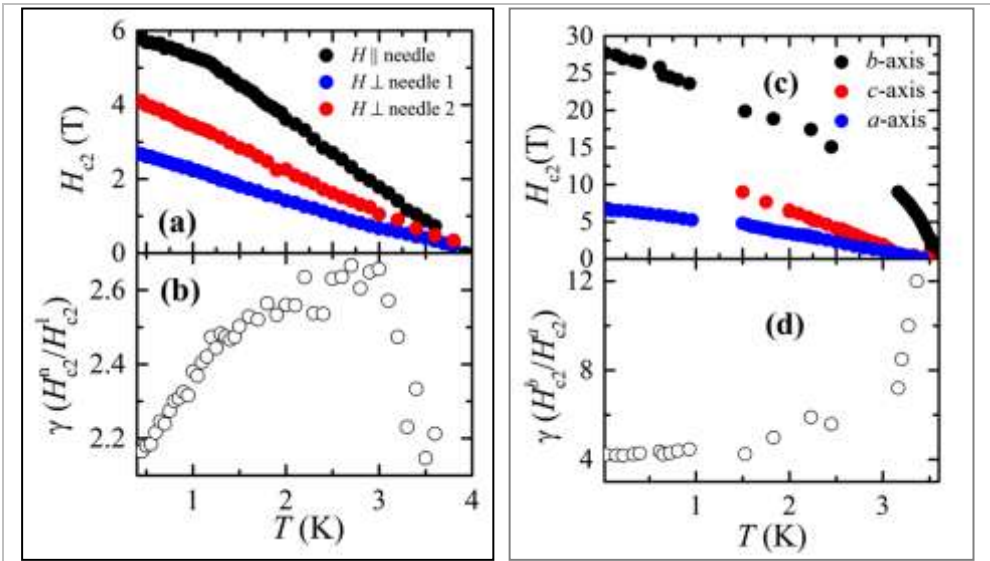


Figure 1. Left panel: (a) Upper critical field H_{c2} , for $\text{Ta}_4\text{Pd}_{3+x}\text{Te}_{16}$ single crystal for fields applied along all three crystallographic axes and as a function of the temperature T . (b) Anisotropy γ between the upper critical fields extracted for fields along the needle axis and the c -axis of the crystal. Right panel: (c) same as in (a) but for a $\text{Nb}_3\text{Pd}_x\text{Se}_7$ single crystal. (d) Same as in (b) but for a $\text{Nb}_3\text{Pd}_x\text{Se}_7$ single crystal.

Magnetic and charge responses of cuprates from the high-temperature limit



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Keywords : cuprates, magnetism, charge order

Magnetic responses at $T > T^*$ are considered in light of the fact that realistically parametrized tight-binding Fermi surfaces commonly predict incommensurate bare responses in the high-temperature (free) limit, while discommensuration is typically observed only at much lower temperatures $T_c < T < T^*$. If the Cu on-site repulsion is taken to infinity, the distinction so induced between the Cu and O orbitals persists to high temperature. The consequence is that a different bare susceptibility, which is always commensurate, becomes relevant for the high-temperature magnetic response. In this way a signature of strong correlations is found within a Fermi-liquid paradigm for the underdoped metal. Postulating a step-like pseudogap allows one to extend the high-temperature paradigm to the magnetic and charge responses of mercury cuprates below T^* . The difference between the hourglass (X) shaped and wine-glass (Y) shaped responses in the lanthanum and mercury cuprates can be traced to an interplay of strong coupling and Fermi surface properties.

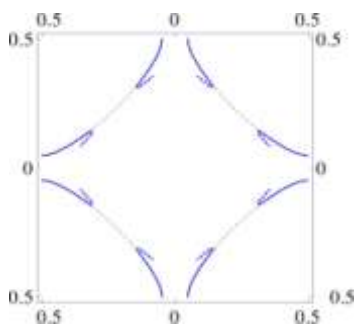


Figure 1: Example of unrealistic Fermi surface, predicted by a diagonal incommensurate bare response

Superconducting Properties and Pseudogap in the Triclinic (CaFe_{1-x}Pt_xAs)₁₀Pt₃As₈



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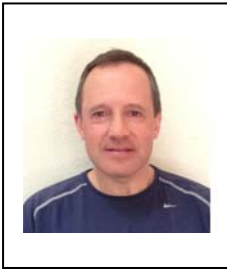
Keywords: iron-based superconductivity, pseudogap, preformed pairs

Using a combination of muon-spin relaxation (μ SR), inelastic neutron scattering (INS) and nuclear magnetic resonance (NMR), we investigated the novel iron-based superconductor with a triclinic crystal structure (CaFe_{1-x}Pt_xAs)₁₀Pt₃As₈ ($T_c = 13$ K), containing platinum-arsenide intermediary layers [1]. The temperature dependence of the superfluid density obtained from the μ SR relaxation-rate measurements indicates the presence of two superconducting gaps, $\Delta_1 \gg \Delta_2$. According to our INS measurements, commensurate spin fluctuations are centered at the $(\pi, 0)$ wave vector, like in most other iron arsenides. Their intensity remains unchanged across T_c , indicating the absence of a spin resonance typical for many Fe-based superconductors. Instead, we observed a peak in the spin-excitation spectrum around $\hbar\omega_0 = 7$ meV at the same wave vector, which persists above T_c and is characterized by the ratio $\hbar\omega_0/k_B T_c \approx 6.2$, which is significantly higher than typical values for the magnetic resonant modes in iron pnictides (~ 4.3). The temperature dependence of magnetic intensity at 7 meV revealed an anomaly around $T^* = 45$ K related to the disappearance of this new mode. A suppression of the spin-lattice relaxation rate, $1/T_1 T$, observed by NMR immediately below T^* without any notable subsequent anomaly at T_c , indicates that T^* could mark the onset of a pseudogap in (CaFe_{1-x}Pt_xAs)₁₀Pt₃As₈, which is likely associated with the emergence of preformed Cooper pairs.

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Nonlinear Goldstone modes and Higgs mechanism chiral helical states



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Keywords: helical states, Goldstone modes, Higgs mechanism

General symmetry arguments dictate that at scales longer than the pitch, the low-energy theory of a chiral nematic liquid crystal (cholesteric) and of a Dzyaloshinskii- Morya (DM) spiral state in a helimagnet (e.g., MnSi, FeGe) is identical to that of a smectic liquid crystal, thereby inheriting its rich phenomenology. Starting with a chiral free-energy (exchange and DM interactions of a helimagnet) we present a transparent derivation of the fully nonlinear Goldstone mode theory, which involves an analog of the Anderson-Higgs mechanism that locks the spiral orthonormal (director/magnetic moment) frame to helical layers. This shows explicitly the reduction of three orientational modes of the state down to a single phonon Goldstone mode that emerges on scales longer than the pitch.

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BCS-BEC crossover physics in iron-based superconductors

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SESSION 23

Tuning superconducting state properties of $\text{FeTe}_{1-x}\text{Se}_x$ and $\text{Rb}_x\text{Fe}_{2-y}\text{Se}_2$: Impact of crystal growth conditions and thermal treatment on mesoscopic phase separation

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The issues concerning the nature and the role of magnetic inhomogeneities in the iron chalcogenide system $\text{FeTe}_{1-x}\text{Se}_x$ and their correlation with superconductivity in this system are addressed. Obtained results suggest that nonhomogeneous distribution of host atoms might be an intrinsic feature of superconducting Fe-Te-Se chalcogenides and a surprising correlation indicating that faster grown crystal of inferior crystallographic properties is a better superconductor is found.

An extended study of the superconducting and normal-state properties of various as-grown and post-annealed $\text{Rb}_x\text{Fe}_{2-y}\text{Se}_2$ single crystals is presented. Magnetization experiments evidence that annealing of $\text{Rb}_x\text{Fe}_{2-y}\text{Se}_2$ at temperature well below the temperature of the onset of phase separation, T_p , neither changes the magnetic nor the superconducting properties of the crystals. In addition, annealing at temperature well above T_p suppresses the superconducting transition temperature T_c and leads to an increase of the antiferromagnetic susceptibility accompanied by the creation of ferromagnetic impurity phases, which are developing with annealing time. However, annealing at $T \approx T_p$ increases T_c , sharpens the superconducting transition, increases the lower critical field, and strengthens the screening efficiency of the applied magnetic field. This suggests that the microstructure of the sample, caused by mesoscopic phase separation, is modified by annealing just at T_p , leading to an improvement of the superconducting properties of $\text{Rb}_x\text{Fe}_{2-y}\text{Se}_2$ and an enhancement of T_c .

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High-Pressure Growth of Solid-State Materials



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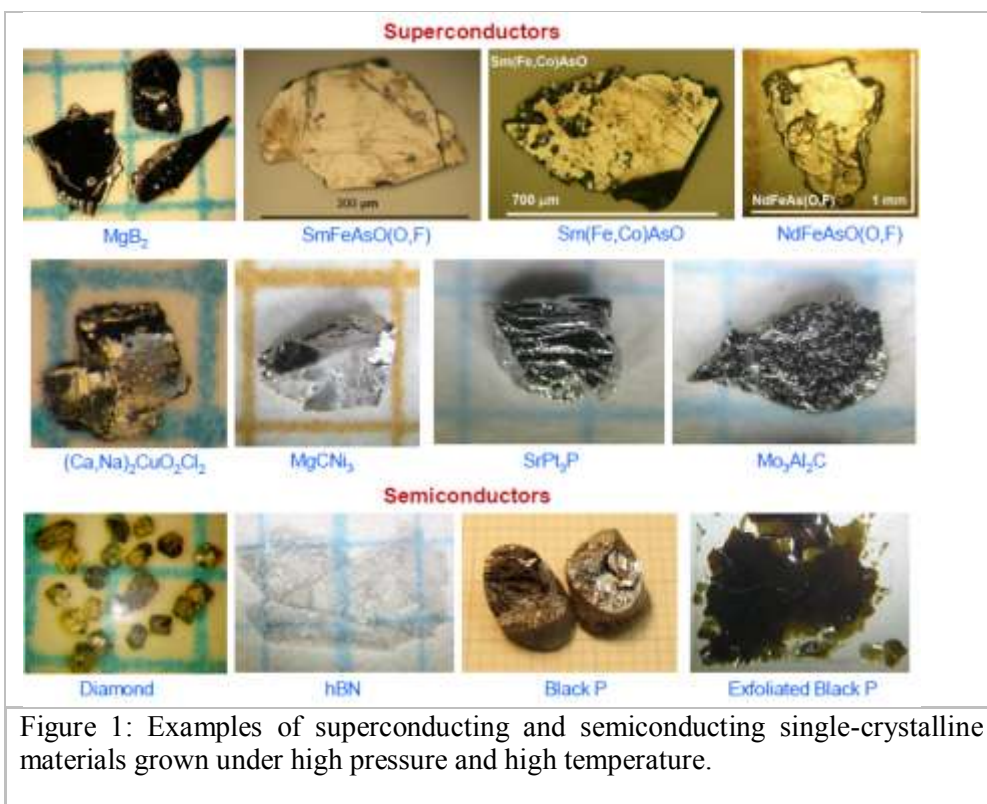
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Keywords: crystals – superconductors – 2D semiconductors

High-pressure conditions are often crucial for the successful synthesis of new materials, including many new modern superconductors and semiconductors. After a short introduction to the technical aspects and the role of high-pressure, high-temperature method in inorganic synthesis, several examples will be presented, including our most recent results (Fig. 1). First, we explore the high-pressure phase diagram of the *Mg-B-N system*, where we discovered the simultaneous growth of completely different types of crystals: a two-band superconductor MgB_2 and a wide-band semiconductor $h\text{BN}$ [1]. Besides the interesting physics, both these materials hold great potential for practical applications. Next, we highlight the critical role played by extreme conditions in the growth of *Fe-based superconductors*, where a systematic evaluation of the composition-structural relations is vital for understanding the microscopic physics. The availability of sizable, high-quality LnFePnO (*Ln*: lanthanide, *Pn*: pnictogen) single crystals with substitution of O by F or H, Sm by Th, Fe by Co, and As by P, allowed us to measure the intrinsic and the direction-dependent superconducting properties, such as H_{c2} , J_c , and their anisotropies [2-5]. In SmFeAs(O,F) we discovered a distinct change in the nature of the vortices: from well-pinned slow-moving Abrikosov-like to weakly-pinned fast-flowing Josephson-like [6]. This transition reflects a delicate balance between key material properties, such as the coherence length perpendicular to the layers and the interlayer separation. In addition, we detected also the sudden appearance of an oscillatory component of the critical current $J_c(H)$ in the hybrid vortex region [7]. Finally, we demonstrate the beneficial role of the high-pressure, high-temperature conditions in exploring the crystal growth of various intermetallic superconductors, such as MgCNi_3 [8], $\text{Mo}_3\text{Al}_2\text{C}$, SrPt_3P [9] and 2D van der Waals semiconductors ($h\text{BN}$, black P). Based on single-crystalline data we determine the underlying correlations and the general trends between composition, structure, and properties in these materials.

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Recent progress on single crystal growth and the study using magnetotransport measurements for trilayer Bi-2223



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Keywords: high- T_c cuprates, Bi-2223, single crystal, TSFZ method, superconductive fluctuation, magnetoresistance, coherence length, superfluid density

In high- T_c cuprates, it is empirically known that their T_c increases on increasing the number of CuO_2 planes in a unit cell, n , from $n = 1$ to $n = 3$. However, T_c slightly decreases for $n \geq 4$ [1]. The microscopic mechanism underlying this behavior is still in dispute. The trilayer cuprate superconductor $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+\delta}$ (Bi-2223: $n = 3$) is a suitable material for such investigations because it is now available in a single-crystal form [2].

Here, we report on the in-plane resistive transition measurements for variously doping-controlled Bi-2223, as well as bilayer $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (Bi-2212: $n = 2$), under various magnetic fields, \mathbf{B} , parallel to the c -axis, ($\mathbf{B} \parallel \mathbf{c}$) [3]. The data are analyzed using the superconducting-fluctuation-renormalized Ginzburg-Landau (GL) theory developed by Ikeda, Ohmi, and Tsuneto (IOT theory) [4]. Subsequent analysis enables us to estimate superconducting parameters such as the in-plane coherence length ξ_{ab} and the superfluid density ρ_s ($\propto 1/\lambda_L^2$: λ_L is the London penetration depth).

Fig. 1 shows the results [3]. The T_c value scales with neither $1/\xi_{ab}$ nor $1/\lambda_L^2$. For example, Bi-2223 sample (3UD90) has much smaller $1/\lambda_L^2$ (i.e., phase stiffness ρ_s) and longer ξ_{ab} (i.e., smaller pairing strength) compared with those of Bi-2212 sample (2OPT89). However, the T_c values of both samples are almost the same. This fact suggests that sample 3UD90 acquires additional superconducting condensation energy compared to sample 2OPT89 from some source other than in-plane pairing strength (or ρ_s). We propose that one possible source is the interlayer tunneling mechanism [5].

Recently, much interests are concentrated on a heavily underdoped state, since antiferromagnetism and superconductivity have been found to coexist in a heavily underdoped single CuO_2 plane for multilayered ($n \geq 3$) cuprates [6]. Here, we also report on the first successful preparation of heavily underdoped Bi-2223 single crystal (zero-resistivity temperatures $\approx 20\sim 35$ K).

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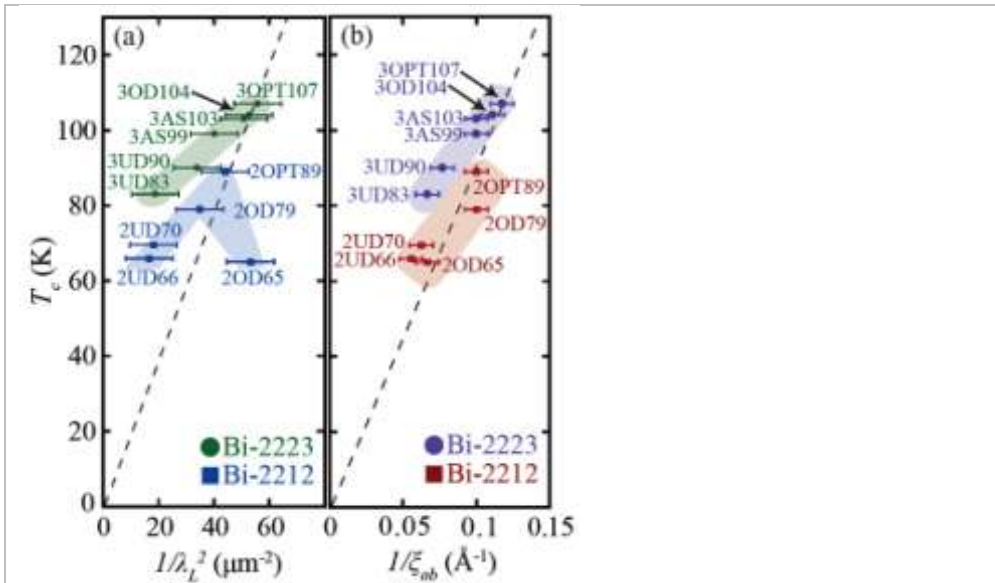


Figure 1: Relationship between superconducting parameters and T_c for Bi-2212 (solid squares) and Bi-2223 (solid circles) [3]. Plots of (a) T_c vs. $1/\lambda_L^2$ and (b) T_c vs. $1/\xi_{ab}$. The dashed lines in each figure represent the scaling relations between the superconducting parameters and T_c .

SESSION 24

Tunable charge and spin order in nickel oxide thin films and superlattices



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Keywords : Charge order – Spin density wave – nickelates

We have recently implemented a new method based on a simple confocal geometry to carry out Raman scattering measurements on very thin films of metal-oxides, whose Raman signal is usually hindered by the strong contribution coming from the substrate. I will discuss the power of this new approach to characterize collective electronic ordering phenomena in nickel-oxide thin films and superlattices [1-3], grown by pulsed laser deposition, on substrates that impose either compressive or tensile strain. More in detail, I will show that a combined analysis of Raman results, resistivity measurements and resonant elastic x-ray scattering data on PrNiO₃ (PNO) clarifies how both epitaxial strain and spatial confinement can be used as “knobs” to control charge [4] and spin [5] order in this system that lies on the verge of a Mott metal-insulator transition. The results directly confirm theoretical predictions for a spin density wave phase, with charge order as a secondary order parameter [6]. Moreover our findings open up new opportunities for device applications, including designs in which metallic antiferromagnets serve as active elements. In addition, our determination of the energies and symmetries of the Raman modes characteristic of charge ordering in PNO, as well as their dependence on strain and spatial confinement, provides specific input for models of charge order and electron-phonon interactions in the nickelates and related transition metal oxides.

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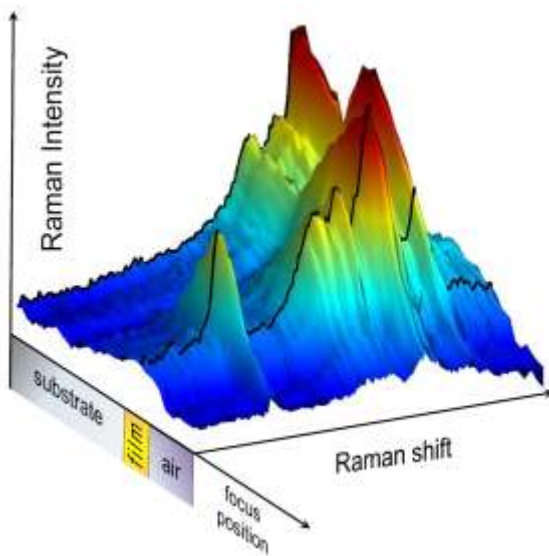


Figure 1: Confocal Raman signal as a function of focus position for a 12 nm PNO film under tensile strain. The PNO phonon modes are only observed within a narrow range when the focus point of the laser coincides with the film position. Some of the new modes observed are due to charge order.

The effects of impurities and disorder on the superconducting gap of Bi-based cuprate superconductors investigated by STM/STS



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Keywords : STM/STS, Bi2212, impurity effects

Recently, it was reported in La214 superconductors that the substitution of Fe for Cu pins down fluctuating stripes in the underdoped region and suppresses the superconductivity markedly [1]. In Bi-based cuprate superconductors, the checkerboard-like modulation of the LDOS develops in a wide doping range [2]. To investigate the Fe substitution effects on the LDOS modulation in the Bi-based cuprates, we performed STM/STS experiments on Fe doped and pure samples of Bi2212. The STS spectra in pure Bi2212 samples are relatively homogeneous and show a d-wave gap, while those in Fe-doped Bi2212 samples are inhomogeneous and the LDOS inside the gap is recovered to some extent although the gap width hardly changes. The LDOS modulation in Fe-doped samples is inhomogeneous and shows a slightly different period from that of pure samples. We will also report the effects of a disorder, the so-called A-site disorder, in Eu-Bi2201.

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Superconductivity and stripes in cuprate high temperature superconductors



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Keywords: mechanisms of high temperature superconductors – strongly correlated electrons – striped states – d-p model – 2D Hubbard model – charge-transfer insulator

It is important to understand the mechanism of high-temperature superconductivity. It is obvious that the interaction with large energy scale is responsible for high critical temperature T_c . The Coulomb interaction is one of candidates that bring about high-temperature superconductivity because its characteristic energy is of the order of eV. There have been many works for electronic models including the Hubbard model and three-band d-p model with the on-site Coulomb repulsion to investigate a possibility of high-temperature superconductivity. It is, of course, not trivial whether the on-site Coulomb interaction leads to a pairing interaction between two electrons. We argue that high-temperature superconductivity is possible in the strongly correlated region by using the variational Monte Carlo method for two-dimensional electronic models. We show the superconducting condensation Energy E_{cond} as a function of U in Fig.1. E_{cond} increases rapidly near $U \sim 8t$ as going into the strongly correlated region. E_{cond} is very small in the weakly correlated region for $U < 8t$ and almost vanishes for $t' = 0$. For such small value of E_{cond} , it is certainly hard to obtain a signal of superconductivity by means of numerical methods such as the quantum Monte Carlo method. It follows from Fig.1 that high temperature superconductivity is possible only in the strongly correlated region. In particular, $U/t \sim 10-14$ is favorable for superconductivity.

Material-parameter dependance in cuprates is important in the search of new superconductors. We also examine the ground state of the three-band d-p model that explicitly includes oxygen p orbitals. There is a strongly correlated region in the d-p model, where superconducting condensation energy is increase considerably, suggesting a possibility of high critical temperature.

The ground state is insulating when the on-site Coulomb repulsion U_d is large in the half-filled case. The ground state undergoes a transition from a metal to a Mott insulator when the level difference $\epsilon_p - \epsilon_d$ is increased.

In the underdoped region, the striped state is stabilized and coexists with superconductivity. In the light-doping region the diagonal striped state of bond-centered

type becomes more stable than the vertical stripe state when the doping hole density is as low as ~ 0.06 . We also show that there is a region where a checkerboard state, composed of 4×4 period checkerboard spin modulation, becomes stable.

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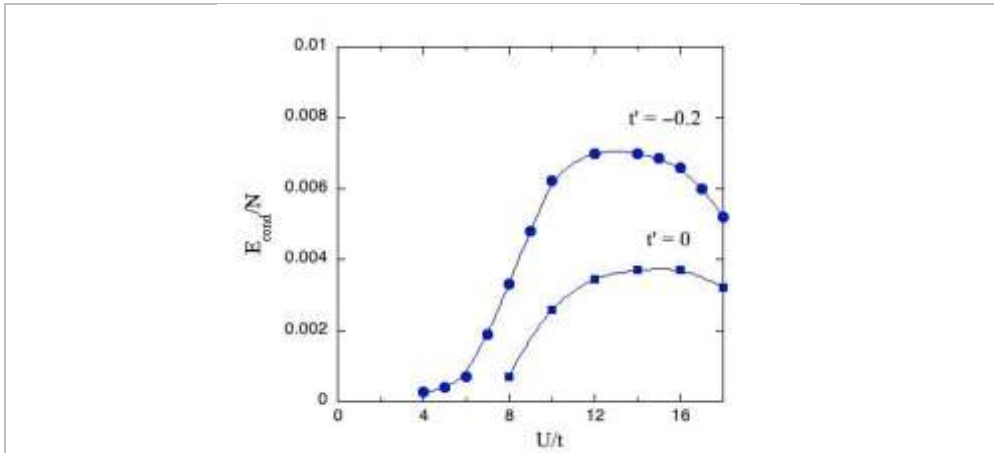


Figure 1: The superconducting condensation energy per site as a function of U in units of t for $t' = 0$ and $t' = -0.2$ on 10×10 lattice. The number of electrons is $N_e = 88$ for $t' = 0$ and $N_e = 84$ for $t' = -0.2$.

Orbital ordering, phase separation and high-pressure neutron scattering study of the iron based superconductors



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Keywords: orbital order, phase separation, Anderson localization, coexistence of superconductivity and antiferromagnetism.

Orbital ordering has been shown in our neutron scattering works on the 1111 [1], 122 [2], 11 [3] as well as the 245 [4] family of the Fe-based superconductors as the unifying mechanism of both the structural and antiferromagnetic transitions [5,6]. For the 245 superconductors, the phase diagram shows a complex phase-separation [7], see Figure 1. In particular, the phase-separation is rather predominant at room temperature in the mixed phase labeled by “Pmna+I4 m+(I4 mmm)” in Figure 1, which has also been observed in TEM [8] and scanning nanofocused x-ray diffraction studies [9], among others, on superconducting as well as insulating samples. A lack of an appropriate appreciation of the correct phase diagram, in particular, the mis-attributing all samples as the 245 phase due to the detection of the signal of the I4/m space group, has led to a lot of confusion in current study on the 245 superconductors. High pressure provides another dimension to the investigation [10]. By simultaneously measuring the Fe vacancy order and the antiferromagnetic order in a high-pressure neutron diffraction work, we demonstrate the concurrence of the vacancy and antiferromagnetic orders with the superconductivity [11], in contrary to the wide-spread *belief* that the 245 phase is irrelevant to the superconductivity [12].

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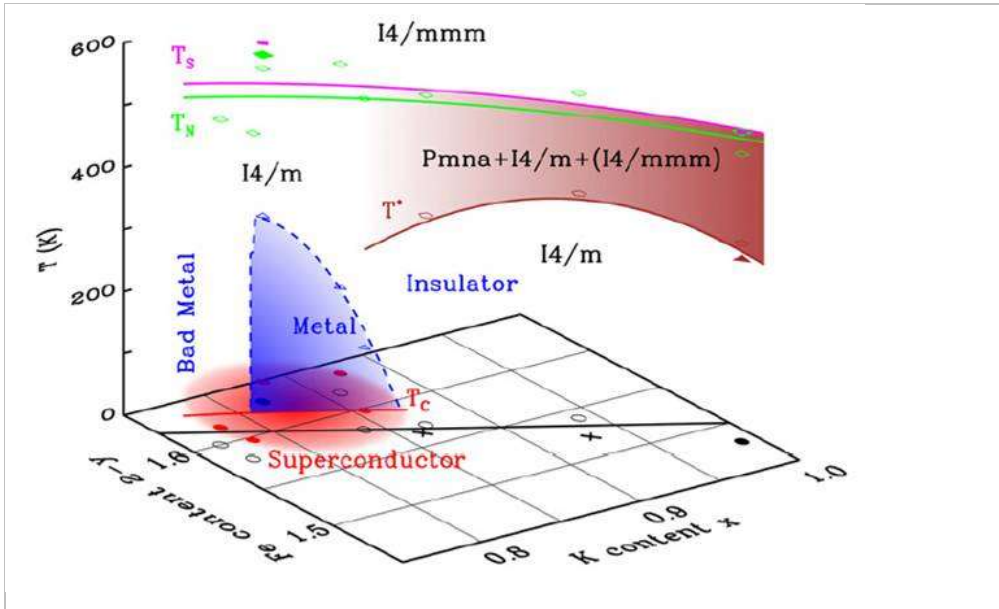


Figure 1: The phase diagram of the 245 superconductor $K_xFe_{2-y}Se_2$ [7]. In the $I4/mmm$ phase, Fe vacancy is randomly distributed. In the order-disorder transition at T_S , the Fe vacancy forms the $\sqrt{5} \times \sqrt{5}$ superlattice of space group $I4/m$ for samples in the neighborhood of $K_{0.8}Fe_{1.6}Se_2$, or $K_2Fe_4Se_5$ (245) on the left, and forms the orthorhombic superlattice of space group $Pmna$ and imperfect $\sqrt{5} \times \sqrt{5}$ superlattice of space group $I4/m$ together with the remnant disordered $I4/mmm$ phase on the right in the shaded phase-separation region. Below the T^* , these phases transform to the imperfect $\sqrt{5} \times \sqrt{5}$ Fe vacancy order in the insulating phase. The occupancy ratio of the Fe1/Fe2 sites measures the perfection of the $\sqrt{5} \times \sqrt{5}$ Fe vacancy order. When the ratio approaches zero, insulator-metal crossover occurs in the blue region, beneath which superconductivity occurs at T_C (red symbols). T_N (green symbols) marks the antiferromagnetic transition.

SESSION 25

Generalized BEC and crossover theories of superconductors and ultracold bosonic and fermionic gases



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Keywords: Cooper pairing, boson-fermion models, Bose-Einstein condensation, superconductors, BEC in ultracold quantum gases.

The generalized Bose-Einstein condensation (GBEC) formalism [1-4] of superconductivity hinges on three separate new ingredients: a) treatment of Cooper pairs as *actual* bosons, b) inclusion of two-hole (2h) pairs on an equal footing with two-electron (2e) ones, and c) inclusion in the resulting ternary ideal boson-fermion gas with boson-fermion vertex interactions that drive formation/disintegration boson processes. Besides subsuming both BCS and BEC theories as well as the well-known crossover picture [5] as special cases, the GBEC formalism leads to several-order-of-magnitude enhancements in the critical superconducting temperature T_c .

The crossover picture is applicable also to ultracold atomic clouds, of either bosonic or fermionic atoms. But known exact low-density expansions (about an ideal gas of the quantum particles) involving the interatomic scattering length diverge term-by-term around the so-called unitary zone about the Feshbach resonance. However, expanding in powers of the *attractive part* of the interatomic potential renders smooth, divergence-free low-density expansions (about an ideal gas of repulsive particles) whose convergence can be accelerated [6] with Padé approximants.

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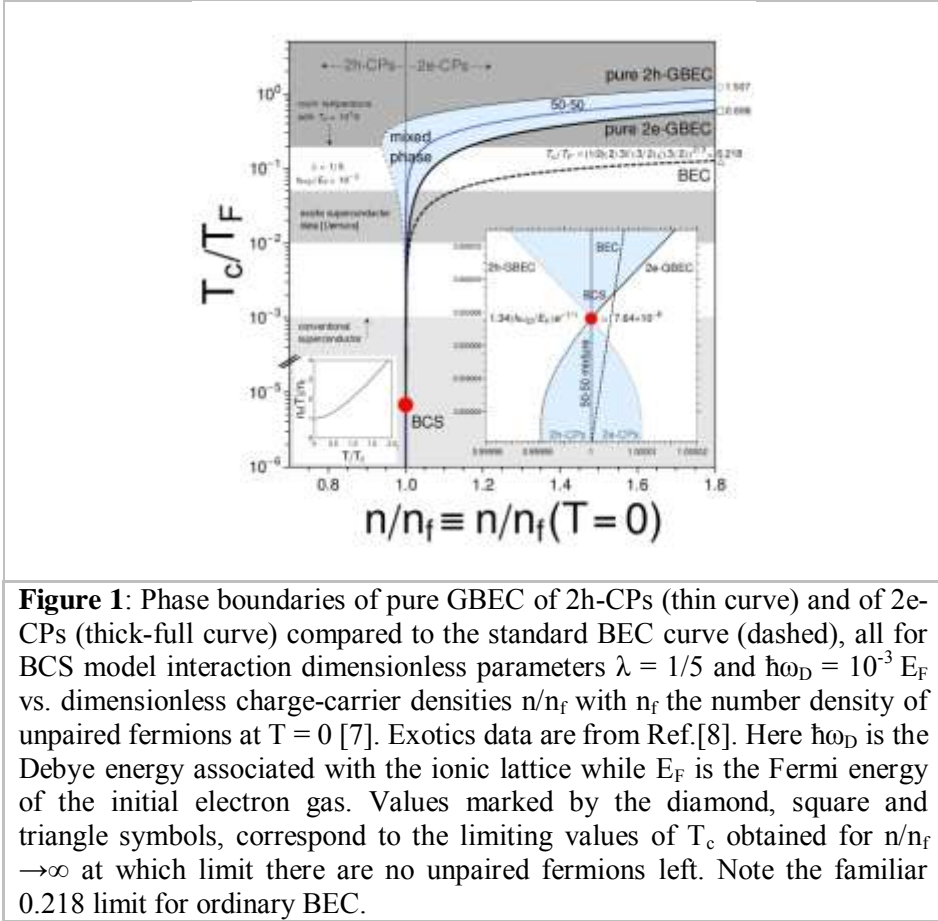


Figure 1: Phase boundaries of pure GBEC of 2h-CPs (thin curve) and of 2e-CPs (thick-full curve) compared to the standard BEC curve (dashed), all for BCS model interaction dimensionless parameters $\lambda = 1/5$ and $\hbar\omega_D = 10^{-3} E_F$ vs. dimensionless charge-carrier densities n/n_f with n_f the number density of unpaired fermions at $T = 0$ [7]. Exotics data are from Ref.[8]. Here $\hbar\omega_D$ is the Debye energy associated with the ionic lattice while E_F is the Fermi energy of the initial electron gas. Values marked by the diamond, square and triangle symbols, correspond to the limiting values of T_c obtained for $n/n_f \rightarrow \infty$ at which limit there are no unpaired fermions left. Note the familiar 0.218 limit for ordinary BEC.

Theory for Higgs oscillations in superconductors



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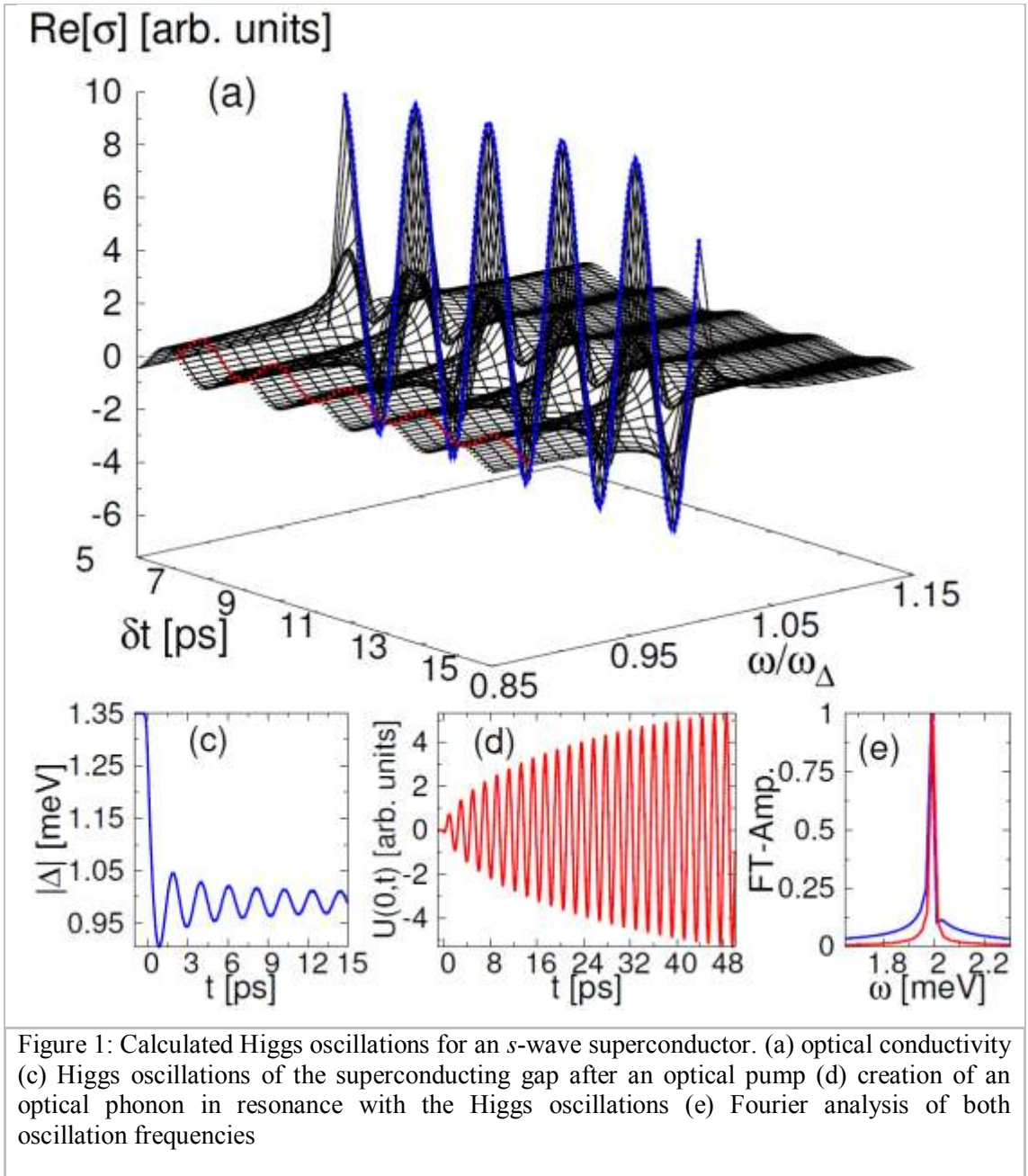
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Keywords : Density Matrix Theory – Higgs – nonequilibrium

Time-resolved pump-probe experiments recently attracted great interest, since they allow to detecting hidden states and they provide new information on the underlying dynamics in solids in real time. Recently, we have established a theory for superconductors in non-equilibrium, for example in a pump-probe experiment [1,2]. Using the Density-Matrix-Theory (DMT) we have developed an approach to calculate the response of conventional and unconventional superconductors in a time-resolved experiment. In particular, DMT method is not restricted to small timescales; in particular it provides a microscopic description of the quench, and also allows also the incorporation of phonons [2]. Furthermore, we employ DMT to time-resolved Raman scattering experiments [3] and make predictions for 2-band superconductors [4]. Very recently, we have focused on the theory for order parameter amplitude (‘Higgs’) oscillations which are the realization of the Higgs mode in superconductors [5,2]. Our prediction has been recently confirmed experimentally [6,7].

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Fluctuation region of a two-band superconductor



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Keywords: two-band superconductor – fluctuation – correlation length – Ginzburg number

In a two-band superconductor, two qualitatively different fluctuation modes related to the gap modules contribute to the free energy and heat capacity, together with the phase fluctuations. The first mode has divergent temperature behaviour since it accounts for critical fluctuations around the phase transition point, T_c , along with pseudo-critical ones associated with the former instability of the weaker superconductivity component. The involvement of these two factors, competing under interband interaction, results in a Ginzburg number that varies with T_c non-monotonically, allowing a reduction of up to 75%. This makes the fluctuations effective in revealing additional superconducting components in the system. The second mode does not diverge, but has a jump at T_c , defined uniquely by the strength of the interband interaction. This mode contributes fundamentally beyond the critical domain.

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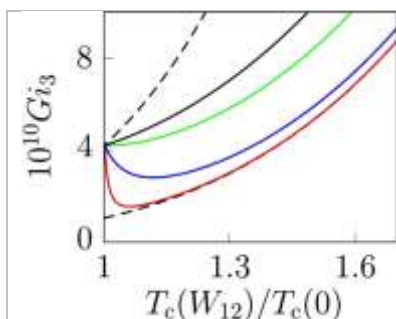


Figure 1: The plot of the Ginzburg number in two-band case vs T_c as former band critical temperatures become closer. The lower dashed curve represents the limiting case when these temperatures coincide. The upper dashed curve corresponds to the single-band dependence.

Novel Phase Sensitive Phenomena in Multi-Band Superconductors with Broken Time-Reversal Symmetry



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Keywords: multi-band, time-reversal symmetry, Josephson effect

Multi-band superconductors attract a lot of interest after discovery of superconductivity in MgB₂ and iron pnictides, where different bands couple to each other. When we have three or more superconducting bands with repulsive couplings, it is possible to have a frustrated state with interband phase differences neither 0 nor π , which breaks the time-reversal symmetry (TRS) [1,2], yielding two degenerate time-reversal symmetry broken (TRSB) states.

Nontrivial interband phase differences lead to novel phase sensitive phenomena. Two coherence lengths are found divergent at critical temperature, with coupled phase and amplitude variations in one of the mode [2]. A novel intermediate phase with vortex cluster appears since changing of sign in interface energy of a presumed superconducting/normal domain and that in the difference between nucleation field and thermodynamic critical field take place separately in parameter space, in sharp contrast to a single point given by GL parameter $\kappa = 1/\sqrt{2}$ for single-band superconductivity [3]. Massless Leggett mode also appears at the phase boundary between TRSB state and time-reversal symmetry reserved state [4].

Recently we focus on the Josephson effects of the TRSB states [5]. We consider a Josephson junction between a three-band TRSB superconductor and a single-band superconductor. Andreev spectra and Josephson current are studied with Bogoliubov-de Gennes equations. It is interesting to find that critical currents are unequal in the two opposite directions, as shown in Fig. 1, as a direct consequence of the broken TRS. In Josephson junctions, opposite currents with the same magnitude are provided by states connected by TRS. When TRS is broken, this connection is not available and thus symmetric critical currents cannot be guaranteed.

Another interesting phenomenon is the appearance of strong 1/3 Shapiro steps.

Due to interference of Josephson tunneling in three condensates, contributions of the third-order harmonics are enhanced while others get cancelled partially, leading to a large 1/3 Shapiro step

It should be mentioned that both of these phenomena can be found in a previous experiment for a Josephson junction between a single-band superconductor and an iron-based superconductor [6], a typical multi-band superconductor. In the light of our theoretical work, TRSB states might have already been realized in iron-based superconductors.

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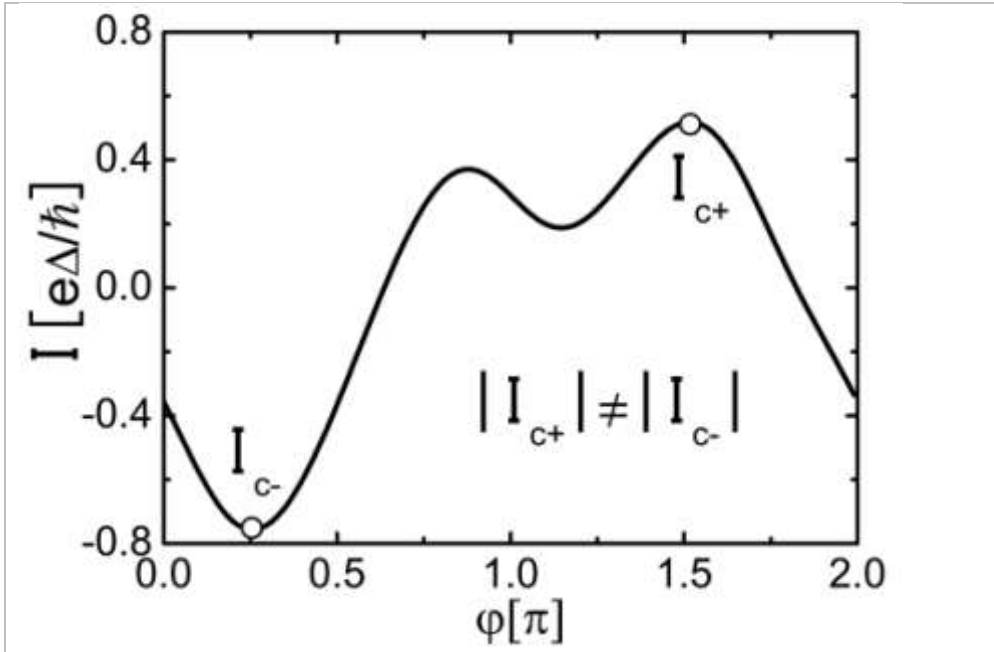


Figure 1: Current phase relation of Josephson junction between single-band and three-band TRSB superconductor, where ϕ is the phase difference between the single-band superconductor and the first component of the TRSB superconductor.

More about the holographic two-band superconductor

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Keywords: Holography, Multi-condensates Superconductivity

In this talk, we continue our previous study on the holographic model of a two-band superconductor constructed in arXiv:1309.0488. We present the static vortex configuration and study its properties especially the effects of interband coupling.

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SESSION 26

Spatially Localized Multiferroicity in magnetic films at room temperature

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Keywords : spin flexoelectricity – domain wall – room temperature magnetoelectricity

The prospects of low power magnetoelectric devices based on electric field control principle tantalizing spintronic engineers that currently resort to high density currents to switch the magnetic state of logic elements. However the majority of magnetoelectric materials demonstrate their properties only in low temperature range.

Magnetic material in the form of epitaxially grown single crystalline film support various type of chiral spin structures: magnetic domain walls (fig 1 a), vortices and skyrmion (fig 1 b). Due to the spin flexoelectric effect [1] this topological structures are associated with a change of symmetry and local multiferroic properties localized on length scales of tens nanometers. This electric polarization of magnetic origin is induced by spin configuration rather than chemical composition and crystal structure.

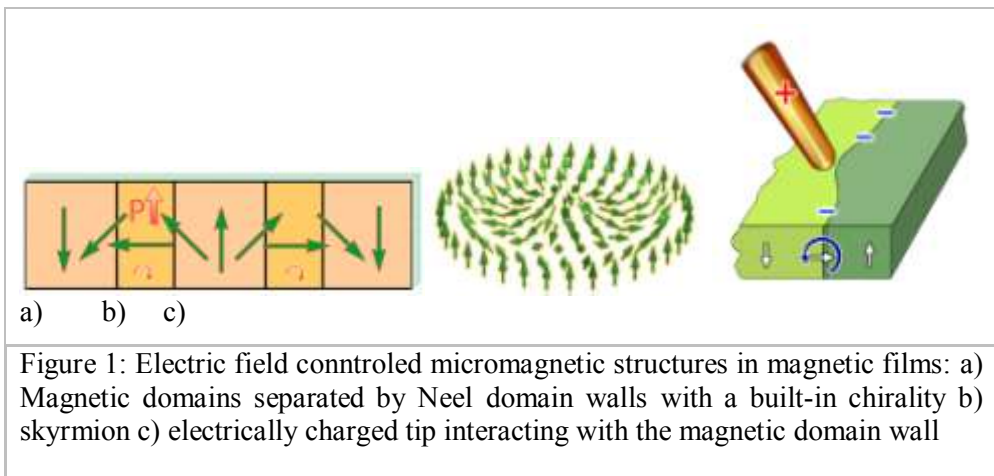
The electric field control of magnetic domain wall was experimentally demonstrated in [2-4]. We used tip electrode that generate high electric field of 1MV/cm only in the immediate vicinity of the tip (fig. 1c). The internal magnetic structure of the wall was controlled by homogeneous magnetic field in the plane of the film. The domain wall displacement up to 30 μm (around the period of the domain structure) and domain wall velocity 30m/s were demonstrated at 1kV voltage bias at the tip.

Thus the electric polarization of magnetic origin localized on micromagnetic structures is particularly promising to circumvent the scarcity of single-phase room-temperature multiferroics. The domain walls and skyrmion can serve as building blocks for spintronics devices and magnetic memory that are controlled by electric field rather than high density current. The spatial localization of magnetoelectric properties is also of high interest for application in magnetoplasmonics where the spatially localized plasmon modes in magnetic material can be effectively controlled by electric field.

The work is supported by RFBR grants #14-29-08216 ofi_m, #14-02-91374 ST_a and TUBITAK (No.213M524).

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Magnetic excitation of hole-overdoped cuprate studied by RIXS and neutron



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Keywords : high T_c cuprates – magnetic excitation

Magnetic fluctuations in high- T_c cuprates play an important role in the superconductivity, which appears typically in the characteristic regime between insulating antiferromagnetic and overdoped metallic regimes. It is an important issue how the dynamical magnetic response can be described in the superconducting regime. In addition to the neutron scattering which made important contributions [1] to understand the magnetic excitations in the low energy region, below 150 meV, the recently developed resonant inelastic x-ray scattering (RIXS) technique at the Cu- L_3 edge provides alternative way to observe single magnons [2,3]. These two techniques are complementary with each other. In this talk, we report high energy magnetic excitations above 100 meV of overdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ ($x = 0.25$) studied by both neutron and Cu- L_3 edge RIXS using identical crystals for the two techniques. The overdoped sample was chosen so that we can also test the doping independence of the paramagnon dispersion relation at high energy (>150 meV) recently observed by RIXS [4,5].

Neutron scattering measurements were done using the chopper spectrometer SEQUOIA at the Spallation Neutron Source of Oak Ridge National Laboratory. Cu- L_3 edge RIXS measurements were done using the AXES spectrometer at the beam line ID08 of the European Radiation Facility. Combination of neutron and RIXS indicates that both data are consistent with each other and that the overall high energy magnetic excitation agrees with the spin-wave dispersion relation of parent compound La_2CuO_4 (LCO) particularly in the $(\pi, 0)$ direction, consistently with the previous RIXS studies. We also draw the magnetic excitation above 100 meV in the (π, π) direction by the complementary use of neutron and RIXS. The magnetic excitation for smaller than $(0.15, 0.15)$ (r.l.u.) measured by neutron follows the LCO spin wave dispersion whereas that for larger than $(0.15, 0.15)$ (r.l.u.) measured by RIXS is apparently less dispersive and the excitation energy near (π, π) is smaller than the LCO spin wave excitation energy. Polarization dependence of RIXS spectra indicates appreciable charge excitations exist in the same energy range of magnetic excitations, which may affect the magnetic excitation.

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A spin jam state of a highly frustrated magnet materials

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Keywords: spin glassy states, spin jam

Can a glassy state exist in the absence of defects? This long-standing problem in condensed matter physics will be addressed in this talk by discussing glassy states found in frustrated magnets. Of particular interest is a quasi-two-dimensional triangular lattice of bi-pyramids. Recently, we found that although classically the ground state of the system is a spin liquid, quantum corrections break the classical degeneracy into a set of aperiodic spin configurations forming local minima in a rugged energy landscape. A consequence of the complex energy landscape is, upon cooling, the system gets trapped in one of the local minima, leading to a glassy state that we call a spin jam.[1] More recently, we have performed systematic neutron scattering experiments on $\text{SrCr}_{1-p}\text{Ga}_p\text{O}_{19}$ (SCGO(p)) with various values of the magnetic concentration, p , covering almost the entire region of p . Our results clearly revealed existence of a unique spin jam state in the vicinity of the clean limit $p=1$. [2]

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SESSION 27

SnS-Andreev spectroscopy of Fe-based oxypnictides: scaling of superconducting parameters with T_C



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Keywords: pnictides, high- T_C superconductivity, multiple Andreev reflections

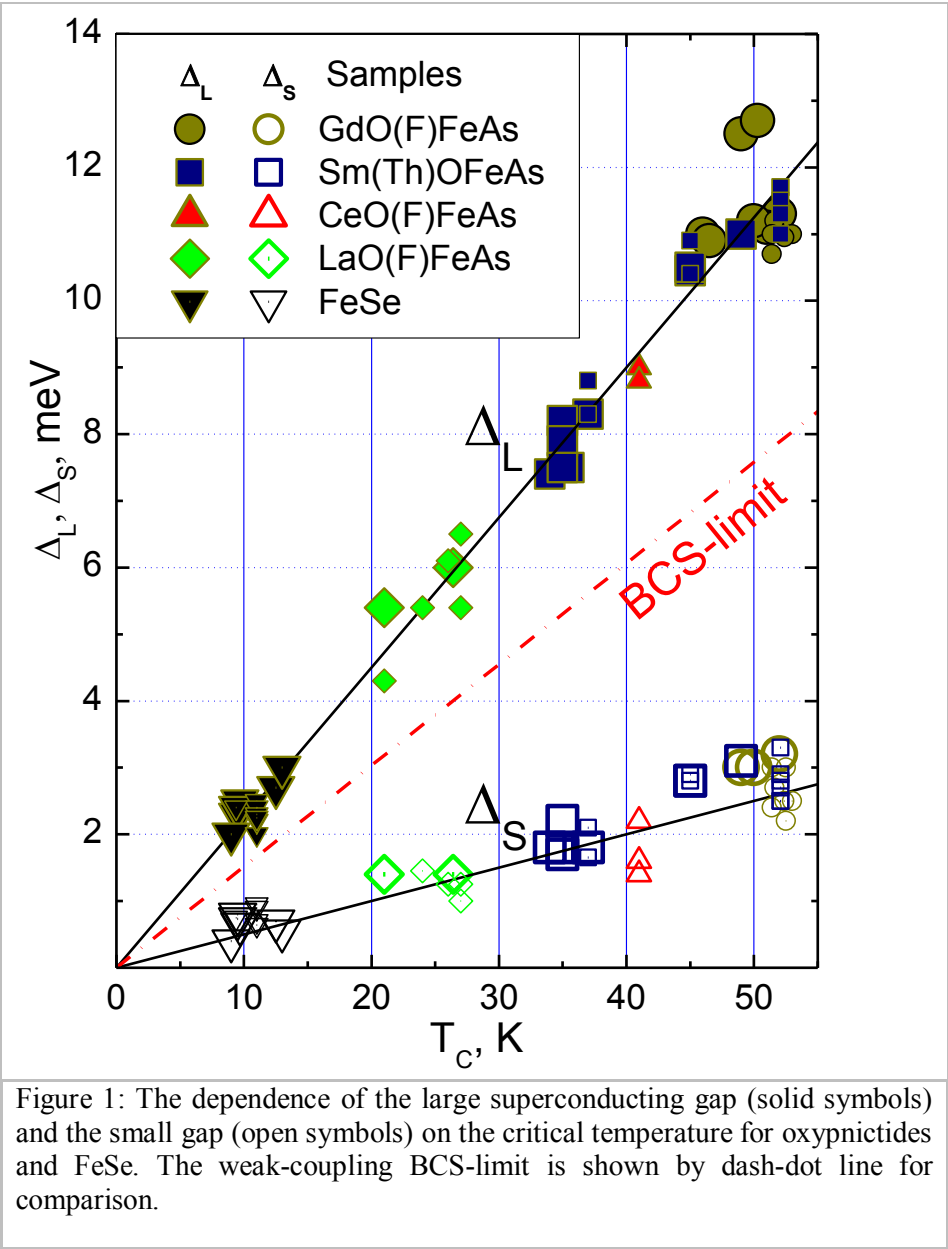
We studied $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$, $\text{GdO}_{1-x}\text{F}_x\text{FeAs}$, $\text{GdO}_{1-\delta}\text{FeAs}$, $\text{Sm}_{1-x}\text{Th}_x\text{OFeAs}$ и $\text{CeO}_{1-x}\text{F}_x\text{FeAs}$ with the T_C range 21–53 K by Andreev and intrinsic Andreev spectroscopies [1,2]. Intrinsic multiple Andreev reflections effect was firstly observed in 1111-oxypnictides, revealing the Andreev-like transport along the c-direction. We determined the values of two bulk superconducting gaps and their BCS-ratios, and demonstrated weak anisotropy of Δ_L (20–30 %) and the absence of nodes in Δ_S . For the maximal $T_C \approx 53$ K, we found $\Delta_L = 11.7 \pm 1.0$ meV, $\Delta_S = 2.7 \pm 0.5$ meV, $\Delta_L/\Delta_S \approx 4.3$.

The gap temperature dependences $\Delta_{L,S}(T)$ agree well with two-band model by Moskalenko and Suhl [3]. Both gaps turn to zero at common critical temperature. Using fitting of the experimental $\Delta_{L,S}(T)$ by the two-band model, we determined some parameters of superconducting state of 1111-materials directly from the experiment.

The estimated relative coupling constants λ_{ij} were shown to be $\lambda_{LL} : \lambda_{SS} : |\lambda_{LS}| : |\lambda_{SL}| \approx 1 : 0.65 : 0.27 : 0.03$ within the range $T_C = 21$ –50 K. We demonstrate scaling of both superconducting gaps with T_C (Fig. 1) and nearly constant BCS-ratio $2\Delta_L/k_B T_C \approx 5.2$. For each condensate, the eigen BCS-ratio was estimated (in a hypothetical case of zero interband coupling, $\lambda_{LS}, \lambda_{SL} = 0$): for the large gap we get $2\Delta_L/k_B T_C^L \approx 4.5$, for the small gap $2\Delta_S/k_B T_C^S \approx 4.2$, $T_C/T_C^L \approx 0.8$. These values exceed the weak-coupling limit but are in frames of Eliashberg theory thus pointing to a strong electron-phonon intraband coupling in two condensates. The spacers lanthanide–O were shown to act as charge reservoirs.

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Directional Point-Contact Josephson Junctions in K-doped Ba 122 single crystals



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Keywords: Fe-based superconductors – Symmetry of the Order Parameter – Josephson Effect – Point Contacts

The symmetry of the order parameter in the Fe-based superconductors (FeBS) has not been unambiguously clarified yet. In this regard, several phase-sensitive experiments have been proposed [0,2] in order to solve this issue, but they are still difficult to realize from the experimental point of view. In particular, some of them should also make use of point contacts between a conventional superconductor and a FeBS [0]. Motivated by these predictions, point-contact Josephson junctions between the conventional *s*-wave superconductor Pb_{0.7}In_{0.3} and K-doped Ba 122 single crystals were investigated.

The samples were optimally doped (Ba_{0.6}K_{0.4}(FeAs)₂, $T_c \approx 36.5$ K) and overdoped crystals (Ba_{0.4}K_{0.6}(FeAs)₂, $T_c \approx 30$ K). A sharpened tip was used for injecting the current along the *c*-axis while a wedge-like one was employed for current injection along the *ab*-plane. Reproducible, non-hysteretic RSJ-like I-V characteristics were observed at low temperature. The junctions were then irradiated with microwaves by using a monopole antenna placed at the end of a semi-rigid coaxial cable. The occurrence of the Josephson

effect was proved by the presence of microwave-induced current steps (Shapiro steps). Subsequently, the power dependence of the current steps was investigated.

The behavior of the Shapiro steps as a function of the square root of the microwave power was studied by means of the RSJ model extended to the nonautonomous case with an rf current-source term [3]. The analysis reveals that, under certain circumstances, the current-phase relation deviates from being simply described by the standard $\sin(\varphi)$. The results are compared with the theory of the dc Josephson effect, formulated by using a method based on the calculation of temperature Green's function in the junction within the tight-binding model [4]. Implications and considerations with respect to the symmetry of the order parameter (in particular with respect to the s_{++} -wave and s_{\pm} -wave symmetries [4,6,7]) will be presented and discussed.

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High-temperature superconductivity from fine-tuning of Fermi-surface singularities in iron oxypnictides



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Keywords: mechanisms for high T_c – Fermiology of iron pnictides – van Hove singularities in superconductors – superconductivity

In the family of iron-based superconductors, LaFeAsO-type materials possess the simplest electronic structure due to their pronounced two-dimensionality. And yet they host superconductivity with the highest transition temperature $T_c=55$ K. Early theoretical predictions of their electronic structure revealed multiple large circular portions of the Fermi surface with a very good geometrical overlap (nesting), believed to enhance the pairing interaction and thus superconductivity. The prevalence of such large circular features in the Fermi surface has since been associated with many other iron-based compounds and has grown to be generally accepted in the field. In this work we show that a prototypical compound of the 1111-type, $\text{SmFe}_{0.92}\text{Co}_{0.08}\text{AsO}$, is at odds with this description and possesses a distinctly different Fermi surface, which consists of two singular constructs formed by the edges of several bands, pulled to the Fermi level from the depths of the theoretically predicted band structure by strong electronic interactions. Such singularities dramatically affect the low-energy electronic properties of the material, including superconductivity. We further argue that the occurrence of these singularities correlates with the maximum superconducting transition temperature attainable in each material class over the entire family of iron-based superconductors.

Superconducting properties and doping effects of (Ca,RE)FeAs₂



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Keywords : iron based superconductor–new material –catenation

Since 2008, series of iron-based superconductors such as REFeAsO (*RE*: rare earth), AFe₂As₂, FeSe have been developed. The structure of iron-based superconductors are composed of superconducting layer(FeAs, FeSe, FeP etc.) and blocking layers, and it is important to find new kinds of blocking layers to understand mechanism of iron-based superconductors as well as enhance superconducting properties. Recently new iron-based superconductor (Ca,RE)FeAs₂ have been discovered[1,2]. The compounds show superconductivity above 40 K is reported[3]. Crystal structure of the (Ca,RE)FeAs₂ is composed of Ca(*RE*) planes, Fe₂As₂ layer and As₂ layer. In As₂ layer of (Ca,Pr)FeAs₂, closest As-As distance is ~2.60 Å, suggesting existence of two As-As bonding for each As atom. Thus, As atoms form catenative chain like structure as shown in the figure, and the catenation is the first example in iron-based superconductors. Features of this compound proved variety of blocking layers as well as arsenic chemistry, and may bring new features in iron-based superconductors. Anisotropy of the compound is lower than that of REFeAsO, though distance between superconducting layers of this compound is longer than that of REFeAsO [4]. It may indicate characteristics of the compound.

In addition, we have synthesized transition metals (*TM* = Mn, Co, Ni) co-doped (Ca,RE)FeAs₂ samples. Mn co-doping suppressed superconductivity, while superconducting transitions became sharp and increase of *T_c* was observed in most of the Co or Ni co-doped samples.

T_c of Co co-doped samples decreased according to the decrease of ionic radii of RE³⁺. *T_c* decreased from 38K(*RE* = La) to 29 K(*RE* = Gd), and Eu doped sample(*T_c* = 21 K) has exceptionally low *T_c* considering the trend of *T_c*. *J_c* value of La and Co co-doped sample estimated from magnetization measurement is approximately 2.0 × 10⁴ Acm⁻² was estimated. In this talk superconducting properties and recent progress of (Ca,RE)FeAs₂ and related topics will be presented.

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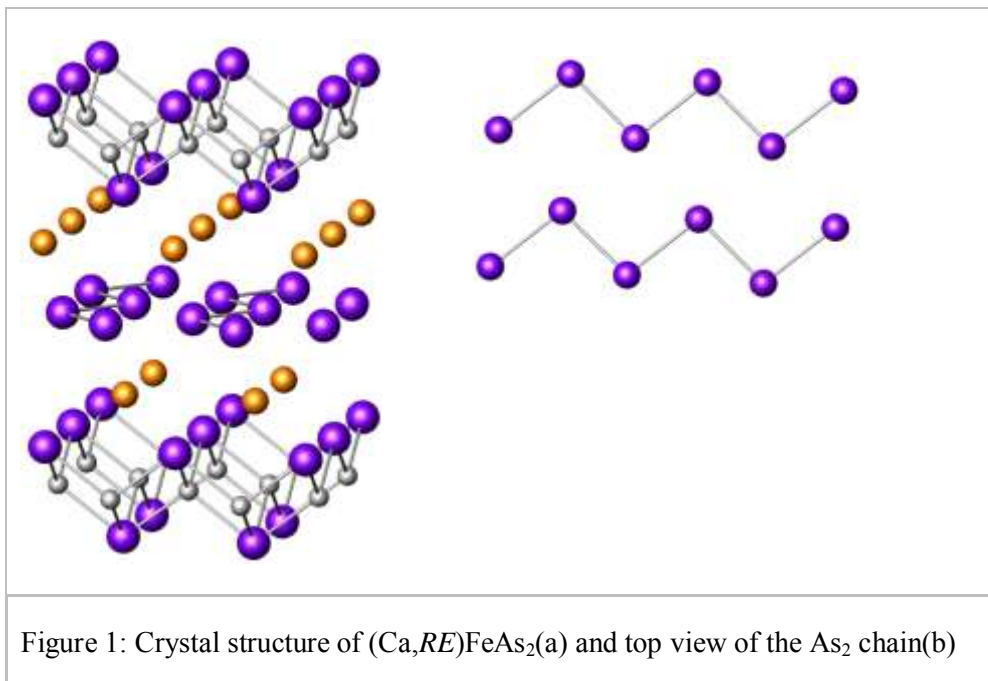


Figure 1: Crystal structure of (Ca,RE)FeAs₂(a) and top view of the As₂ chain(b)

SESSION 28

Hidden and Apparent Mott Physics in Iron Superconductors



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Keywords : Electron-Electron Correlations – Mott Transition – Orbital Selective Mott Physics

The link between high-temperature superconductivity and strong electron-electron correlations has been forged and strengthened by thirty years of investigation in the cuprates, where superconductivity emerges doping a Mott insulator. In this light, the debate about the strength and the role of electron correlations in iron-based superconductors (FeSC) maintains a crucial importance. The phenomenology of these materials does not provide a self-evident answer. In these materials superconductivity appears doping a metallic spin-density-wave parent compound and, even if the metallic state is highly incoherent, the standard fingerprints of strong correlations, like the Hubbard bands, are not universally observed.

A crucial difference with the cuprates is the multiorbital nature of the bands close to the Fermi energy, which involve all the d orbitals. Non-perturbative studies of the effect of the interactions have highlighted a novel behavior in multiorbital systems, in which the Hund's coupling J plays a big role, despite being much smaller than the Hubbard U . In particular, for 6 electrons in 5 orbitals, the configuration of the parent compounds of FeSC, we have a strongly correlated state for a wide range of intermediate and realistic U , despite the Mott transition is pushed to huge values [1].

Here we argue that Mott physics is however the key understand the phase diagram of these materials. In particular, we show that the doping degree of correlation in the 122 family is controlled by the distance from a putative Mott insulator that would be obtained for 5 electrons per iron (one hole per iron). A second crucial result is that the different orbitals are decoupled by the Hund's coupling, so that each of them behaves like a single-band Hubbard model. This unifies the phase diagram with the cuprates and leads to "orbital selectivity" of the electronic properties [2].

Finally, we show that also stoichiometric materials can be in a Mott state as a consequence of relatively small changes in the bandstructure. In particular $\text{LaO}_3\text{Fe}_2\text{Se}_2$ is indeed a Mott insulator with four half-filled orbitals because of a larger crystal field-splitting and a smaller kinetic energy per band [3]. Another interesting system is $\text{K}_2\text{Fe}_4\text{Se}_5$, which is

indeed found in an orbital-selective Mott state, which becomes fully insulating breaking the magnetic symmetry, in agreement with experiments [4]. This work is financed by ERC/FP7 through the StG-2009 SUPERBAD (GA 240524)

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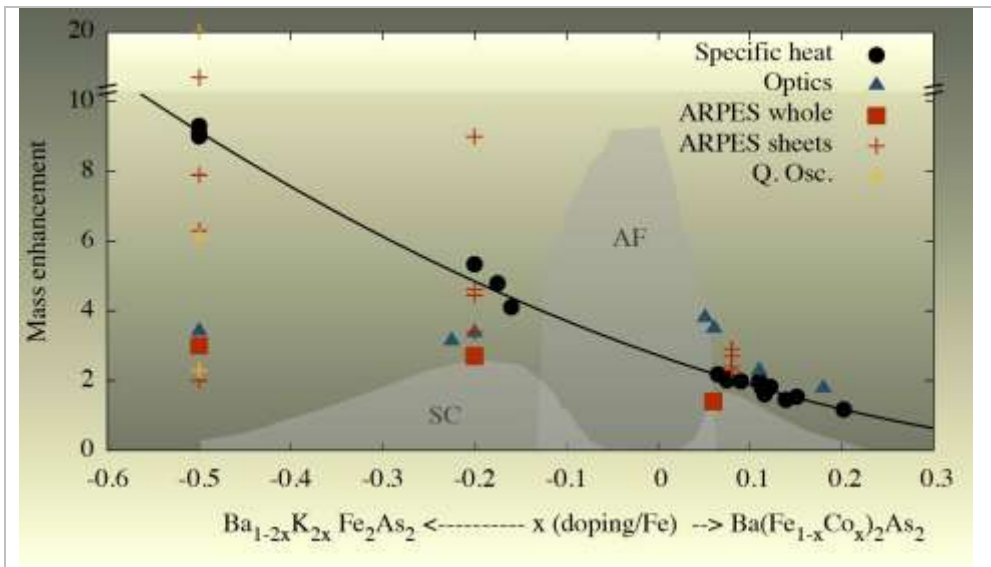


Figure 1: Experimental data for the effective mass of doped BaFe_2As_2

Electronic correlations in AFe_2As_2 iron-based superconductors ($\text{A} = \text{K}, \text{Rb}, \text{Cs}$)



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Keywords : superconductivity – strong correlations – thermal expansion

Superconductivity in iron pnictides and chalcogenides occurs in close proximity to antiferromagnetic order, giving rise to the assumption that the superconducting state originates from electron-electron interactions. So far, experimental and theoretical studies underpin this assumption but have failed to unravel the pairing mechanism. A central question is what is the role played by electronic correlations in these materials. We have investigated the thermal expansion and magnetostriction of the stoichiometric compounds AFe_2As_2 with $\text{A} = \text{K}, \text{Rb},$ and Cs . Our measurements reveal a remarkable increase of the effective masses of the quasiparticles with increasing ionic radius, while the superconducting transition temperature T_c decreases. Our measurements provide valuable input to explore the relation between crystal structure, electronic correlations and superconductivity on a more quantitative basis.

Competing magnetic double-Q phases in iron pnictides



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Keywords : Pnictides-Magnetic properties-Superconductivity

We perform a microscopic theoretical study of the generic properties of competing magnetic phases in iron pnictides. As a function of electron filling and temperature, the magnetic stripe (single-Q) order forms a dome, and we find that competing non-collinear and non-uniform double-Q phases exist at the foot of the dome in agreement with recent experiments [1,2]. We compute and compare the electronic properties of the different magnetic phases, investigate the role of competing superconductivity, and show how disorder may stabilize double-Q order. Superconductivity competes more strongly with double-Q magnetic phases, which can lead to re-entrance of the C2 (single-Q) order in agreement with recent thermal expansion measurements on K-doped Ba-122 crystals [2].

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Can disorder really enhance superconductivity?



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Keywords : superconductivity, disorder, percolation, multifractality

There is growing evidence, from experiments and numerical simulations, that a key feature of sufficiently disordered superconductors is the spatial inhomogeneity of the order parameter. However not much is known analytically about the details of its spatial distribution or the associated global critical temperature that signals the breaking of long-range order. Here [1] we address this problem for disordered systems around an Anderson transition characterized by multifractal one-body eigenstates. In the limit of weak multifractality and for weakly coupled superconductors we compute the superconducting order parameter analytically, including its energy dependence and statistical distribution in space. The spatial distribution of the order parameter is found to be always log-normal. The global critical temperature, computed by percolation techniques and neglecting phase fluctuations, is enhanced with respect to the clean limit only for very weakly coupled superconductors. Some enhancement still persists even in the presence of moderate phase fluctuations crudely modelled by increasing the percolation threshold. Our results are also consistent with experiments, where enhancement of the critical temperature is observed in Al thin films, a weakly coupled metallic superconductor, but not in more strongly coupled materials.

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Transient regime of single-molecule magnets



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Single-molecule magnets (SMM) coupled to ferromagnetic leads are promising candidates for solid state implementation of quantum information protocols [1]. The exchange coupling between electrons tunneling through unoccupied molecular orbitals and the localized molecular spin S allows the electrical switching of the latter. A key ingredient here is the magnetic anisotropy characterized by two parameters D and E controlling the uniaxial anisotropy term DS^2_z and the transverse anisotropy effects $E(S^2_x - S^2_y)$. We present a theoretical description of the time-dependent transport through SMM in the framework of the Generalized Master Equation (GME) method [2].

We analyze the effects of the transverse anisotropy on the transient currents and molecular spin dynamics, generalizing some previous results [3]. The possibility to read the dynamics of the molecular spin from transient current measurements and the effect of a perpendicular magnetic field are discussed.

Finally we investigate the effect of time-dependent signals applied at the contacts between the molecule and particle reservoirs, particular attention being paid to the quantum turnstile setting [4,5] which we propose as a new way to manipulate molecular spins. In particular, we show that for ferromagnetic leads with antiparallel spin polarizations the turnstile protocol allows the stepwise writing and reading of molecular states with well defined spin S_z . The efficiency of this operation depends crucially on the ratio $E=D$.

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CHAPTER 4

SESSION 29

Is FeSe a nematic quantum paramagnet?

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For spin-1/2 systems when quantum fluctuations destroy the N\'eel long-range order and open a spin gap, the resulting state usually breaks the lattice translation and rotation symmetries.

This can be understood as reflecting a Berry's phase associated with the magnetic monopole of the N\'eel order parameter. Here we point out the same Berry phase causes spin-1 systems to spontaneously break the discrete rotational symmetry of the crystal while preserving its translation symmetry. We support this claim by presenting an exactly solvable microscopic model whose ground state is a nematic quantum paramagnet. In addition we derive a field theory to describe the continuous, Landau-forbidden phase transition between a N\'eel ordered state and a nematic quantum paramagnet, and compare the theory with existing numerical results. We propose that the nematic quantum paramagnetic state captures essential features of bulk FeSe which becomes nematic around 90K but does not develop any spin long range order down to the lowest measured temperature.

Strange metals, fermion signs and long range entanglement.



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Keywords: non-Fermi liquids, quantum critical states

The strange metals as observed in high T_c superconductors and other correlated electron systems are arguably the greatest enigma of condensed matter physics. The difficulties are rooted in the fundamentals of physics: the lack of a general mathematical framework to deal with strongly interacting fermions at finite density, the “fermion sign problem”. The holographic duality as discovered in string theory is the first method yielding a precise description of non-Fermi liquids [1]. These holographic strange metals are suggestively similar to the laboratory variety, at the same defeating the basic principles of bosonic field theory. These are quantum critical phases with scaling properties alien to those computable with conventional methods. Remarkably their entanglement entropies demonstrate that their ground states are more densely entangled than deemed possible [1]. I will present some first indications that this is rooted in the sign structure. Using the so-called nodal surface (zero’s of the wavefunction) as a measure, this fermionic entanglement structure can be addressed in a geometrical language. The nodal surface of a Fermi liquid is characterized by a scale but using a particular Ansatz a quantum critical state can be described characterized by a fractal nodal surface [2]. We show that such states are characterized by entanglement entropies, which are strikingly similar as to those of the holographic strange metals [3].

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Spin-orbit interaction vs. nematicity in multiband iron-based superconductors as seen by ARPES



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Keywords: IBS, ARPES

Spin-orbit coupling (SOC) is a fundamental interaction in solids which can induce a broad spectrum of unusual physical properties from topologically non-trivial insulating states to unconventional pairing in superconductors. In iron-based superconductors (IBS) its role has so far been considered insignificant with the models based on spin- or orbital fluctuations pairing being the most advanced in the field. Using angle-resolved photoemission spectroscopy we directly observe a sizeable spin-orbit splitting in all main families of IBS. We demonstrate that its impact on the low-energy electronic structure and details of the Fermi surface topology is much stronger than that of possible nematic ordering. Intriguingly, the largest pairing gap is always supported exactly by SOC-induced Fermi surfaces.

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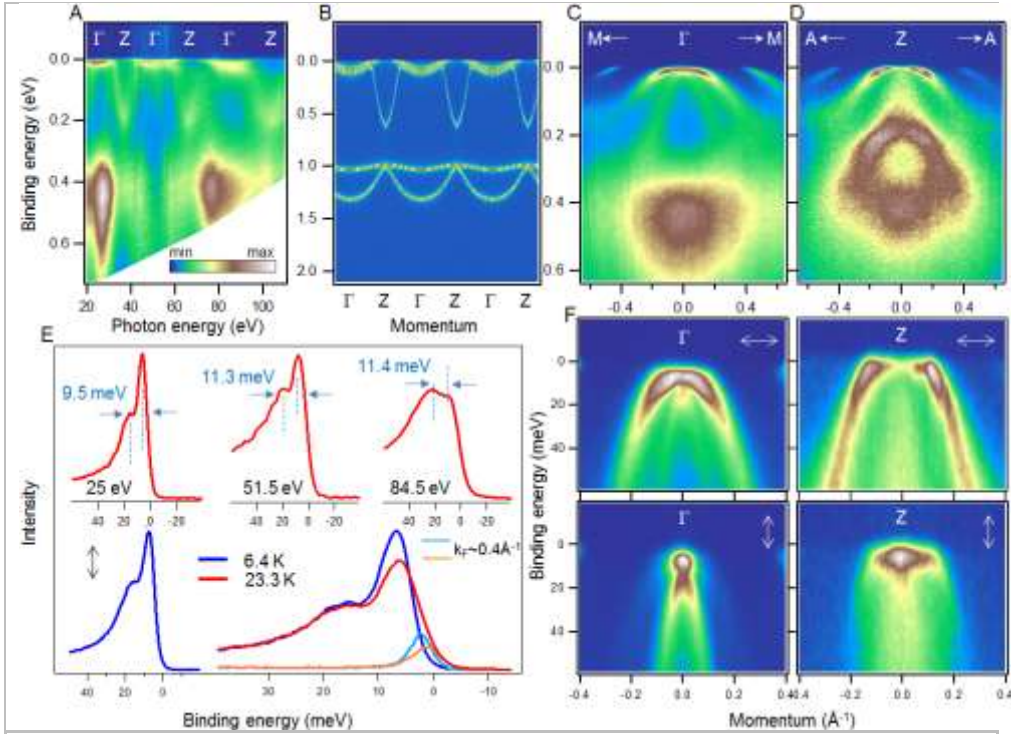


Figure 1: Determination of spin-orbit splitting at Γ -point. (A) Photon-energy dependence of the normal emission EDC representing the band structure along Γ Z-direction at T = 23.3 K (B) Calculations with SOC along the Γ Z-direction for comparison with (A). (C) Energy-momentum intensity distribution recorded along the M- Γ -M direction at T = 23.3 K using the 25 eV photons. (D) Same as (C), but along A-Z-A directions using 35.5 eV photons. (E) EDCs from the Γ -point taken at T = 23.3 K (red curves) and at T = 6.4 K (blue curves) using different photon energies and polarizations. Orange and light blue kF-EDCs taken above and below T_c respectively are shown for comparison. (F) High-resolution low-temperature ARPES data near Γ - and Z-points recorded with the light of horizontal (upper) and vertical (lower) polarizations.

Orbital-driven nematicity and superconductivity in FeSe: NMR study



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Keywords: orbital-driven nematicity – superconductivity – NMR study

Since the discovery of the iron based superconductors, the origin of the nematic tetragonal-to-orthorhombic transition has been hotly debated. Since in most iron pnictide families, the nematic transition occurs very close to the antiferromagnetic instability, it has been argued that the nematicity stems from the magnetic spin fluctuations, coupled to the lattice degrees of freedom. The iron selenide FeSe is different in that the structural transition occurs at $T_s \sim 90$ K without any sign of antiferromagnetism, and it is therefore tempting to conclude that an alternative scenario for nematicity, based on orbital (rather than spin) degrees of freedom, takes place. To establish whether this is indeed the case, we have conducted extensive nuclear magnetic resonance (NMR) measurements on FeSe. Below the nematic transition temperature T_s , we observe a clear splitting of the Se NMR line, which we show to be of electronic origin. Moreover, by measuring the spin-lattice relaxation rate and Knight shift, we establish unequivocally that this line splitting is driven by orbital nematic order. We furthermore establish a connection between orbital nematicity and superconductivity, showing that the two order parameters compete with each other. Intriguingly, this may provide an explanation for the very high superconducting transition temperature reported in the single-layer FeSe.

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Stripe Domains in Multiferroics and near Quantum Critical Points in Ferroelectrics

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We have examined stripe dynamics in three families of ferroelectrics near their Quantum Critical Points. these are O-18 isotopic SrTiO₃, Br-substituted tris-sarcosine calcium chloride (TSCC), and BaFe₁₂O₁₉ M-type hexafluoride. The latter two materials are uniaxial and have effective dimensionality $d+1=5$ rather than 4, as in the pseudocubic perovskites, and hence the susceptibility exponent γ is predicted to be $(d+z+1)/z = 3$ (Khmelnitskii). We have also examined domain wall behavior in some room-temperature multiferroics, including GaFeO₃ and PbFe_{1/2}Nb_{1/2}O₃ and its single-phase mixtures with PZT.

SESSION 30

Meissner-like effect in neutral trapped Fermi gases with arbitrary Interaction



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Keywords: BCS-BEC crossover, rotating superfluids, vortices

Vortex arrays in type-II superconductors admit the translational symmetry of an infinite system. There are cases, however, like ultra-cold trapped Fermi gases and the crust of neutron stars, where finite-size effects make it quite more complex to account for the geometrical arrangement of vortices. Here, we self-consistently generate these arrays of vortices at zero and finite temperature through a microscopic description of the non-homogeneous superfluid based on a differential equation for the local order parameter, obtained by coarse graining the Bogoliubov-de Gennes (BdG) equations [1]. In this way, the strength of the inter-particle interaction is varied along the BCS-BEC crossover, from largely overlapping Cooper pairs in the BCS limit to dilute composite bosons in the BEC limit. Detailed comparison with two landmark experiments on ultra-cold Fermi gases [2,3], aimed at revealing the presence of the superfluid phase, brings out several features that makes them relevant for other systems in nature as well.

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Effects of spin-orbit coupling on the Berezinskii-Kosterlitz-Thouless transition.

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Keywords: superfluidity/superconductivity, spin-orbit coupling, two-dimensions.

We investigate the Berezinskii-Kosterlitz-Thouless (BKT) transition in a two-dimensional (2D) neutral Fermi system with spin-orbit coupling (SOC), as a function of the two-body binding energy and a perpendicular Zeeman field [1]. By including a generic form of the SOC, as a function of Rashba and Dresselhaus terms, we study the evolution between the equal Rashba-Dresselhaus (ERD) and the Rashba-only (RO) cases. We show that in the ERD case, at fixed non-zero Zeeman field, the BKT transition temperature T_{BKT} is increased by the effect of the SOC for all values of the binding energy. We also find a significant increase in the value of the Clogston limit compared to the case without SOC. Furthermore, we demonstrate that the superfluid density tensor becomes anisotropic (except in the RO case), leading to an anisotropic phase-fluctuation action that describes elliptic vortices and anti-vortices, which become circular in the RO limit. This deformation constitutes an important experimental signature for superfluidity in a 2D Fermi system with ERD SOC. Finally, we show that the anisotropic sound velocity exhibit anomalies at low temperatures in the vicinity of quantum phase transitions between topologically distinct uniform superfluid phases.

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Composite bosons in the 2D BCS-BEC crossover



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Keywords: ultracold atoms – crossover BEC-BCS – dimensional regularization

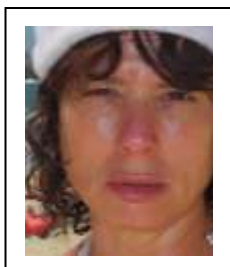
We study the finite-temperature attractive Fermi gas in the 2D BCS-BEC crossover showing that Gaussian fluctuations are crucial to get a reliable equation of state in the BEC regime of composite bosons, bound states of fermionic pairs [1]. Performing dimensional regularization of the ultraviolet-divergent Gaussian fluctuations we find that in the BEC regime the renormalized grand potential gives exactly the Popov's equation of state of 2D interacting bosons, and allows us to identify the scattering length a_B of the interaction between composite bosons as $a_B = a_F / (2^{1/2} e^{1/4})$, with a_F is the scattering length of fermions [2]. Remarkably, the value from our analytical relationship between the two scattering lengths is in full agreement with that obtained by recent Monte Carlo calculations [3].

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SESSION 31

$\sqrt{3}\times\sqrt{3}$ -Ag/Si(111)7×7: A Template for Silicene Growth



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Keywords: Multilayer silicene, LEED, AES, XRD, EDXR, RAMAN

Silicene, a single layer of silicon atoms ordered in a two-dimensional (2D) honeycomb structure, was synthesized in one layer 2D sheets [1], as well as bilayer and multilayer silicene on Ag(111) [2-3]. These films can grow in sequential flat terraces, after the initial formation of 3×3 reconstructed monolayer, which is in a 4×4 coincidence super cell respect to silver (111) unit cell. All terraces have a honeycomb $\sqrt{3}\times\sqrt{3}R(30^\circ)$ surface symmetry, with respect to 1×1 silicene. As detected in Scanning Tunnelling Microscopy (STM) and Low Energy Electron Diffraction patterns (LEED), thick epitaxial multilayer silicene films were obtained either on Ag(111) [2] or $\sqrt{3}\times\sqrt{3}R(30^\circ)$ -Ag/Si(111)-7×7 and studied by LEED, Auger electron spectroscopy, X-ray diffraction, energy dispersive X-ray reflectivity, Fourier transform infrared as well as Raman spectroscopy. Presently, there is a scientific debate on whether these multilayers silicene were indeed thin films of bulk-like silicon [4]. A key parameter to control the silicene growth is the substrate temperature during Si deposition. It strongly affects the nature of these films, by passing amorphous, multilayer silicene and bulk Si(111). These outcomes are of crucial importance for using silicene in conventional silicon based electronics, taking into account that the first single layer silicene FET was successfully realized [5] and a new type multilayer silicene based could be realized in the near future.

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Emergence of New Dirac Fermions in Twisted Silicene



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Keywords: silicene – twisted – STM – Dirac fermion – Moiré pattern

The band theory dictates that the propagation of the wave function of the nearly free electrons in a weak periodic potential results in the opening of bandgaps near points of the reciprocal lattice known as Brillouin zone boundaries [1]. However, in the case of massless Dirac fermions, it has been predicted that the pseudospin of the charge carriers prevents the opening of a bandgap and instead new Dirac points appear in the electronic structure of the material [2]. Silicene, a silicon-based two-dimensional Dirac fermion system, possesses a honeycomb structure, hence would exhibit a Moiré pattern if interlayer rotation exists [3-6]. Here, we report the emergence of new Dirac fermions in twisted silicene layers led by a honeycomb Moiré potential. Using low-temperature scanning tunneling microscopy and spectroscopy, we observed an interlayer rotation between adjacent stacking silicene layers which creates periodic ordered potential modulating the local density of states in a honeycomb arrangement. A set of new Dirac cones are consequently generated at the energy determined by the periodicity of Moiré pattern. Moreover, the Moiré pattern manifests Van de Waals interactions between neighboring silicene layers, which demonstrates layered structure of silicene.

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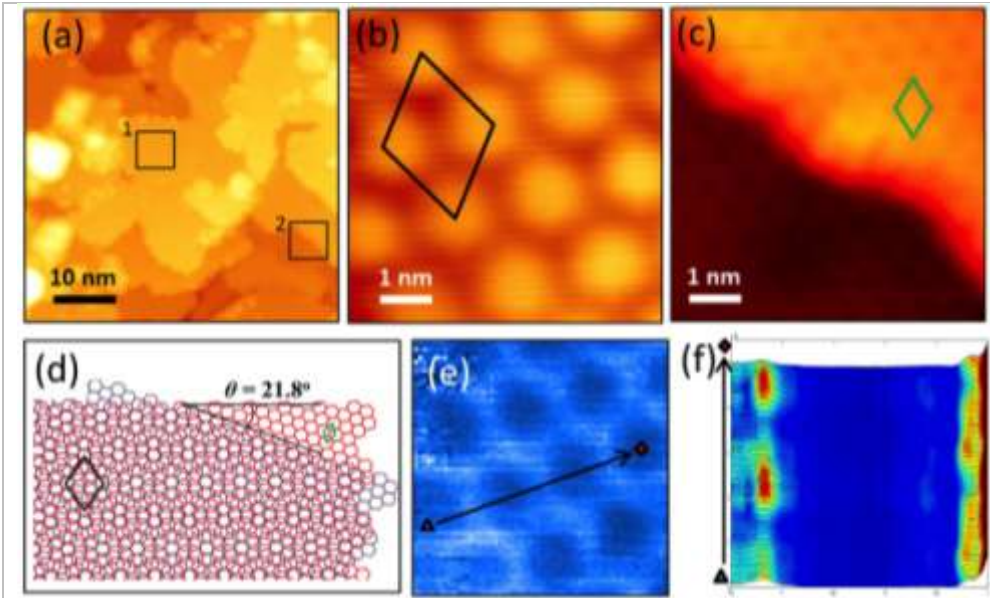


Figure 1: STM and STS on twisted silicene multilayers. (a) STM topographic image of multilayer silicene. (b) and (c) are high-resolution STM images corresponding to twisted silicene multilayers in Area 1 and normal stacking silicene multilayers in Area 2 in (a), respectively. (d) An obvious Moiré pattern demonstrates interlayer rotation angle of 21.8° in twisted silicene layers. (e) and (f) are STS mapping obtained in Area 1 in (a), which demonstrate a set of new Dirac-cone structures created by a Moiré-pattern-modulated honeycomb potential field in twisted silicene.

Reactivity of silicene towards atoms and molecules



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Keywords: silicene – reactivity – doping – ARPES

Silicene is a novel synthetic two-dimensional allotrope of silicon with a honeycomb structure similar to graphene [1,2]. Because of its potential compatibility with microelectronics technologies and its fascinating predicted characteristics, silicene is attracting a lot of attention [2,3]. Yet, fundamental knowledge about silicene is still in its infancy. To contribute to the state of the art, we have undertaken an experimental work to study the reactivity of silicene with respect to organic molecules as well as hydrogen atoms.

We have studied the effect of a strong electron acceptor organic molecule on the electronic properties of silicene grown on Ag(111). Indeed, similarly to graphene, a multilayer film of silicene appears to be intrinsically n-type doped. A possible issue to circumvent this intrinsic doping is to adsorb strong electron acceptor molecules that will act as a p-type dopant. With that aim, we combined several surface sensitive techniques to study the adsorption of 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4-TCNQ) on silicene-($\sqrt{3}\times\sqrt{3}$)R30°. We demonstrate that while there are strong modifications on the vibrational modes of the molecules, suggesting a strong charge transfer from the silicene to the molecule, there is unexpectedly no significant modification of the silicene's valence band.

We also present a study of the interaction between silicene and atomic hydrogen. Focusing on the Si-H vibrational modes, we demonstrate that depending on the film thickness, the reactivity and electronic properties of the silicene films are different. By studying the structural properties of the silicene sheets we also evidence an etching of the surface upon adsorption.

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Exploring Silicene mono- and multilayers of Silicene and Graphene with soft X-ray spectroscopy and DFT



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Keywords: 2D-Materials – Silicene – Graphene

2012 brought the first reports of a new member of the 2D material family: a hexagonal honeycomb of Si atoms deposited on the Ag(111) surface called “silicene”[1]. The characteristics and stability of freestanding silicene had previously been theoretically explored [2], and there was a strong push to determine if the epitaxial sheets possessed the promising qualities of their hypothetical freestanding counterparts. Initially, the results of angle-resolved photoemission spectroscopy (ARPES) experiments were thought to indicate that epitaxial silicene had a gapped Dirac cone in its electronic structure [1], as would be expected of freestanding silicene with a broken inversion symmetry. This enticing result, however, would be later overturned through a combination of experimental and theoretical techniques [3-5], and it would eventually be concluded that the epitaxial silicene sheet was in fact metallic with a strong cohesion to the underlying Ag(111) face. However, this conclusion would prove controversial [6,7], as the ambiguity of the ARPES data left some room for interpretation as to whether specific electronic features belonged to the epitaxial Si, the Ag substrate, or represented a hybridization between the two.

Soft X-ray emission and absorption spectroscopy (XES and XAS) are synchrotron-based experimental techniques for probing the element-specific projected density of electronic states (PDOS) in the valence and conduction bands of a material. When performed in combination at the Si $L_{2,3}$ emission and Si $2p$ absorption edges, XES and XAS allowed us to unambiguously show that the Si valence and conduction states were continuous across the Fermi energy; i.e. that the silicene overlayer was indeed metallic [3]. Complementary DFT simulations also showed a large degree of bonding between the Si overlayer and the Ag substrate. This result is an important but unfortunate finding, as it limits the future utility of epitaxial silicene monolayers on Ag(111). If they are to come into use they must be all at once isolated from their substrates, stable and possessing the linear band dispersion that is responsible for the desirable characteristics unique to 2D electronic systems.

One suggested way of achieving these characteristics is to produce a multilayer of silicene on the Ag(111) surface. These materials have been briefly described in the literature, and early indications suggest that they might play host to a Dirac cone structure [8]. However,

other reports insist that bilayers and multilayers are inherently unstable, collapsing into bulk Si nanocrystals shortly after the monolayer deposition is complete [9].

Our DFT calculations predict a stable, AA-stacked silicene bilayer on Ag(111) that corresponds nicely to the scanning tunneling microscopy (STM) bilayer observations. Unfortunately, these same DFT calculations predict a similar electronic structure as that of the monolayers, namely metallic and bound to the Ag(111). However, our XES and XAS measurements indicate a transition to bulk, sp^3 -hybridized Si beginning shortly after the completion of a monolayer, supporting the low-energy electron microscopy study that first suggested the nucleation of the silicene sheets to bulk crystals [10] (see Figure). In this way, XES, XAS and DFT provide us with a method for evaluating structural models, predicting and measuring electronic characteristics and determining the composition of a particular sample simultaneously.

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SESSION 32

Temperature- and Si deposition-dependence of epitaxial silicene on $\text{ZrB}_2(0001)$



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Keywords: Silicene, $\text{ZrB}_2(0001)$

The experimental observation of silicene, the silicon analogue of graphene, demonstrates that crystalline silicon can possess a much wider variety of physical and chemical properties than believed until recently. Due to its π electronic system, and its two-dimension character, silicene is of great technological interest as it is expected to offer new functionalities to silicon-based technologies.

Silicene exists only in epitaxy on a limited number of substrates. Among them, silicene on zirconium diboride (ZrB_2) buffer layers grown on $\text{Si}(111)$ [1-6] has the particularity to form spontaneously upon annealing in vacuum. The honeycomb lattice made of Si atoms segregating from the substrate adopts a $(\sqrt{3}\times\sqrt{3})$ -reconstructed structure to accommodate to the (2×2) unit cell of $\text{ZrB}_2(0001)$. The deviation of the structure from that of free-standing silicene causes the opening of a gap, as shown in Fig. 1 [1,2,4]. The epitaxial silicene sheet is textured by a large-scale one-dimension array of stress-domain [1,6]. Due to the high reproducibility of its formation, its high stability and the single orientation of its structure with respect to the $\text{ZrB}_2(0001)$ surface, this form of silicene is a suitable system for the study of the two-dimensional allotrope of silicon.

In particular, the evolution of the domain-structure with the temperature or upon the deposition of silicon adatoms is expected to give insight into the mechanical properties of epitaxial silicene and the origin of its stability on $\text{ZrB}_2(0001)$.

By means of scanning tunneling microscope (STM), we investigated at atomic scale the temperature-dependence of the silicene structure which manifests itself by the disappearance of the large-scale-ordering observed at 600°C by low-energy electron diffraction.

We also demonstrated that the deposition of a Si amount corresponding to the atoms missing at the boundaries is also able to turn the domain structure into a single-domain silicene sheet with very similar properties. The deposition of an additional silicon monolayer gives rise to the formation of a silicon bilayer with distinct structural and

electronic properties. This observation further demonstrates the ability of the $\text{ZrB}_2(0001)$ surface to stabilize two-dimensional forms of silicon.

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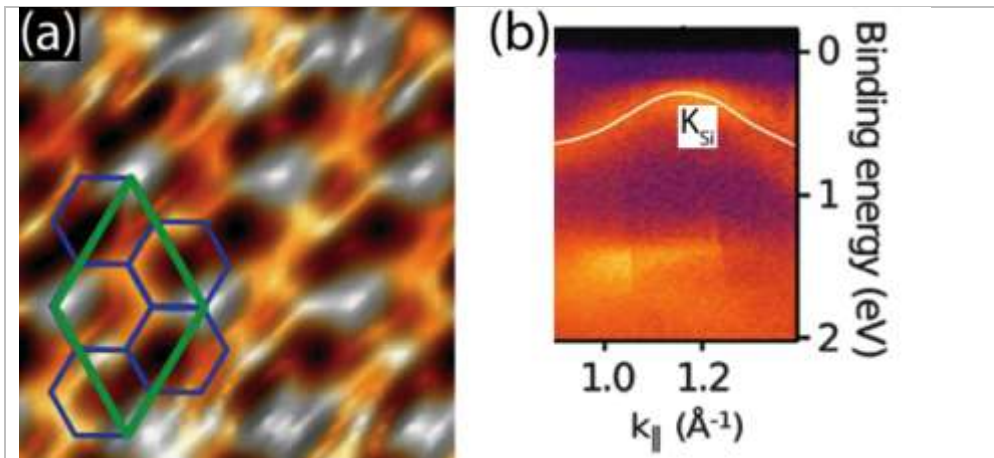


Figure 1: Epitaxial silicene on $\text{ZrB}_2(0001)$. (a): STM image of silicene. The atomic structure is brought out by the blue honeycomb. The green rhombus indicates the $(\sqrt{3}\times\sqrt{3})$ -reconstructed unit cell of silicene which corresponds to the (2×2) unit cell of $\text{ZrB}_2(0001)$. (b) Silicene π -band observed by angle-resolved photoemission spectroscopy. The gap found instead of the Dirac cone predicted for free-standing silicene is a result of the buckling of the reconstructed unit cell.

The ordered and reversible hydrogenation on silicene



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Keywords: silicene, hydrogenation, STM, DFT, Ag(111)

We present the investigation of the hydrogenation of monolayer silicene-3x3 and r7xr7 structure on Ag(111) using scanning tunneling microscopy experiments and density functional theory calculations.

For silicene-3x3, the fully hydrogenation at room temperature result in 7 hydrogen atoms reacted with Si atoms in one 3x3 unit cell. We find that the hydrogenated silicene will undergo an interesting structural transition, in which the buckled degree of Si atoms will be rearranged.

For silicene-r7xr7, the fully hydrogenation at room temperature result in the ordered structures with lattice identical to silicene-1x1 unit cell, which reveals that the original silicene with r7xr7 superstructure is an ideal defectless single-crystal monolayer film.

Combined with density functional theory calculations, both structures of hydrogenation can be explained by the “sub-lattice adsorption-picture”, in which H atoms prefer to adsorb on Si atoms in one sub-lattice of silicon.

Moreover, by annealing to a moderate temperature, about 450 K, de-hydrogenation process occurs and the clean silicene with original superstructure can be fully recovered. The easy reversible hydrogenation of monolayer silicene suggests that silicene may be a promising material for hydrogen storage.

Defect and oxidation of silicene on Ag(111) surface



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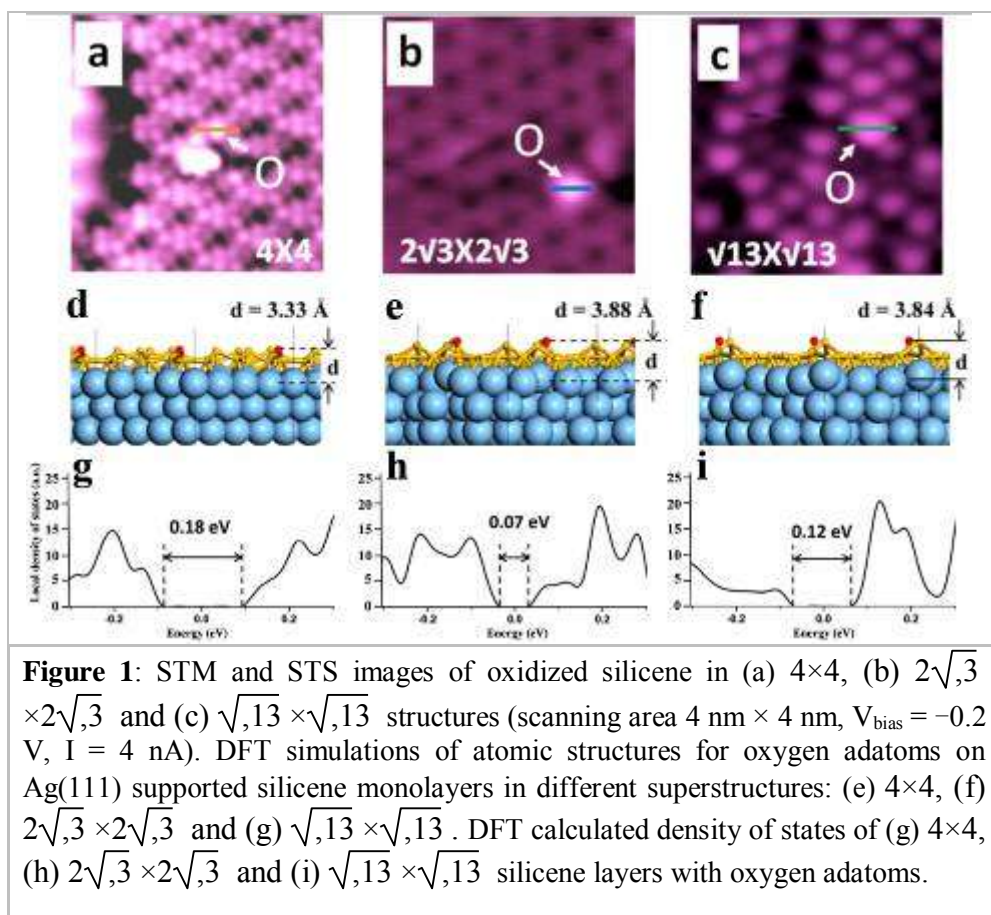
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Keywords: silicene, defect, oxidation, electronic properties

Silicene, a monolayer of silicon atoms arranging in a honeycomb lattice, is undergoing a rapid development in recent years due to its superior electronic properties and its compatibility with the mature silicon-based semiconductor technology. Defects are nearly inevitable in the growth of silicene and are widely found in the epitaxial growth in experiments. Thus, identifying the structural defects and understanding the defect effects on the electronic properties of silicene become important issues. For different silicene superstructures on Ag(111) surface [1], including (4×4) , $(\sqrt{13} \times \sqrt{13})R13.9^\circ$, $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$ with respect to Ag(111), various point defects of silicene and Ag surface are constructed. The STM images for these structures are simulated by first-principle calculations and compared with those observed in experiments. The simulated STM images agree well with those from experiments. Defects can effectively modify the electronic properties of silicene, transforming silicene to semiconductor or metallic [2]. Moreover, scanning tunneling spectroscopy (STS) and first-principle calculations suggest that an electronic band gap can be induced in monolayer silicene on Ag(111) surface by oxygen adatoms [3]. The Si-O-Si bonds are the most energetically favored species formed on $\sqrt{13} \times \sqrt{13}$, 4×4 and $2\sqrt{3} \times 2\sqrt{3}$ structures under oxidation, which is verified by *in situ* Raman spectroscopy as well as first-principles calculations. These results demonstrate the feasibility of tuning the band gap of silicene with oxygen adatoms, which, in turn, expands the base of available two-dimensional electronic materials for devices with properties that is hardly achieved with graphene oxide. It is noteworthy that quasi-free-standing silicene sheet can be obtained by oxygen intercalation of bilayer silicene epitaxial on Ag(111). After oxidation, the bottom layer silicene is oxidized forming amorphous SiO_2 , but the top layer silicene with $\sqrt{3} \times \sqrt{3}$ superstructure retains its structure due to the relative chemically resistance of $\sqrt{3} \times \sqrt{3}$ silicene to oxygen. Consequently, the top layer $\sqrt{3} \times \sqrt{3}$ silicene is quasi-free-standing.

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Construction of 2D Materials on Solid Surfaces: Silicene, Germanene, and Hafnene



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Keywords: 2D Materials – Silicene – Germanene – Graphene

The novel properties of graphene honeycomb structure have spurred tremendous interest in investigating other two-dimensional (2D) layered structures beyond graphene. In this talk, besides high quality and large scale single crystal graphene, we will report the fabrication of several graphene-like materials, silicene, germanene and hafnene, wherein silicon (germanium or hafnium) atoms are substituted for carbon atoms in graphene. Molecular beam epitaxial (MBE) growth technique is used to form the large scale 2D crystalline materials on metal surfaces, for example, Ru(0001), Pt(111), and Ir(111). The stacking heterolayers based on these kinds of 2D materials will be also introduced. As-prepared graphene/Si(or Hf)/metal architectures were characterized by scanning tunneling microscopy /spectroscopy (STM/STS), Raman, and angle resolved electron photoemission spectroscopy (ARPES) and proves the high structural and electronic qualities of the new complex. We expect that on the solid surfaces more new 2D crystalline materials could be found and these materials will show very interesting physical property and its promising potential applications in nanoscale devices.

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Figure 1: Buckled silicene fabricated on Ir(111).

Quantum Phase Transition from Superconducting to Metallic state in Diluted Arrays of Tin Dots on Graphene



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Keywords: Quantum Phase transition, superconducting proximity effect, superconducting to insulator transition, graphene, Bose Metal.

When subjected to an external field, quantum phases such as a disordered superconductor, terminates into either metallic or insulating states. This remarkable phase transition in the vicinity of a quantum critical point has been intriguing both theoretically and experimentally and is still subject of an active debate in condensed matter physics. Here, we focus on a specific type of quantum phase transition: the superconductor-to-metal transition in 2D, which is believed to be driven by quantum phase fluctuations. The main interesting feature of this transition is that it can be precisely controlled by the conductance of a 2D metallic film [1,2] which can be tuned in case of a semiconducting system.

Graphene turns out to offer a highly suitable platform for addressing this study: its surface-exposed and chemically inert 2D electron/hole gas is open to the intimate coupling of superconductors, giving rise to long range superconducting proximity effect [3–6]. Meanwhile, gate-tunability of the electron mean free path opens the possibility to study the stability of the superconducting phase against quantum fluctuations [7]. In this work, graphene monolayers were surface-conjugated to arrays of superconducting disk-shaped islands, whose inter-island distances were patterned to be in the quasi-ballistic limit of the underlying 2D electron gas. Arrays can be made on a large range of geometry and density, up to the highly diluted limit with less than 5% surface coverage and few micrometers in between islands.

In the lower temperature limit (<100 mK), despite of the long distance in between islands, a supercurrent was observed among the whole graphene sheet. Interestingly, the superconducting state vanishes exponentially in gate voltage and rests in a metallic state. This peculiar behaviour provide a hint to the understanding of long-standing issue of “zero-temperature” bosonic metallic state observed earlier in a other systems.

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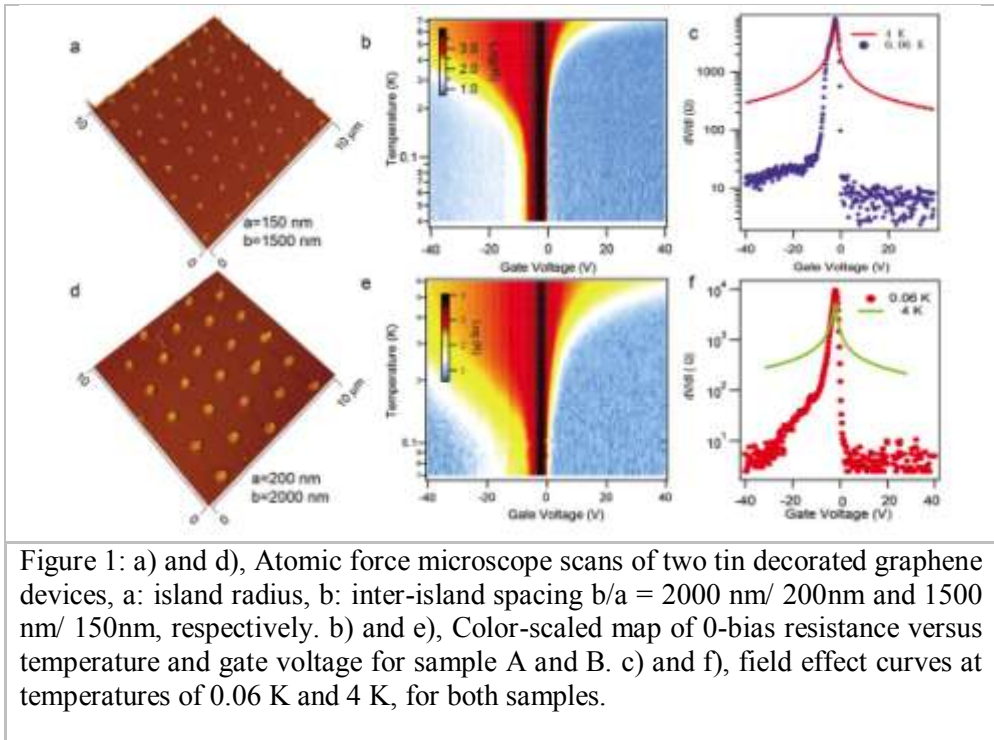


Figure 1: a) and d), Atomic force microscope scans of two tin decorated graphene devices, a: island radius, b: inter-island spacing $b/a = 2000$ nm/ 200nm and 1500 nm/ 150nm, respectively. b) and e), Color-scaled map of 0-bias resistance versus temperature and gate voltage for sample A and B. c) and f), field effect curves at temperatures of 0.06 K and 4 K, for both samples.

SESSION 33

CDW in the underdoped cuprates



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Keywords: high T_c – CDW – competing orders

I will present an overview of the results obtained from various x-ray scattering experiments on high temperature superconducting cuprates in the last couple of years. I will first focus on Cu L-edge resonant scattering experiments that led us to uncover charge density wave (CDW) correlations competing with superconductivity in the YBCO family [1-3], for which a complete temperature and doping dependent phase diagram has been worked out [4]. These investigations have been extended to other families of cuprates Bi2201 [5], Bi2212 [6] and Hg1201 [7] demonstrating the ubiquity and the universality of the phenomenon. Further information was gained from high resolution inelastic x-ray scattering. The observation of a quasi-elastic ‘central peak’ unraveled the static nature of the CDW correlations, attributed to the pinning of CDW nanodomains on defects. Low energy phonons exhibit anomalously large superconductivity induced renormalizations close to the CDW ordering wave vector, providing new insights regarding the long-standing debate of the role of the electron-phonon interaction, a major factor influencing the competition between collective instabilities in correlated-electron materials [8]. Finally I will discuss new results obtained in a heterostructure comprising YBCO and metallic ferromagnet La₂/3Ca₁/3MnO₃, where a stabilization of the CDW phase is concluded and discussed within the scope of tuning the equilibrium conditions of metastable phases via heterostructuring [9].

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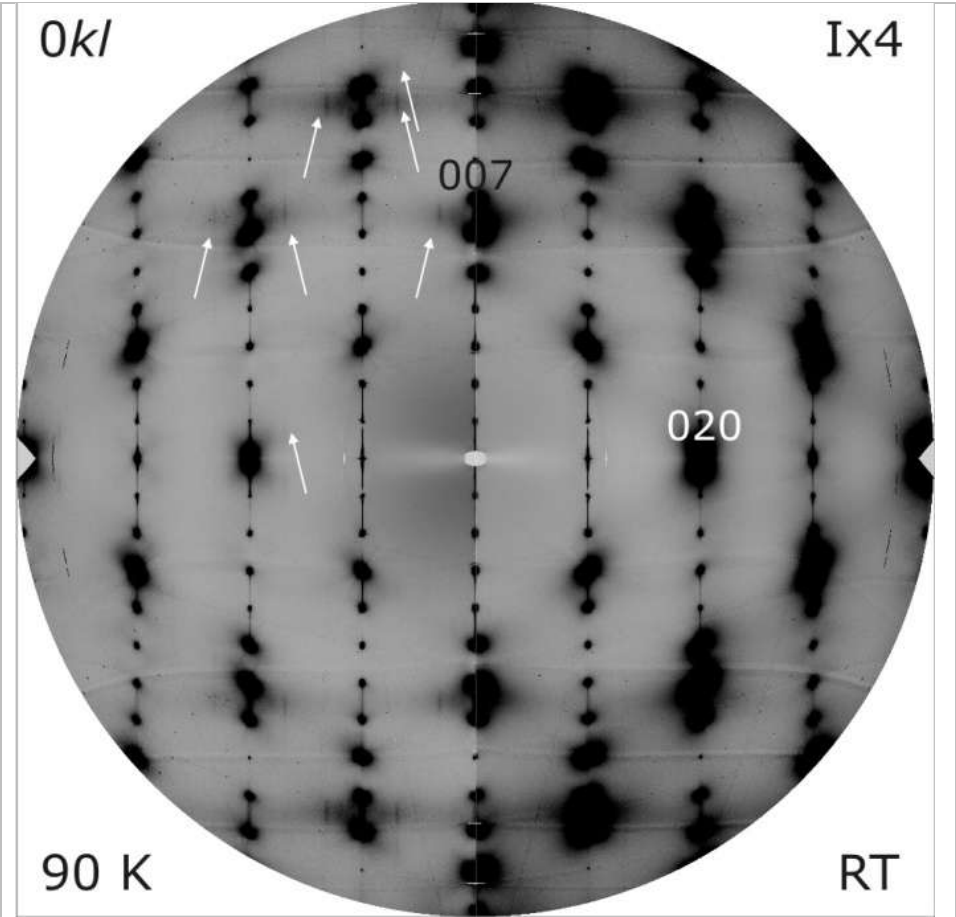


Figure 1: Diffuse scattering mapping of the $(0\ k\ l)$ of $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ plane at $T = 90\ \text{K}$ (left) and at room temperature (right)

On the vortex core states seen by STM in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$



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Keywords: Scanning Tunneling Spectroscopy – YBCO – Vortex core

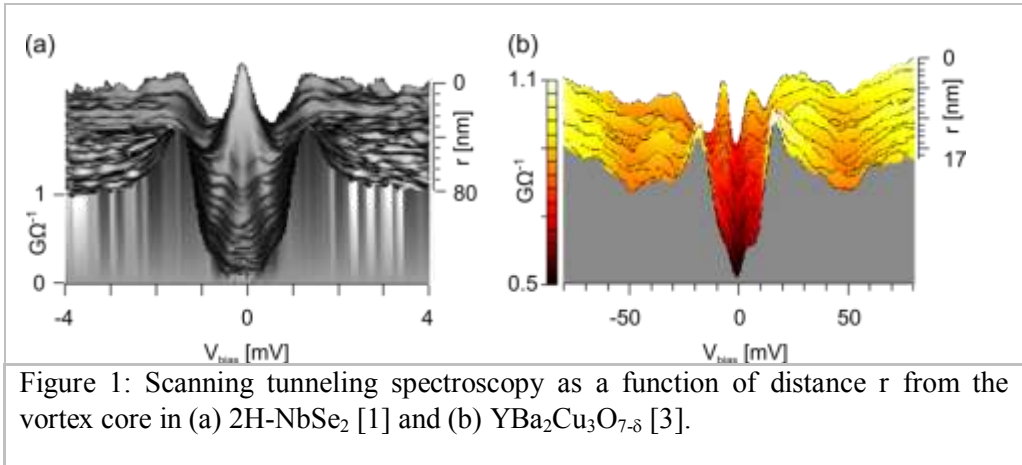
The normal state of high temperature superconductors (HTS) has been puzzling the scientific community as much as the superconducting phase itself. In the simplest description of a type II superconductor in the presence of a magnetic field, the vortex cores should provide insight into the normal state of superconducting materials. The electronic local density of states can be measured as a function of position in a vortex core using scanning tunneling spectroscopy (STS). The first successful STS vortex core spectroscopy was carried out by Hess et al [1] on 2H-NbSe_2 and their findings (Fig. 1a) could be fully explained in the framework of conventional s-wave superconductivity and Caroli de Gennes quasiparticle states bound to the normal core. Theory predicts a minigap at the core center and dispersing states as a function of distance r from the core. While the experiment clearly shows the latter, it measures a conductance peak at the Fermi level at the core center. This was explained in terms of finite resolution and temperature, as well as the level of cleanliness of the material [2].

The situation is more difficult and not yet settled in the case of high temperature superconductors. The first detailed STS mapping of a vortex core in any HTS was carried out on $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (Y123) and revealed a very different signature (Fig. 1b). STS finds a clear gap at the Fermi level at the core center and two non-dispersing states vanishing with increasing distance from the vortex core. Theory has so far not been able to fully describe this spectroscopic signature of a vortex core in the context of the d-wave superconductivity prevailing in Y123.

We will present a new scanning tunneling microscopy study of Y123 showing that the electronic states best resolved at the vortex center are in fact not a characteristic feature of the vortices [4]. We observe the same spectroscopic features independent of position with respect to the vortex core and even in the absence of any applied magnetic field. We discuss the implications of these new observations and their possible link with the normal state and recently reported electronic (ordered) phases competing, cooperating or coexisting with superconductivity.

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Breaking the Waves – Experiments and theories on fractional excitations from 1D to 2D



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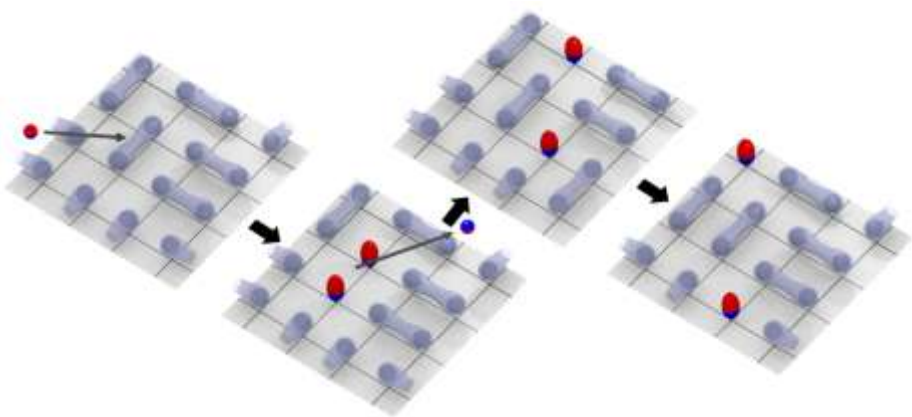
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Quantum magnets have occupied the fertile ground between many-body theory and low-temperature experiments on real materials since the early days of quantum mechanics. However, our understanding of even deceptively simple systems of interacting spin-1/2 particles is far from complete. The quantum square-lattice Heisenberg antiferromagnet, for example, exhibits a striking anomaly of hitherto unknown origin in its magnetic excitation spectrum. This quantum effect manifests itself for excitations propagating with the specific wavevector $(\pi, 0)$. We use polarized neutron spectroscopy to fully characterize the magnetic fluctuations in the metal-organic compound $\text{Cu}(\text{DCCO})_2 \cdot 4\text{D}_2\text{O}$, a known realization of the quantum square-lattice Heisenberg antiferromagnet model. Our experiments reveal an isotropic excitation continuum at the anomaly, which we analyse theoretically using Gutzwiller-projected trial wavefunctions. The excitation continuum is accounted for by the existence of spatially extended pairs of fractional $S = 1/2$ quasiparticles, 2D analogues of 1D spinons. Away from the anomalous wavevector, these fractional excitations are bound and form conventional magnons. Our results establish the existence of fractional quasiparticles in the high-energy spectrum of a quasi-two-dimensional antiferromagnet, even in the absence of frustration.

Illustration of fractionalization in the square lattice antiferromagnet: The electron's magnetic moments pair up into a non-magnetic quantum entangled state called a singlet (connected pairs of blue spheres) forming a singlet sea. An incoming particle (red and blue sphere), for instance a neutron, polarize a singlet into two fractional particles called spinons (elongated red and blue spheres). Once created, the two spinons can float free of each other onto the singlet sea.

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SESSION 34

Vortices and Emergent Defects in Iron-based superconductors

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The pronounced electronic anisotropy observed in several experiments probing the iron-based superconductors is currently a topic of great interest and controversy.[1] I will discuss novel disorder effects in the nematic phase above the transition temperature to the $(\pi, 0)$ stripe ordered magnetic state but below the orthorhombic structural transition. The anisotropic spin fluctuations in this region can be frozen by disorder, to create elongated magnetic droplets whose anisotropy grows as the magnetic transition is approached. Such states act as strong anisotropic defect potentials that scatter with much higher probability perpendicular to their length than parallel, although the actual crystal symmetry breaking is tiny. From the calculated scattering potentials, relaxation rates, and conductivity in this region we conclude that such emergent defect states are essential for the transport anisotropy observed in experiments.[2] Thus, a full understanding of the transport anisotropy in iron pnictides requires both intrinsic nematic susceptibility and concomitant emergent impurity response. Below the spin density wave transition the nematogens freeze into dimer states that show many characteristics in agreement with STM measurements.[3] Finally, I will discuss our recent modeling of the vortex states in iron-based materials.[4]

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Magnetism without tetragonal symmetry breaking in iron-based superconductors



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Keywords: unconventional superconductivity – magnetic stripes – electronic liquid-crystalline phases

Superconductivity in the iron-based materials is observed in close proximity to a uniaxial magnetic stripe state, which breaks both the $O(3)$ spin-rotational symmetry and also the tetragonal C_4 symmetry of the lattice. One of its most remarkable properties is that fluctuations can cause the symmetry-breaking to take place in two steps: first, at higher temperatures, the Ising-like symmetry related to lowering the point group symmetry from tetragonal C_4 to orthorhombic C_2 is broken, but the $O(3)$ spin-rotational symmetry is preserved. Then, at lower temperatures, spin-rotational symmetry is broken and the system goes to the magnetically ordered state. The paramagnetic-orthorhombic state is called nematic and can be understood as a vestigial order of the underlying stripe magnetic instability.

Recent experiments in a series of hole-doped iron pnictides, however, reported a new magnetically ordered state, near optimal doping, that does not break tetragonal symmetry despite displaying magnetic Bragg peaks at the same momenta as the stripe magnetic phase. These magnetic ground states are compatible with biaxial (double-Q) magnetic stripes, forming C_4 -symmetric spin configurations that are either non-collinear (a spin-vortex crystal) or non-uniform (a charge-spin density-wave). In this talk, we show that these phases are naturally captured by a microscopic itinerant approach for the magnetism of the iron pnictides [1,2,3]. In particular, deviations from perfect nesting, allied to residual electronic interactions not responsible for the magnetic instability, favor these C_4 magnetic phases at the edges of the magnetic dome. We present the signatures of these C_4 phases in the electronic and spin-wave spectra, and also demonstrate that they compete stronger with the superconducting state than the C_2 magnetic stripe phase. Finally, we discuss the vestigial states associated with these tetragonal magnetic phases. While the non-uniform C_4 configuration supports a vestigial charge density-wave state, which breaks translational symmetry but preserves tetragonal symmetry, the non-collinear C_4 configuration supports a vestigial spin-current density-wave state, which, besides the translational symmetry, also breaks a chiral symmetry of the system. We discuss the importance of the magnetic tetragonal phases to understand

the origin of magnetism in the iron-based superconductors, and their impact on the superconductivity displayed by these materials.

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Static and dynamical correlations of strongly disordered superconductors

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Keywords: disordered superconductors, electromagnetic response, attractive Hubbard model

In the last decades the failure of the BCS paradigm of superconductivity in several correlated materials led to a profound modification of the description of the superconducting phenomenon itself. A case in point is the occurrence of Cooper pairing and phase coherence at distinct temperatures, associated respectively with the appearance of a single-particle gap and a non-zero superfluid stiffness. This particular behavior is observed in several materials, which range from high-temperature cuprate superconductors to strongly-disordered films of conventional superconductors. For the latter systems scanning tunneling microscopy measurements have revealed that the superconducting state becomes inhomogeneous, segregating into domains of large and suppressed superconducting order parameter.

In this contribution we will discuss the static and dynamical response of such systems based on studies of the attractive Hubbard model with strong on-site disorder and by including fluctuations beyond the Bogoljubov-de Gennes approach.

We find a decoupling of charge and amplitude correlations with increasing disorder due to the formation of superconducting islands. This emergent granularity also induces an enhancement of the charge correlations on the SC islands whereas amplitude fluctuations are most pronounced in the 'insulating' regions. While charge and amplitude correlations are short-ranged at strong disorder we show that current correlations have a long-range tail due to the formation of percolative current paths in agreement with the constant behavior expected from the analysis of the one-dimensional xy-model

Moreover we show that for strongly disordered superconductors phase modes acquire a dipole moment and appear as a subgap spectral feature in the optical conductivity.

Tunable Multifractality in Quantum Matter



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Keywords: Multifractality, Anderson localisation, Reentrant Superconductivity

In strongly disordered materials, electronic wavefunctions develop multifractal spatial distributions in the vicinity of the Anderson transition between extended and localised states [1]. Such multifractal ordering has been predicted to enhance electron-electron interactions [2]. One may therefore envisage the possibility of tuning the ground state of a correlated electron material via disorder. For the case of disordered superconductors, a large multifractal enhancement is expected in the pairing interaction (and hence the critical temperature T_c), provided that the Coulomb repulsion is weak [3,4]. However, no such rise in T_c has yet been observed experimentally, due to the suppression of superconductivity by emergent granularity and a dynamically-augmented Coulomb repulsion in highly disordered materials [5].

Using a range of experimental techniques (including electrical transport, magnetization and X-ray diffraction/scattering), we demonstrate that multifractal pairing enhancement does in fact occur in the quasi-one-dimensional superconductor $\text{Na}_{2-\delta}\text{Mo}_6\text{Se}_6$. This enhancement develops due to the combination of random Na vacancy disorder with an intrinsically screened Coulomb interaction. We observe the pairing temperature T_{ons} to rise monotonically as the Anderson-Mott mobility edge is approached from the metallic side, in quantitative agreement with a multifractal enhancement model [4]. Strikingly, T_{ons} continues to rise in the localised phase after crossing the mobility edge, in accordance with theoretical predictions [3]. The upper critical field H_{c2} exceeds the weak-coupling Pauli limit by a factor of at least 4 in the localised regime, indicating a large increase in the superconducting gap energy.

Our results provide the first experimental perspective onto the unknown physics of correlated electron materials in the absence of Coulomb repulsion. We also show that the unique interplay between superconductivity and localisation in nanofilamentary materials renders them ideal building blocks for functional superconductors. In an inhomogeneous matrix of disordered nanowires, electron delocalisation leads to reentrant phase coherence upon raising the temperature, magnetic field or electric current, in direct contrast to the behaviour of conventional homogeneous superconductors.

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SESSION 35

Heterogeneous and complex superconductors as seen by synchrotron x-ray (sub)micron beam measurements



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Keywords : X ray microdiffraction – Charge Density Waves – Interstitial Oxygen

Outstanding structure-function relationship of new advanced materials are often due to the composition heterogeneity and/or the competition between two or more coexisting phases at different length scales [1-3]. In oxygen doped copper oxides, the competition between interstitial oxygen, i-O, ordering and charge density waves, CDW, is believed to play a fundamental role in High Temperature Superconductivity (HTS) [4, 5]. Taking advances from X ray synchrotron radiation features and from optical focusing devices, we visualize spatial distribution of interstitial oxygen and electronic CDW fluctuations with fine details in real space. We report recent results about the possibility to control the nanoscale phase separation generated by i-O and charge ordering, affecting the functionality in different superconducting systems such as $\text{La}_2\text{CuO}_{4+y}$, $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ and $\text{HgBa}_2\text{CuO}_{4+y}$ [6].

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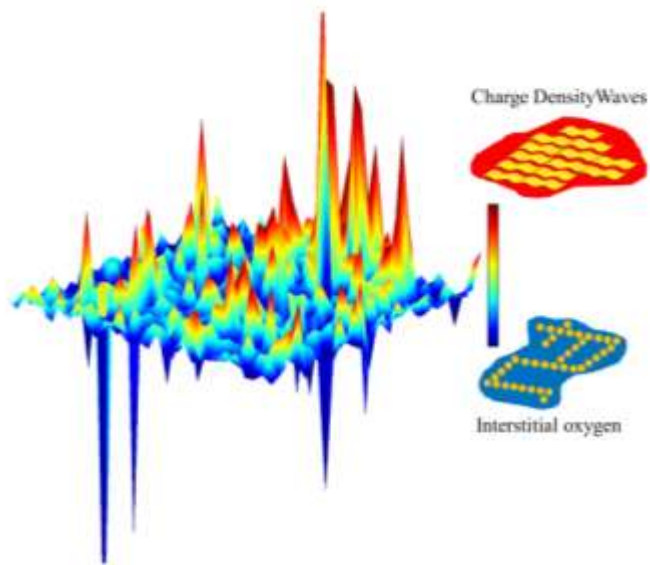


Figure 1. Spatial anticorrelated distribution of charge density waves on the CuO_2 atomic plane and interstitial oxygen dopants in the spacer rock salt layers in the single layer Hg1201 superconductor at optimum doping. [6]

Heavy fermion liquid formation, superconductivity and the ‘hidden order’ in URu₂Si₂



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Keywords: heavy fermions – superconductivity – hidden order

The interactions between localized and delocalized electrons in the heavy fermion materials result in fascinating and unexpected quantum phenomena, which continue to challenge condensed matter researchers. A most prominent example is the enigmatic ‘hidden order’ (HO) state in URu₂Si₂, which is characterized by a large loss of entropy at T_{HO} = 17.5 K [1]. We first present a high-resolution angle-resolved photoemission of the heavy-fermion superconductor URu₂Si₂. Detailed measurements as a function of both photon energy and temperature allow us to disentangle a variety of spectral features [2], revealing the evolution of the low-energy electronic structure as a function of temperature (see Figure 1). Upon crossing the Kondo temperature T_K at around 70 K, heavy fermion states form below the Fermi level, which remain incoherent and do not show any significant dispersion as long as T > T_{HO}. Upon entering the hidden order phase, these incoherent states begin to disperse and rapidly transform into a coherent heavy fermion liquid. This experimentally observed temperature evolution of the low-energy electronic structure is found to be in excellent agreement with a many-body analysis of the Kondo lattice Hamiltonian by means of the projective renormalization method [3,4]. This analysis together with our experimental results implies that the hidden order of URu₂Si₂ is, in fact, not a long-range ordered state. Rather it turns out to be characterized by a sudden reorganization of heavy quasiparticle states close to the Fermi energy mediated by the RKKY interaction.

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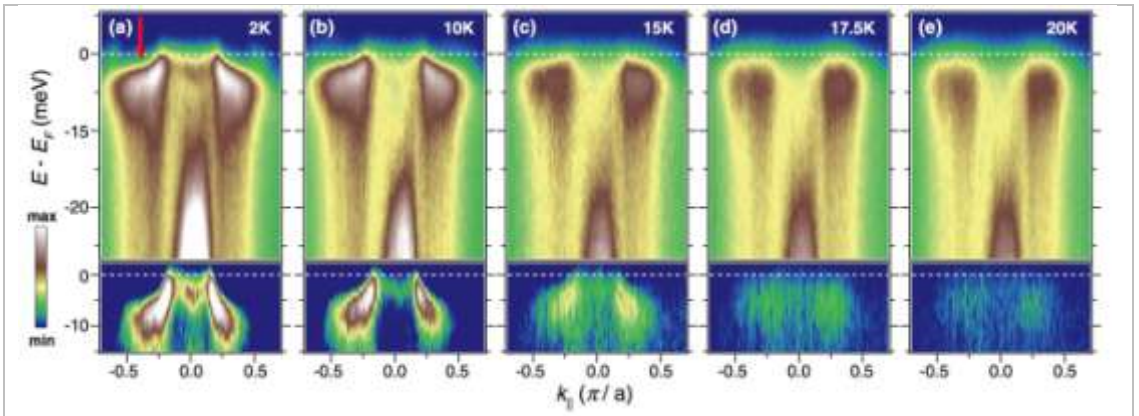


Figure 1: a)–(e): Temperature evolution of the ARPES intensity plots of URu_2Si_2 measured along the $(0,0)$ - $(\pi,0)$ direction at 31 eV photon energy over the temperature range 2–20 K. In the lower panel, ARPES spectral maps obtained after subtracting the corresponding intensity map at 25 K are shown. The color scale has been adjusted to show only the positive part of the subtracted spectrum. Note that all the spectral maps in the lower panel are plotted keeping the range of the color scale fixed. Below T_{HO} a coherent heavy fermionic band rapidly emerges which simultaneously becomes sharper and more dispersive as the sample is cooled down. From Ref. 2.

Momentum-space structure of quasielastic spin fluctuations in $\text{Ce}_3\text{Pd}_{20}\text{Si}_6$



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Keywords: magnetically ordered materials – electron states – condensed matter

Among heavy-fermion metals, $\text{Ce}_3\text{Pd}_{20}\text{Si}_6$ is one of the heaviest-electron systems known to date [1, 2]. Here we used high-resolution neutron spectroscopy to observe low-energy magnetic scattering from a single crystal of this compound in the paramagnetic state. We investigated its temperature dependence and distribution in momentum space, which was not accessible in earlier measurements on polycrystalline samples. At low temperatures, a quasielastic magnetic response with a half-width $\Gamma \approx 0.1$ meV persists with varying intensity all over the Brillouin zone. It forms a broad hump centered at the (111) scattering vector, surrounded by minima of intensity at (002), (220) and equivalent wave vectors. The momentum-space structure distinguishes this signal from a simple crystal-field excitation at 0.31 meV, suggested previously [3,4], and rather lets us ascribe it to short-range dynamical correlations between the neighboring Ce ions, mediated by the itinerant heavy f-electrons via the RKKY mechanism. With increasing temperature, the energy width of the signal follows the conventional $T^{1/2}$ law [5], $\Gamma(T) = \Gamma_0 + A\sqrt{T}$. The momentum-space symmetry of the quasielastic response suggests that it stems from the simple-cubic Ce sublattice occupying the 8c Wyckoff site, whereas the crystallographically inequivalent 4a site remains magnetically silent in this material.

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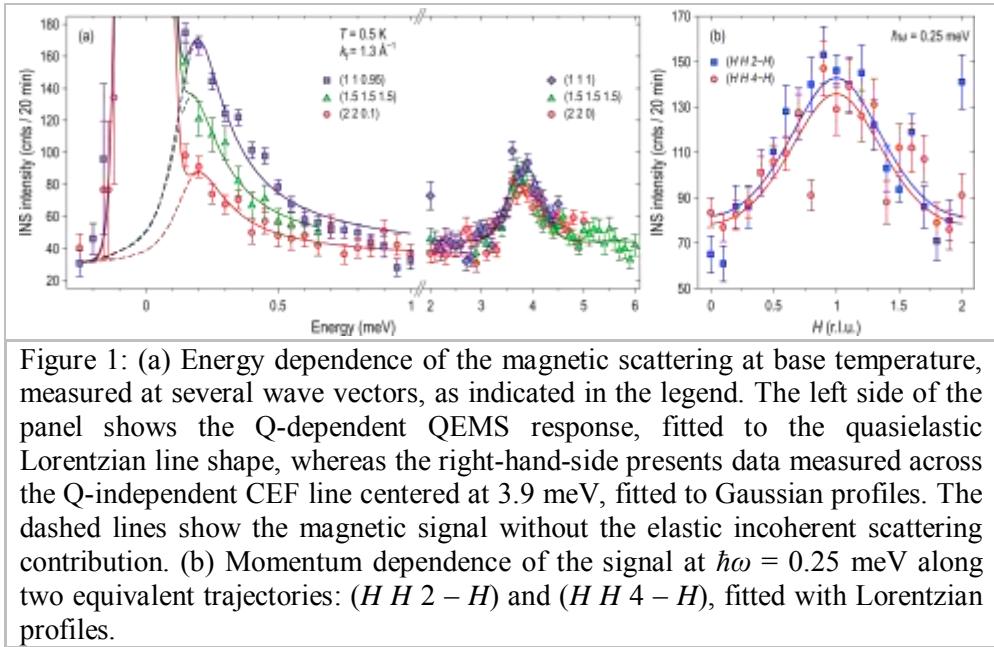


Figure 1: (a) Energy dependence of the magnetic scattering at base temperature, measured at several wave vectors, as indicated in the legend. The left side of the panel shows the Q-dependent QEMS response, fitted to the quasielastic Lorentzian line shape, whereas the right-hand-side presents data measured across the Q-independent CEF line centered at 3.9 meV, fitted to Gaussian profiles. The dashed lines show the magnetic signal without the elastic incoherent scattering contribution. (b) Momentum dependence of the signal at $\hbar\omega = 0.25 \text{ meV}$ along two equivalent trajectories: $(H H 2 - H)$ and $(H H 4 - H)$, fitted with Lorentzian profiles.

Interplay of disorder and spin frustration near the critical point: A case study of CoAl_2O_4 by local spin probe techniques



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Keywords: spin frustration, disorder, critical point, magnetic resonance

We present a detailed experimental study with three local spin probe techniques, NMR, μSR and ESR, of magnetic properties of the CoAl_2O_4 single crystal where the Co spins form a frustrated spin lattice with the diamond structure.

We find that in the studied single crystal the degree of structural disorder due to the Al-Co site inversion is optimally tuned to obtain insights onto its influence on the ground state and on the low energy magnetic dynamics of the frustrated diamond spin lattice. Inhomogeneous broadening of ESR and NMR lines at temperatures below 30 – 50 K indicates the growth of short-range spin correlations. The analysis of the NMR and μSR relaxation rates evidences a critical slowing down of spin fluctuations at a characteristic temperature $T^* = 8$ K which suggests the onset of a quasi-static order at this temperature. Most probably the spin order is short-range and unconventional which is manifested by the overdamped oscillations of the muon spin polarization and a continuous line broadening of ESR and NMR lines below T^* .

Since in the phase diagram of the diamond spin lattice CoAl_2O_4 is located close to the special critical point which separates collinear and noncollinear spin phases [1], it appears in our results that Al atoms at the Co sites acting as quenched impurities smear the phase boundary between the two phases. This can yield a competition between the two ground states with the low-lying spin spiral excitations responsible for an inhomogeneous magnetic dynamics. We argue that our experimental findings may have important implications for recent theories of an "order by disorder" mechanism in the frustrated diamond spin lattice.

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Triplet pairing and memory effect in S/F nanostructures as a base for superconducting spintronics



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Keywords: proximity effect, heterostructures superconductor/ferromagnet, triplet pairing

Superconducting state in proximity coupled heterostructures superconductor/ferromagnet (S/F) has a lot of peculiarities in comparison with uniform BCS- state of conventional superconductors. The theory of non-uniform superconductivity predicts existing together with a short-range singlet pairing generation of two additional components: an even-in-frequency and a long-range, odd-in-frequency triplet pairing in samples with two ferromagnetic (F) layers at non-collinear alignment (NCA) of the magnetizations of the F-layers [1-3]. This triplet pairing we have detected experimentally in a Nb/Cu₄₁Ni₅₉/NL/Co/CoO_x spin-valve-type proximity effect coupled heterostructure (with a spacer of normal conducting metal, NL- thin layer between two F-layers) [4]. The resistance of the sample as a function of an external magnetic field shows that the system is superconducting at a collinear alignment of the Cu₄₁Ni₅₉ and Co layers magnetic moments, but switches to the normal conducting state at a NCA configuration. The last is the evidence that the superconducting transition temperature T_c for NCA is lower than the fixed measuring temperature. The existence of a minimum T_c , at the NCA regime below that one for parallel or antiparallel alignments of the F-layer magnetic moments, is consistent with the theoretical prediction of the appearance of the long-range triplet pairing. We have found, that the resistive state of the nanolayered hybrid superconductor/ferromagnet spin-valve structure (SSV) depends on the preceding magnetic field polarity. The detected effect is based on a strong exchange bias (about 2 kOe) in the diluted ferromagnetic copper-nickel alloy and generation of a long range odd in frequency triplet pairing component. The difference of high and low resistance states at zero magnetic field is 90% of the normal state resistance for a transport current of 250 mA and still around 42% for 10 mA. Both logic states of the structure do not require biasing fields or currents in the idle mode. This detected memory effect opens perspectives for design of logic elements for superconducting spintronics.

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SESSION 36

Superconductivity and Magnetism in Iron Selenides

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Keywords: pairing mechanism, iron-based superconductors, Mössbauer effect, pressure

The pairing mechanism in Fe-based superconductors is still an opened question. Appear more experimental facts evidencing that SC can be mediated by AF spin fluctuations acting as “glue” for superconducting pairing [1,2]. FeSe-based superconductors do not reveal magnetically ordered parent phase and spin density waves. However, the doping of copper into the FeSe introduces local moments localized on the iron and glassy magnetic interactions appear. Application of pressure leads to restoration of superconductivity in Cu-doped FeSe under pressure [3] which could be associated with disappearance of spinglass-type magnetic state. Corresponding Mössbauer Synchrotron spectroscopic pressure studies of non-SC Fe_{0.97}Cu_{0.04}Se are in progress. Mössbauer spectroscopic studies of FeSe intercalated with LiNH₂ showing the superconducting transition temperature of 43 K [4] have revealed pronounced magnetic fluctuations which increase in the superconducting state below T_C scaling with a superconducting transition. These features are not seen in de-intercalated samples as well as in the precursor FeSe with T_C lower than 10 K [6]. Based on mentioned experiments we conclude that the superconducting pairing in FeS-based SC is mediated by antiferromagnetic spin fluctuations [7].

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Superconductivity of iron selenides intercalated with molecular spacers



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Keywords: iron selenides, intercalated, organic spacer

Single crystals of $A_x\text{Fe}_{2-y}\text{Se}_2$ ($A = \text{K}, \text{Rb}, \text{Cs}$) are superconducting at relatively narrow iron and alkali metal contents. Furthermore, the transformation from a superconducting to an insulating antiferromagnetic state is intimately related to their composition, which in fact deviates from the ideal 122 stoichiometry and is extremely difficult to control during synthesis by conventional high temperature methods. The whole system is already known since 2010 but there are many open questions and controversies regarding the origins of superconductivity and stoichiometry of superconducting phases. It has been shown in recent years that the single crystals of intercalated iron chalcogenides manifest reversible phase separation at low temperatures. The questions about the exact nature of superconducting phases led to further investigations on alternative low temperature synthetic routes. The first intercalated material prepared by solvothermal technique revealed a whole list of compounds with significantly improved $T_c \sim 40 - 46\text{K}$, but with superconducting volume fractions between 0.5 and 30%. The possibility of additional modifications of layered structure of FeSe by molecular spacers attracted the attention of researches to soft chemistry. Further investigations of solvothermal routes brought intercalated materials with nearly 80% shielding fractions. Despite some discrepancies regarding the nature of guest molecules (complexes of alkali metals with ammonia, lithium amide or both of them) all the reports are consistent with regards to the value of superconducting transition and the crystal structure of the intercalated material. The structure of the solvothermally intercalated superconductor adopts body centered tetragonal unit cell with $I4/mmm$ symmetry with slightly compressed in-plane lattice parameters and significantly expanded c-axis in comparison to single crystalline alkali metal intercalated iron chalcogenides. The solvent molecules co-inserted to the host structure significantly modify not only the superconducting properties but also the stability of the whole system. Layered iron chalcogenides seem to be quite flexible with regards to the possibility of their intercalation with spatial molecular spacers, which in most cases, results in the significant enhancement of transition temperature.

Superconducting Properties of $\text{Ln}_4\text{Fe}_2\text{As}_2\text{Te}_{1-x}\text{O}_{4-y}\text{F}_y$ ($\text{Ln}=\text{Pr}, \text{Sm}, \text{Gd}$)



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Keywords: superconductivity – iron based superconductors – pressure effect – upper critical field – electrical anisotropy.

Recently new type of iron based superconductor $\text{Ln}_4\text{Fe}_2\text{As}_2\text{Te}_{1-x}\text{O}_{1-y}\text{F}_y$ ($\text{Ln}=\text{Pr}, \text{Sm}, \text{Gd}$) has been found [1, 2]. This superconductor reveals T_c up to 46 K upon substitution of the rare earth element and optimum fluorine-doping. The tetragonal crystal structure, labelled “42214”, presents an alternation of FeAs conducting layers and Ln_2O_2 spacing layers separated along the c direction by Te atoms (Fig. 1a). The lattice constants a and b are comparable to those found in the “1111” or “122” structures but the c axis parameter is considerably larger.

In this presentation we will report a detailed electrical transport study of $\text{Ln}_4\text{Fe}_2\text{As}_2\text{Te}_{1-x}\text{O}_{4-y}\text{F}_y$ single crystals under pressure and in high magnetic fields.

Measurements of upper critical fields along different crystallographic directions result in $\mu_0 H_{c2}(0) \sim 50$ T for $\text{Sm}_4\text{Fe}_2\text{As}_2\text{Te}_{1-x}\text{O}_{4-y}\text{F}_y$. This compound shows an unprecedented superconducting anisotropy $\gamma_H = H_{c2}^{ab}/H_{c2}^c = \sqrt{m_c/m_{ab}} \simeq 32$ near T_c , that decreases at lower temperatures. Hydrostatic pressure up to 2 GPa linearly decreases the critical temperature as observed in overdoped cuprate superconductors. Direct measurement of electronic anisotropy is performed with the support of microfabrication techniques, showing a value of $\rho_c/\rho_{ab}(300\text{K}) \simeq 5$ that raises up to 19 near T_c .

In contrast, the pressure dependence of T_c for fluorine free $\text{Pr}_4\text{Fe}_2\text{As}_2\text{Te}_{1-x}\text{O}_4$ measured (up to ~ 2 GPa) reveals increasing of T_c from 26 to 27 K. Upper critical field is considerably smaller for fluorine free samples $\mu_0 H_{c2}(0) \sim 7$ T.

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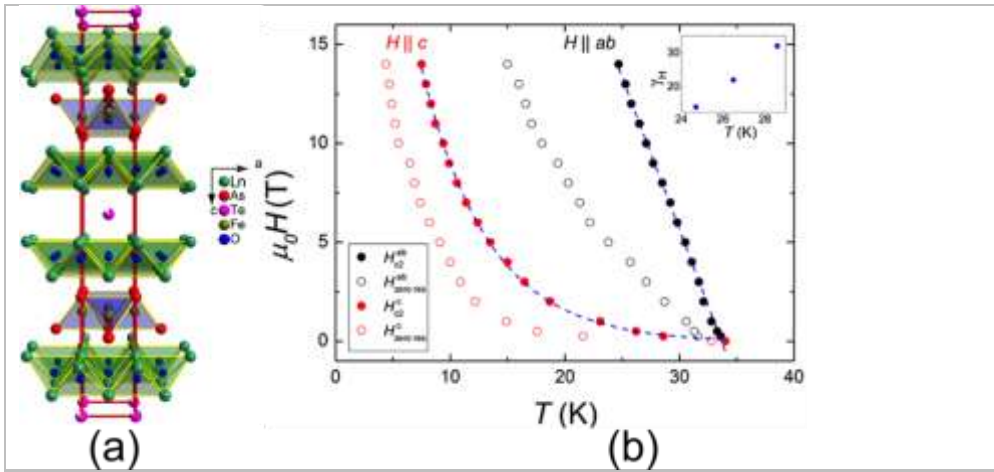


Figure 1: a) Crystal structure fragment of $\text{Ln}_4\text{Fe}_2\text{As}_2\text{Te}_{1-x}\text{O}_4$ ($\text{Ln}=\text{Pr}, \text{Sm}, \text{Gd}$). Blue and green polyhedra indicate FeAs_4 and PrO_4 tetrahedra, respectively. The unit cell is outlined in red; b) Phase diagram for $\text{Sm}_4\text{Fe}_2\text{As}_2\text{Te}_{1-x}\text{O}_{4-y}\text{F}_y$ from resistivity measurement with $H \parallel ab$ (black points) and $H \parallel c$ (red points) as a function of temperature. Filled dots correspond to values of upper critical field (H_{c2}) estimated from the midpoint of resistive transitions while empty dots represents the fields evaluated at the zero-resistivity point. The inset shows the magnetic field anisotropy as function of temperature near T_c . Blue dashed line are the fits used to extract the values of $H_{c2}^{ab}(0)$ and $H_{c2}^c(0)$.

SESSION 37

Nanoscopic inhomogeneity, intrinsic charge instability and metal-to-superconductor transition in oxide heterostructures



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Keywords: superconducting oxide interfaces, electronic phase separation, density-driven quantum criticality

Experiments in oxide interfaces like $\text{LaAlO}_3/\text{SrTiO}_3$ or $\text{LaTiO}_3/\text{SrTiO}_3$ (LXO/STO) heterostructures, strongly indicate that the 2D electron gas at the interface is strongly inhomogeneous on the nanoscopic scale. Disorder induces a distribution of local superconducting critical temperatures accounting well for transport and tunnel experiments [1]. With lowering the temperature, global superconductivity establishes as soon as percolation occurs within the superconducting clusters. Microscopic mechanisms for electronic phase separation (EPS) based on Rashba spin-orbit coupling (RSOC) [2] and/or electrostatic electron confinement at the interface [3] (see Fig.1) are investigated to establish a possible intrinsic origin for this inhomogeneous character of LAO/STO or LTO/STO interfaces.

The density dependence of the RSOC on the local inhomogeneous electron density also opens the way to novel spin-Hall effects.

Both RSOC and electrostatic confinement not only provide an intrinsic mechanism for the observed inhomogeneity, but also open the way to new interpretations of the observed quantum critical behaviour of LTO/STO [4]. We investigate the effects of temperature, gating, and magnetic field on the charge instability finding a novel type of quantum critical point related to the vanishing of the critical temperature of the EPS [2,3,5].

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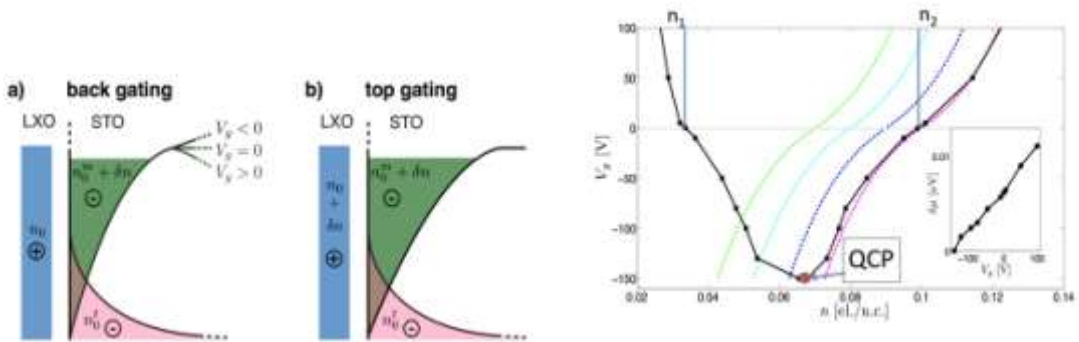


Figure 1: (Top) Sketch of the interface for back (a) and top (b) gating. The confining potential depends on both mobile (green) and trapped (pink) charges. Applying a positive (negative) voltage, δn electrons per unit cell are added to (subtracted from) the interface and the potential changes accordingly.

(Bottom) Gating versus density phase diagram for the back gated LXO/STO interface. n_1 and n_2 are determined by the Maxwell construction. The colored curves correspond to (from right to left) $n_0 = 0.07, 0.08, 0.09, 0.1$ el./u.c. at $V_g = 0$.

Inset: Energy gain due to phase separation as a function of gating potential.

Reconstruction effects at complex oxide interfaces studied with resonant x-ray scattering



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Keywords: electronic reconstruction, orbital reconstruction, complex oxides

Different reconstruction phenomena can occur at solid-state interfaces and surfaces, especially in complex transition-metal oxide heterostructures, which offer a rich phenomenology due to their multivalent character and non-trivial orbital configuration. These degrees of freedom allow the reconstruction not only by chemically disrupting the interfaces or by structural displacements, but also through electronic paths: Electronic, magnetic and orbital reconstructions are under intense scrutiny. Resonant x-ray reflectivity (RXR) is the only tool with sufficient spatial and energy resolution, element specificity and sensitivity to address virtually all aspects of reconstructions in transition metal oxide heterostructures [2].

The $\text{LaAlO}_3/\text{SrTiO}_3$ (LAO/STO) system is being studied due to the polar-non-polar character of the interface and the idea that the observed high-mobility electron liquid (2DEL) at the interface is due to electronic reconstruction [1]. However, the reported electron density at the interface vary widely [3,4], from values close to the expected 0.5 electrons per unit cell to values deviating orders of magnitude.

Here, we demonstrate how RXR can be used to determine the chemical, electronic and valence state profiles and solve the above discrepancy following the scheme in Fig. 1.

Next to the LAO/STO system, we also study electronic reconstruction at the surfaces of other polar systems such as LaCoO_3 , which have the advantage of having only one polar/non-polar (vacuum) interface, rendering the analysis more robust.

Finally, we will report the observation and analysis of orbital reconstruction at the surface of SrTiO_3 films and discuss its implications for the physics of this system.

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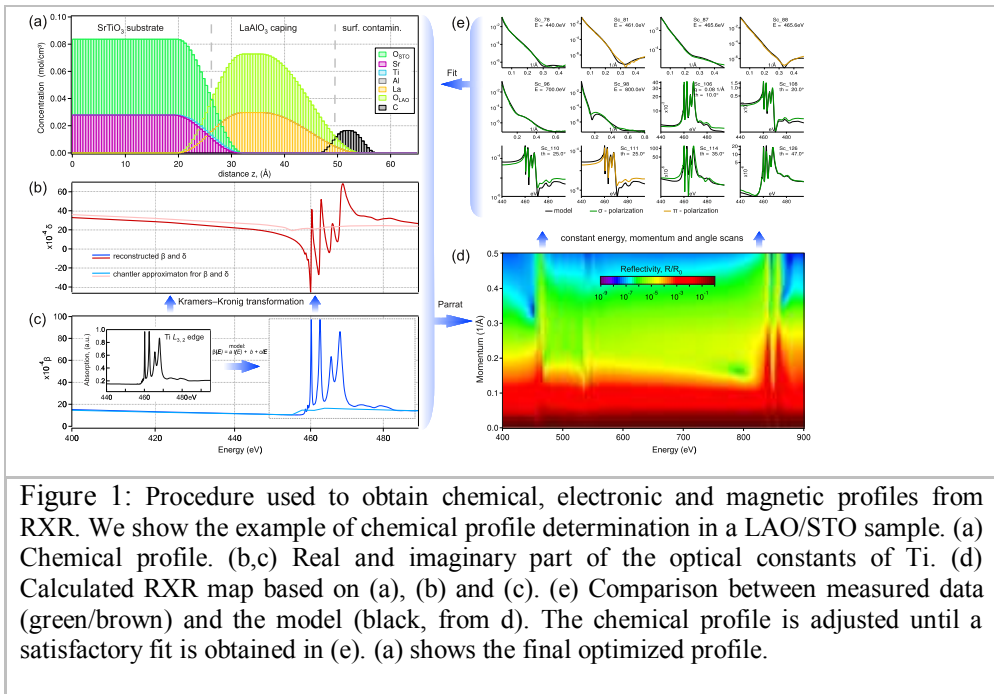


Figure 1: Procedure used to obtain chemical, electronic and magnetic profiles from RXR. We show the example of chemical profile determination in a LAO/STO sample. (a) Chemical profile. (b,c) Real and imaginary part of the optical constants of Ti. (d) Calculated RXR map based on (a), (b) and (c). (e) Comparison between measured data (green/brown) and the model (black, from d). The chemical profile is adjusted until a satisfactory fit is obtained in (e). (a) shows the final optimized profile.

Top-gating control of the 2-DEG at the LAO/STO interface



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Keywords: oxides interfaces –superconductivity –Rashba spin-orbit coupling

Recent results show material and electronic complexity in transition metal oxides. Transition metal oxides display a great variety of quantum electronic behaviors where correlations often play an important role. The achievement of high quality epitaxial interfaces involving such materials gives a unique opportunity to engineer artificial materials where new electronic orders take place. It has been shown recently that a superconducting two-dimensional electron gas 2DEG could form at the interface of two insulators such as LaAlO₃ and SrTiO₃ or LaTiO₃ (a Mott insulator) and SrTiO₃ [1]. An important feature of these interfaces lies in the possibility to control their electronic properties, including superconductivity and spin-orbit coupling (SOC) with field effect [3-5]. However, so far, experiments have been performed almost exclusively with a metallic gate at the back of the substrate, which makes difficult to control these properties at a local scale.

In this presentation, we will report on the realization of a top-gated LaAlO₃/SrTiO₃ device whose physical properties, including superconductivity and Rashba SOC, can be tuned over a wide range of electrostatic doping. In particular, we will present a phase diagram of the interface and compare the effect of the top-gate and back-gate on the mobility, superconducting properties and Rashba SOC [6]. Finally, we will discuss the field-effect modulation of the Rashba spin-splitting energy extracted from the analysis of magneto-transport measurements. Our result paves the way for the realization of mesoscopic devices where both superconductivity and Rashba SOC can be tuned locally.

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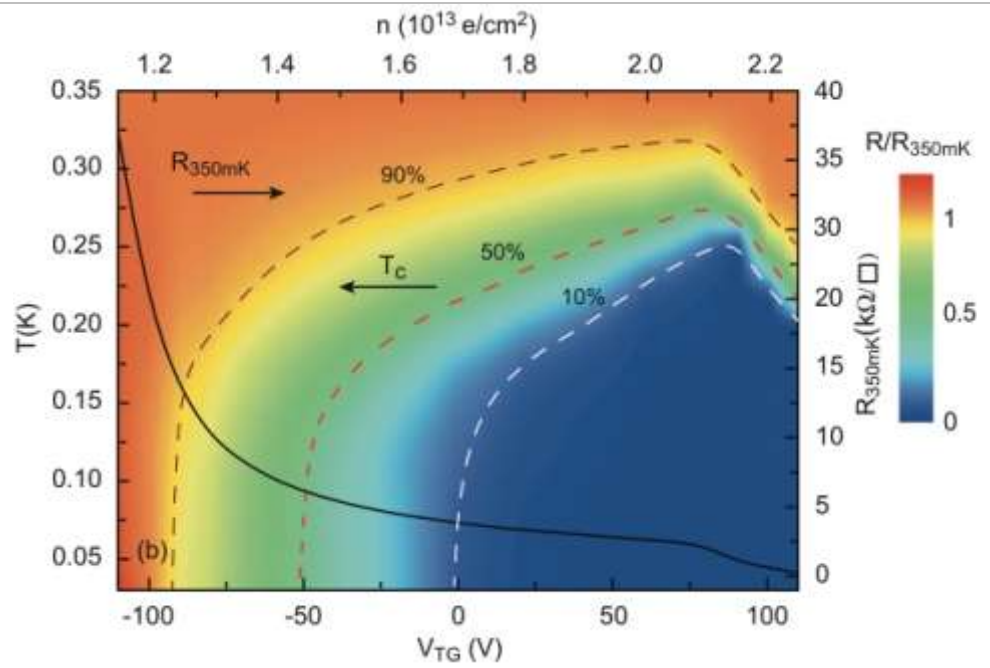
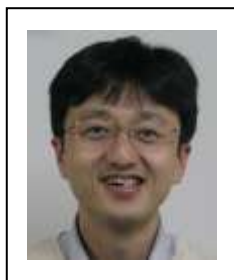


Figure 1: Sheet resistance normalized by its value at $T=350\text{mK}$ plotted with a colour scale as a function of temperature (left axis) and top-gate voltage. The carrier densities corresponding to the top-gate voltages have been added in the top axis. The sheet resistance at $T=350 \text{ mK}$ is plotted as a function of top-gate voltage on the right axis and the critical temperature T_c is plotted as function of the top-gate voltage on the left axis.

Effects of high pressure on spin-driven ferroelectricity



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Keywords: Multiferroics, high pressure, magnetoelectric effect

A class of multiferroics such as TbMnO₃ exhibit a remarkable change in electric polarization by the application of a magnetic field, i.e., gigantic magnetoelectric effects. In these multiferroics, their ferroelectricity originates from complex magnetic ordered structures which breaks the inversion symmetry. Since such complex magnetic ordered states often arises from keen competitions between nearest-neighbor and further-neighbor magnetic interactions, the application of a magnetic field to such multiferroics often causes magnetic phase transitions which contributes to the gigantic magnetoelectric effect. In the field of condensed matter physics, not only the application of magnetic field but also that of high pressure sometimes leads to new states of matter, as well as to higher performances of materials' functionalities which cannot be reached in ambient-pressure condition. In the present study, we show effects of pressure up to 10 GPa (plus magnetic field) on multiferroic properties in some multiferroics showing complex spiral magnetic ordered state.

By using a home-made high-pressure measurement system with a diamond anvil cell [1], we investigated high-pressure effects on thermal, ferroelectric, and magnetoelectric properties of CuCrO₂ [2], Mn₂GeO₄ [3], and TbMnO₃ [4]. Our study has revealed that TbMnO₃ exhibits a pressure-induced magnetoelectric phase transition and that the high-pressure phase shows the largest ferroelectric polarization ($\sim 1 \mu\text{C}/\text{cm}^2$) among spin-driven ferroelectrics ever reported. Moreover, the ferroelectric polarization is further enhanced by applying a magnetic field and reaches $1.8 \mu\text{C}/\text{cm}^2$ whose magnitude is comparable to that of conventional ferroelectrics.

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SESSION 38

Out equilibrium Polaron Formation



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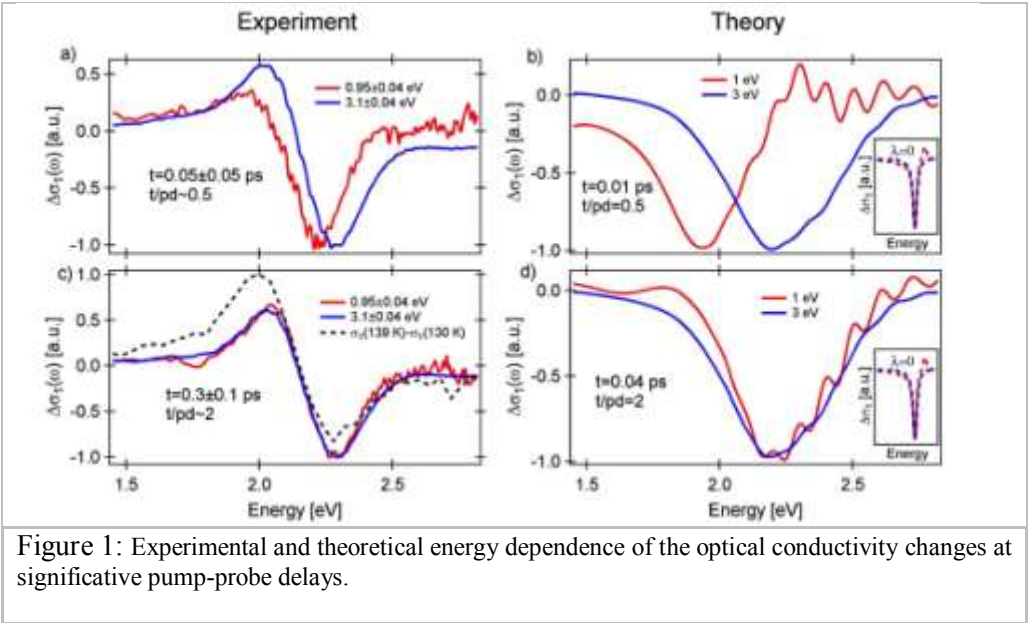
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Keywords: polaron, strongly correlated electron, out of equilibrium

Starting from a general theoretical framework (Hubbard-Holstein Hamiltonian), we characterize the wavelength dependent excitation processes of strongly correlated charge transfer insulators. We demonstrate that variations of the pump wavelength across the charge transfer gap results in completely different electronic dynamics. While pump pulses with photon energy larger than the charge-transfer gap lead to an effective electronic heating, excitation in the excitation tail pilots an instantaneous increase of the coherent motion followed by an ultrafast reaction of the bosonic field. Our results force a revision of multi-temperature approaches to correlated electron systems and disclose an anomalous behavior of electron-boson interaction if abetted by strong correlation between electrons.

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Time-domain spectroscopy of the Berezinskii-Kosterlitz-Thouless transition in highly underdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$



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Keywords: thermally-driven superconductor-normal transition – underdoped cuprates – dynamics

The possibility to observe the Berezinskii-Kosterlitz-Thouless (BKT) transition in bulk highly underdoped cuprates has been a subject of debate [1]. We investigated the nature of the thermally driven transition to a superconducting state on 100 nm thick $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ films with $x=0.07$ and 0.08 by studying a) superconducting fluctuations (SCFs), as determined from the magnetoresistance, b) current-voltage (I - V) characteristics, and c) fluctuations of the resistance with time (noise). We observe and discuss the main signatures of the BKT transition [2]: a) The contribution of the SCFs to the conductivity increases monotonically with decreasing temperature T and diverges exponentially at T_{BKT} , where resistance also goes to zero. b) The I - V characteristics exhibit power-law behavior $V \sim I^{\alpha(T)}$ with $\alpha(T) \geq 3$ for $T \leq T_{BKT}$. Here we focus on the resistance noise measurements, which can provide a direct probe of correlations. In the regime of T where phase fluctuations are dominant, we find that the resistance noise increases exponentially as T_{BKT} is approached, probably reflecting the exponential divergence of the correlation length at the BKT transition. At the same time, the dynamics slows down and becomes correlated. Furthermore, the higher-order spectrum analysis indicates the existence of some kind of interacting domains. A possible origin of these domains and the role of disorder will be discussed.

This work was supported by NSF DMR-1307075 and NHMFL via NSF DMR-1157490 and the State of Florida.

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Photoinduced Carrier Dynamics in Charge-Ordered Insulator and Mott Insulator

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Keywords: Ultrafast dynamics, Cuprates, Charge Order, Theory

Ultrafast carrier dynamics in strongly correlated electron systems have significantly attracted much attention, because a number of time-resolved experimental techniques and theoretical calculation methods for non-equilibrium states are rapidly developed in the last decade. A lot of experiments and theoretical analyses for transient carrier dynamics have been done in several classes of correlated electron systems. In this talk, we introduce recent our theoretical studies in the photo-induced transient electron dynamics in correlated electron systems.

I will talk about the following topics:

1) Photo-excited charge dynamics of interacting charge-frustrated systems are studied using a spinless fermion model on an anisotropic triangular lattice [1]. We find that the photo-induced excited states from the two types of charge orders are distinct. The observations are attributable to the charge frustration effects appearing in the photo-excited states. We also touch the effect of the electron-phonon interaction in the photoinduced carrier dynamics [2].

2) Transient dynamics of hole carriers injected into a Mott insulator with antiferromagnetic long range order are studied based on the two dimensional t-J model [3]. Time dependences of the optical conductivity spectra and the one-particle excitation spectra are calculated based on the Keldysh Green's function formalism combined with the self-consistent Born approximation. Time profiles are interpreted as doped bare holes being dressed by magnon clouds, and are relaxed into spin polaron quasi-particle states. The present works are in collaboration with H. Hashimoto (Tohoku), H. Matsueda (Sendai college), H. Seo (RIKEN), and E. Iyoda (Tokyo).

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Relaxation dynamics of many-body systems



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Keywords: relaxation dynamics, correlated electron systems,

I will present a fundamental study of the relaxation dynamics of a single hole in the two dimensional t - J model initially excited by a strong quench. Taking fully into account quantum effects we follow the time-evolution of the system from a highly excited state until it reaches a steady state. Relaxation occurs on the time- scale of 10 fs due to inelastic scattering of a photo-excited carrier on spin excitations [1,2]. Within this ultrafast relaxation time an excess of 1 eV of initial photo absorbed energy by the doped charge carrier is distributed among neighboring spin bonds, thus decreasing the kinetic energy of the carrier. In this process less than 20meV of bond energy is stored in neighboring spin bonds, see Fig.1.

I will also present relaxation dynamics of a carrier coupled to spin and lattice degrees of freedom based on the one dimensional t - J -Holstein under the influence of an external staggered field [3]. After an initial ultrafast relaxation a subsequent energy transfer from lattice to spin degrees of freedom is observed.

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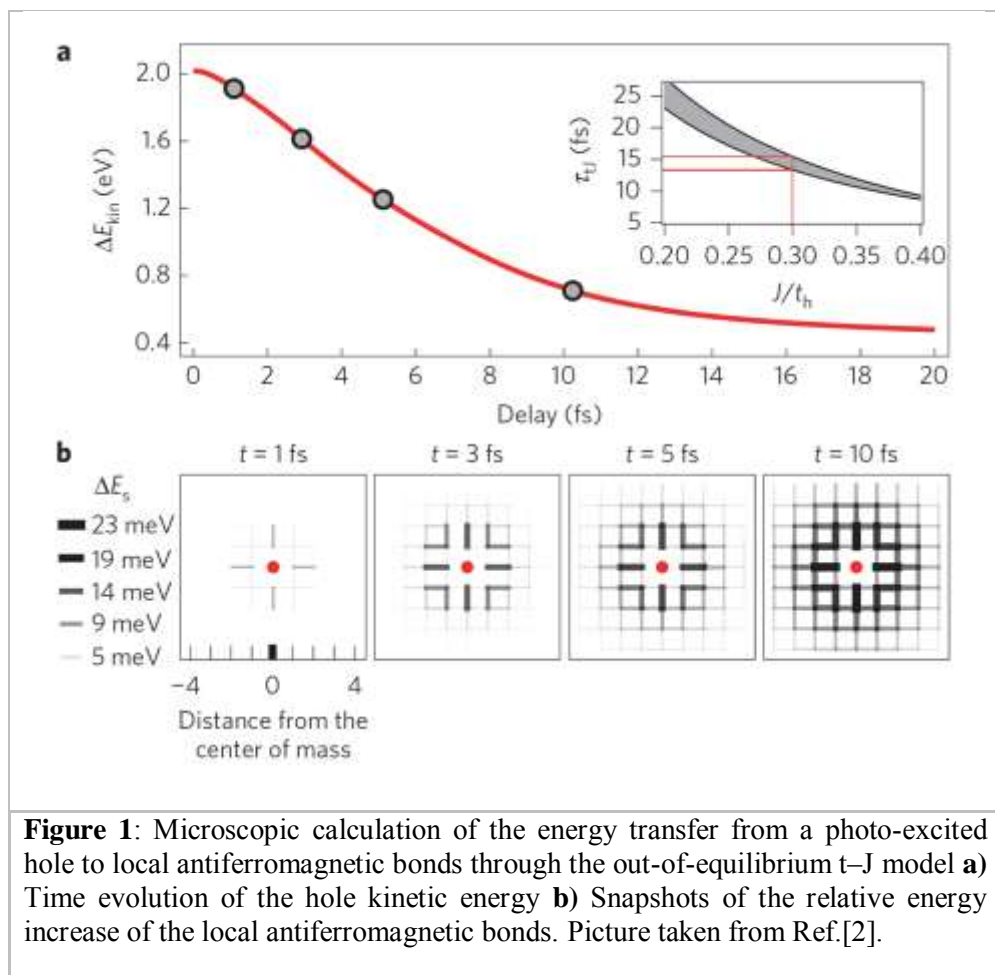


Figure 1: Microscopic calculation of the energy transfer from a photo-excited hole to local antiferromagnetic bonds through the out-of-equilibrium t - J model **a)** Time evolution of the hole kinetic energy **b)** Snapshots of the relative energy increase of the local antiferromagnetic bonds. Picture taken from Ref.[2].

SESSION 39

Negative capacitance? 1000% enhancement of the carrier density at the surface of non-doped SrTiO₃.



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Keywords: Negative capacitance – SrTiO₃ – many-body effects

We have fabricated a field effect transistor (FET) on the (100) surface of a highly insulating SrTiO₃ single crystal utilizing a bilayer gate insulator of 6nm Parylene-C and 20 nm HfO₂ [Fig. 1(a)-(c)]. Although our Parylene-C film is extremely thinner than that of conventional usages ($\sim 1\mu\text{m}$), we confirmed it can sufficiently prevent the degradation of vulnerable SrTiO₃ surface during the device fabrication.

The obtained clean interface of our SrTiO₃ FET channel has eventually shown a surprisingly small sub-threshold swing ($\Delta V_G / \Delta \log_{10} I_D$) of 170 mV/decade (theoretical minimum value is 60mV/decade, and even the very clean Si FET shows the value of $\sim 100\text{mV/decade}$ [1]). We also observed a large field-effect mobility of $7.3\text{cm}^2/\text{Vs}$ at room temperature, where V_G is the gate voltage and I_D is the drain current.

Moreover, sheet carrier density of $4 \times 10^{13}\text{cm}^{-2}$ of our FET channel deduced by Hall effect measurements is nearly 1000% of the classical value, *i.e.*, the capacitance of the bilayer gate insulator. This enormous enhancement suggests the novel "negative capacitance" of the SrTiO₃ surface, since the negative capacitance raises the chemical potential of the channel and facilitate the accumulation of more carriers. It is likely to be originating in the many body effects of the electronic systems on the surface of SrTiO₃ [2, 3]. However, the observed enhancement is too large. The anomaly might be related to an enhancement of the Coulomb interaction by surface effects and longer-range hopping [4] ferroelectricity as reported in the strained surface [5], contribution of the spin-orbit effect [6], and some other quantum effects.

It is very interesting to note that, even though SrTiO₃ is not a Mott insulator, we have successfully realised the small subthreshold swing and large carrier accumulation simultaneously in this SrTiO₃ FET, both of which are the main characteristics expected for the futuristic Mott FET: that is, the FET with Parylene-C/HfO₂ bilayer gate insulator with non-doped SrTiO₃ is an ideal mockup to explore the physics of yet-to-be-developed Mott FET.

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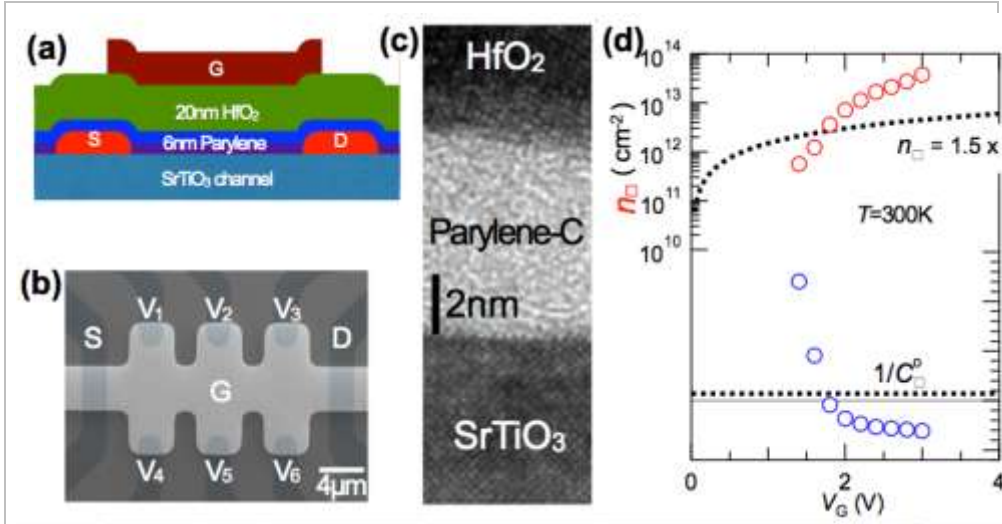


Figure 1: (a) Schematic picture of the cross section of our FET with HfO_2 (20nm)/Parylene-C (6nm) solid-state bilayer gate insulator fabricated on a non-doped SrTiO_3 single crystal. (b) Scanning electron microscopy images of a multi-terminal device. G, S, and D stand for gate, source, and drain electrodes, respectively. $V_1 - V_6$ are potential probes. (c) Cross sectional TEM image of the channel. (d) Top: sheet carrier density n_{\square} (open circles) in the strong accumulation region ($V_G > V_{\text{th}}$) obtained by the Hall effect measurement of the multi-terminal FET device. n_{\square} of the classical limit (dashed line) is depicted for comparison. Bottom: comparison of n_{\square} to the classical limit gives the gate voltage V_G dependence of $1/C_{\text{STO}}$ (open circles), where C_{STO} is the sheet capacitance of the SrTiO_3 channel. The large deviation of n_{\square} from the classic limit is reflected in the negative $1/C_{\text{STO}}$.

Microscopic details of orbital and electronic reconstructions at oxide interfaces from resonant x-ray reflectometry



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Keywords: Oxide Heterostructure – 2D Electron Gas – X-ray Spectroscopy – Electronic Reconstruction – Orbital Reconstruction

Interfaces in oxide heterostructures exhibit a wide range of emergent phenomena, such as interface charge transfer, two dimensional electron gases (2DEGs), superconductivity, and ferromagnetism between non-magnetic materials [1]. Such phenomena result from the interface-induced tuning of the various spin, charge, orbital, and lattice degrees of freedom, and show great promise for electronics applications. However, while the emergent phenomena are readily apparent, obtaining electronic structure information specific to the nanometer-scale interface region—in order to understand and further tune the emergent phenomena—is an understandably difficult task. Here we study the electronic structure of heterostructures directly at the interface region using resonant x-ray reflectometry (RXR), an experimental technique which combines the powerful electronic structure probing capability of x-ray absorption spectroscopy with the interface sensitivity provided by reflectivity. By tuning to various different reflection geometries and resonance energies, we can obtain information on the element-specific electronic structure directly at and near the interface. For the paradigmatic LAO/STO which exhibits orbital and electronic reconstructions [2,3], we extract layer-resolved, reconstructed Ti orbital energies within a few unit cells of the interface, and determine the quantity of charge in the 2DEG, as well as its spatial distribution. These results provide important insight into the physics behind the intriguing emergent phenomena and show RXR to be an ideal tool for studying oxide interfaces.

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Studying emergent phenomena at surfaces and interfaces of complex matter using resonant soft x-ray reflectivity



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Keywords: x-ray reflectivity – spectroscopy – thin films – interfaces – proximity effects – electronic reconstruction

Development in the synthesis of transition metal oxide materials at the atomic scale has provided a vast playground for exciting novel physics that takes place especially at their surfaces and interfaces [1]. Some examples are the formation of a 2D electron gas at the LaAlO₃/SrTiO₃ interface [2], the observation of superconductivity at interfaces of non-superconducting copper oxides [3], among others [4,5]. The nature of these new phenomena has been addressed to be closely related to reconstruction of the charge, spin and orbital states that takes place as a consequence of the local symmetry breaking at these interfaces. Notwithstanding, since these interfaces are normally buried deep below the sample's surface, the study of their electronic and structural properties is an experimental challenge. In this regard, resonant x-ray reflectivity (RXR) is the ideal tool. It is non-destructive, interface sensitive and, since the experiment is performed at energies close to absorption edges, it yields depth resolved element specific spectroscopic information.

In this talk, the capability of RXR in studying electronic properties at surface and interfaces will be demonstrated based on two examples. First, an element and valence specific description of RXR is used in order to obtain the electronic density z-profile of Co in a LaCoO₃ film along the polar (001) direction. The analysis of the experimental reflectivities shows that whereas Co in the film bulk has a typical 3+ ionic state, at the

surface Co undergoes a reconstruction into a $2+$ state (cf. Fig. 1). These results provide strong evidence of genuine electronic reconstruction at a polar surface.

Finally, a single (001) oriented YBCO thin film is studied using RXR at the Cu L_{2,3} edges. The presence of the structural (001) Bragg reflection at the measured Q range, enables us to accurately describe the observed interference pattern using classical models approaches to reflectivity. Therefore, a new scheme is introduced where atomic planes with anisotropic scattering factors for Cu at chains and planes are explicitly defined. First calculations will be presented and discussed.

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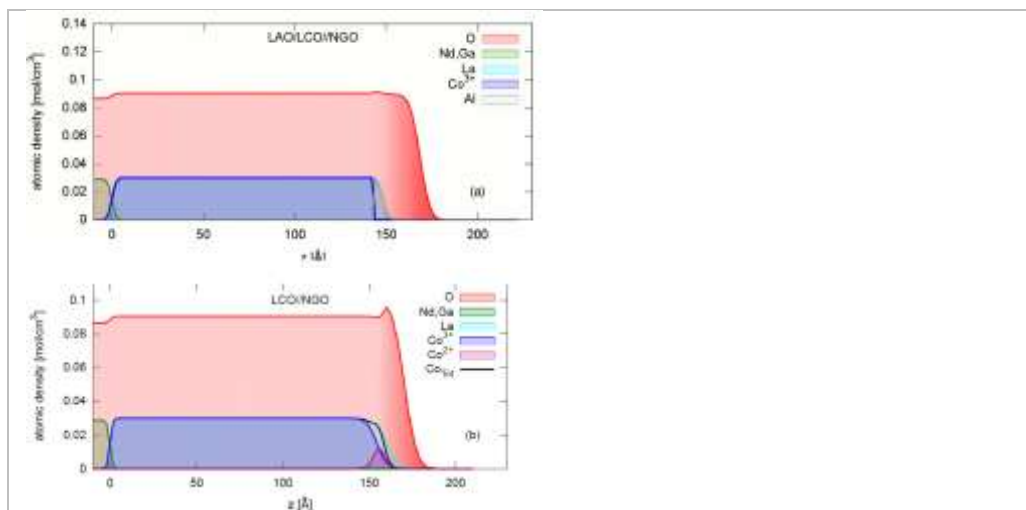


Figure 1: Element and valence depth profiles of LaCoO_3 thin films. (a) Profiles for a LCO film capped with an LAO layer showing only a Co^{3+} valence state. (b) Profiles for an uncapped LCO film exhibiting the appearance of Co^{2+} at the surface. The region at the surface of the samples marked in darker red is likely to contain further light adsorbed elements such as carbon, in addition to oxygen.

SESSION 40

Renormalization group approach to quantum topological phase transitions



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Keywords: quantum phase transitions – topological phase transitions – p-wave superconductors

Topological phase transitions cannot be described by the usual Landau paradigm for critical phenomena. They do not have a natural order parameter and in general there is no symmetry breaking as the system moves through the transition by varying some control parameter. On the hand the renormalization group (RG) provides the appropriate framework to describe these phenomena. It associates the transition with an unstable fixed point of a RG transformation and this allows to calculate the critical exponents that characterize the critical behavior of the system at the topological transition. Since, this is a quantum phase transition there is a dynamical quantum critical exponent z that plays a fundamental role. This is related by a *quantum hyperscaling relation* [1] to the dimension of the system, to an exponent characterizing the critical behavior of the compressibility and to that related to the divergence of a characteristic length. Here we will distinguish between a *Lifshitz* transition and a topological phase transition between phases with different topological properties. We will show that one can distinguish at least two different universality classes of topological transitions and will give examples of these two classes. One is the usual band-filling transition in a metallic system and the other is the topological transition that occurs in the p-wave superconductor model introduced by Kitaev [2].

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Multiple condensate of composite bosons

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Keywords: composites condensation-fermion number conservation

I will present an exact bosonization procedure that generates a Hamiltonian of composite bosons interacting among themselves and with fermionic quasiparticles ^[1]. The interaction among composites whose mixing is allowed by symmetries is strong. I will give the conditions of decoupling from the other composites and I will compare the results with the Random Phase Approximation and the BCS theory.

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Fluctuations of “hidden order” as Cooper pairing glue



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Keywords: Euclidean crystallization – “hidden order” – Landau-Ginzburg-Wilson functional – double-periodic order parameter

Fluctuations of the “hidden order” as an origin of the Cooper pairing glue in high-T_c superconductors is discussed. New scenario is based on the recent publications [1]-[3] that introduced Euclidean crystallization in correlated fermi-system as an origin of a “hidden order”, breaking translational invariance of the system along the Matsubara’s time axis. Matsubara time-periodic spin-density wave manifests “hidden order”. Fluctuations of this peculiar order parameter provide a Cooper pairing glue in the fermi-system. It is proven analytically [1] that self-consistent Matsubara time-periodic order parameter, built of Jacobian elliptic function, has zero scattering cross section and, therefore, is a candidate for a “hidden order”, emerging in the fermi-system. Simultaneously, it is proven now analytically that this order parameter itself is only a metastable state of the fermi-system. But, fluctuations around it form a discrete spectrum [2], [3] and may play a role of Cooper pairing glue, that stabilizes the multiply-ordered state via formation of the superconducting Cooper pairs condensate. The discrete spectrum of the “hidden order” fluctuations is found using Lamé functions theory. The self-consistent solution minimizing the effective Euclidean action of the fermi-system in a form of Landau-Ginzburg-Wilson functional with two coupled orders is found analytically. Measurable predictions for the fermionic excitation spectrum and cross section of the neutron scattering by the “hidden order” fluctuations are derived in analytic form. Possible relation of the theory to the physics of high-T_c cuprates is discussed.

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Cluster Luttinger Liquids and supersymmetry in an extended Hubbard model



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Keywords: Luttinger liquids, supersymmetry

We investigate the quantum phases of hard-core bosonic atoms in an extended Hubbard model where particles interact via soft-shoulder potentials in one dimension. Using a combination of analytical and numerical methods, we demonstrate that the low energy phase can be a conformal cluster Luttinger liquid (CLL) where the microscopic degrees of freedom correspond to mesoscopic ensembles of particles. The CLL phase is separated from a conventional Tomonaga-Luttinger liquid by a critical point with central charge $c=3/2$. The latter is expression of an emergent conformal supersymmetry, which is not present in the original Hamiltonian. All these phases should be observable in experiments with weakly-dressed Rydberg atoms confined to optical lattices.

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SESSION 41

“Light Fermion” Problem in the Low-Density Electron Gas



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Keywords: Critical points – effective mass – momentum distribution function

The electron-gas model (namely, an interacting many-electron system in a compensating uniform positive background) plays a very useful role in the discussion of the many-body properties of conduction electrons in metals. This model becomes even more important in low-density systems in which $a_0 p_F$ is much smaller than unity (a_0 : the lattice constant and p_F : the Fermi wave number), because the first-principles Hamiltonian is reduced to this model in this limit, indicating that the universal behavior in the low-density metals can be captured by the investigation of the electron gas at low densities.

This model is completely specified by the parameter r_s which is defined by $r_s = (3/4\pi n)^{1/3} a_B^{-1}$ with n the electron density and a_B the Bohr radius. In usual metals in which r_s is in the range 1-5, this model can be well treated by the appropriate combination of ring diagrams, ladder ones, and their exchange partners, but the situation becomes complex and difficult for r_s larger than 5.25 at which the electronic compressibility κ diverges and subsequently the dielectric catastrophe occurs in the sense that the static dielectric function in the long-wave-length region is negative. In close connection of this dielectric catastrophe, we have already discussed an anomalous behavior of the interatomic distance in the alkali fluid metals in the supercritical region, namely, for r_s between 5 and 8 [1,2]. We have also reported the calculated results on various physical quantities including the momentum distribution function $n(p)$ and the one-electron spectral function $A(p, \omega)$ in the same r_s region [3] with employing the nonperturbative scheme of the GW method [4].

In my talk, we will report on our recent results on the electronic states such as the effective mass at the Fermi level m^* and $A(p, \omega)$ but mainly on $n(p)$ for r_s larger than 10. We will emphasize on the possibility of a new critical point at r_s around 20, which is much smaller than 100 where the Wigner crystallization is expected to occur, on the basis of the anomalous behavior of $n(p)$ and, in particular, the observation that our numerical result on m^* tends to zero at the critical point, indicating a new problem of “light fermion” due to exchange and correlation. We will explain the physics behind this anomalous behavior of m^* from the viewpoint of competition with the excitonic instability.

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Phase fluctuation in overdoped cuprates? Superconducting dome due to Mott-ness of the tightly bound preformed pairs



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Keywords: high T_c superconductivity, cuprates, phase diagram

In contrast to the current lore, we demonstrate that even the overdoped cuprates suffer from superconducting phase fluctuation in the strong binding limit. Specifically, the Mott-ness of the underlying doped holes dictates naturally a generic optimal doping around 15% and nearly complete loss of phase coherence around 25%, giving rise to a dome shape of superconducting transition temperature in excellent agreement with experimental observations of the cuprates. We verify this effect with a simple estimation using Gutzwiller approximation of the preformed pairs, obtained through variational Monte Carlo calculation. This realization suggests strongly the interesting possibility that the high-temperature superconductivity in the cuprates might be mostly described by Bose-Einstein condensation, without crossing over to amplitude fluctuating Cooper pairs.

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Electronic structure, doping, order and disorder in cuprate superconductors.



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Keywords: mechanisms for high T_c – cuprates, band structure, thermal disorder, oxygen ordering

The superconducting T_c 's are calculated from estimations of electron-phonon and spin-phonon coupling in typical high- T_c cuprates, like LSCO and HBCO. It is shown that the couplings are peaked for just a few q -vectors because of the 2-dimensional Fermi surface shape.

The involvement of few spin-phonon modes compensates for the low electronic density-of-states, and T_c can be high [1]. Thermal disorder of the lattice perturbs the strongly coupled modes already at moderately high temperatures. This happens because of incoherent potential fluctuations of the Madelung term, and electronic structure calculations show that the effective spin-phonon coupling is reduced. This effect puts a limit on long-range superconductivity, while fluctuations can persist to higher temperature [2]. BCS-type model calculations are used to show how disorder modifies the superconducting gap and reduces T_c . Some ideas of how to recuperate a higher T_c from superconducting fluctuations are discussed. Ordering of dopants into stripes has been suggested to improve superconducting properties, mainly through an increased DOS. Such mechanisms have been investigated for ordering of excess O in HBCO and for a nickelate system [3].

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Iridates realizing complex spin-orbital physics



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Keywords: spin-orbit coupling – iridates – quantum magnetism

While correlations are widely believed to be relevant in iridates, they are weaker than in many $3d$ compounds and the picture of a spin-orbital Mott insulator can thus not be taken for granted. In this picture, the low-energy manifold consists of $j=1/2$ pseudospins, separated from higher-energy $j=3/2$ state as well as from states with two holes on a site. We investigate excitations of the low-energy $j=1/2$ system in square-lattice iridates, in particular spin-orbital excitons into the $j=3/2$ states [1]. The analysis supports the interpretation as a spin-orbit-assisted Mott insulator. Moreover, the $j=3/2$ excitations show a sharp quasi-particle-like peak as expected for a hole in a Mott insulator, even though the spin-orbit excitation is charge neutral. These two different excitations – the hole and the orbital excitation – turn in fact out to be described by the same effective microscopic t - J Hamiltonian [2]. We then move beyond the square lattice and theoretically investigate potential ground states of frustrated Kitaev-Heisenberg models in hexagonal symmetry. We find a persistent tendency towards incommensurate non-coplanar patterns. In particular, we find regular lattices of topological defects, somewhat similar to skyrmion lattices, in the ground state for both triangular and honeycomb lattices [3].

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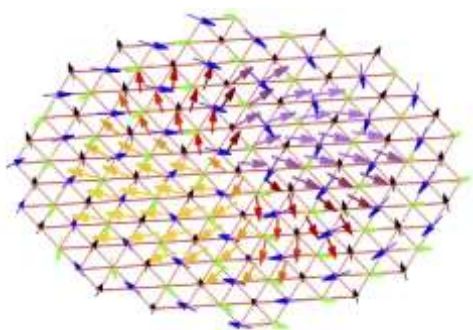


Figure 1: Topological defect (Z_2 vortex) in the triangular-lattice Kitaev-Heisenberg model.

CHAPTER 5

SESSION 42

Complex Phase Diagrams of Models for Iron Based Superconductors



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Keywords: iron based high T_c superconductivity, states with exotic magnetic and orbital order, competition and cooperation of quantum states, Hartree Fock and Monte Carlo simulations.

This presentation will focus on three recent results: (1) the much studied spin nematic state of iron superconductors and its diverging susceptibility above the critical temperature T_s analyzed from the perspective of Monte Carlo simulations of the spin fermion model [1]; (2) the complex phase diagram of multiorbital Hubbard models varying couplings and temperatures, including the orbital selective Mott physics regime, obtained with recently developed techniques that combines mean field and Monte Carlo techniques [2]; and (3) the many competing states found in real-space zero-temperature Hartree-Fock studies of Se-based compounds when in the presence of regularly spaced iron vacancies and also in the case of two-leg ladders [3]. Moreover, an analysis of experimental and theoretical results indicates that iron superconductors are in an “intermediate” coupling regime [4]. Overall, the picture emerging is that of many competing exotic states that it is starting to resemble the historical path followed in Cu-based high-T_c superconductors and in colossal magneto resistance manganites that eventually led to a variety of nonlinear effects and states with nanoscale phase separation.

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Relaxor Ferroelectrics, Spin-Glass and Real Glass



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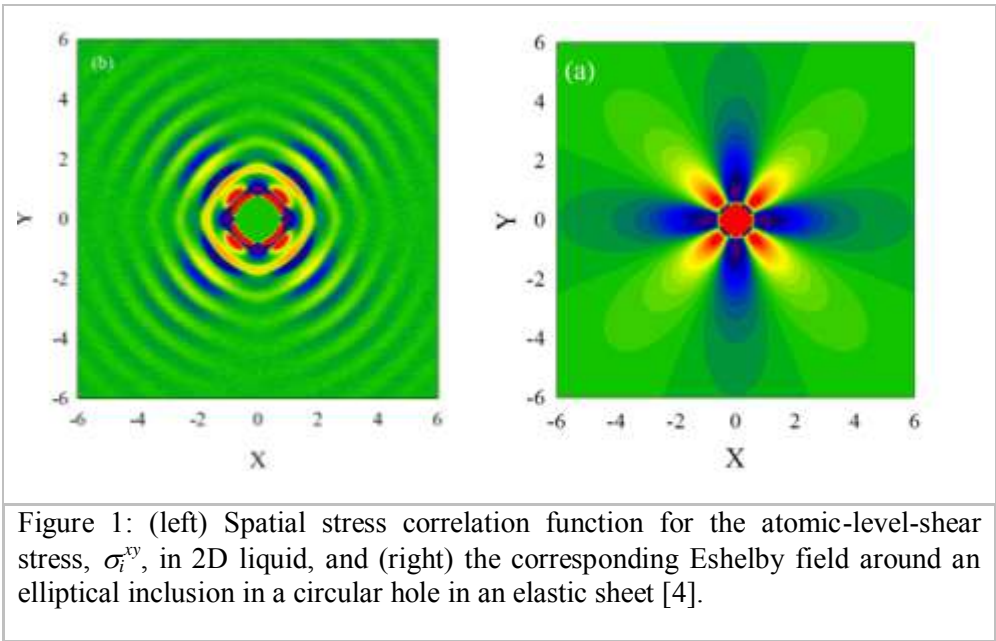
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Keywords : relaxor ferroelectrics – glass transition – spin glass

Similarities and differences among the relaxor ferroelectrics, spin-glasses and real glasses are discussed, in the hope of elucidating the glassy behavior in general by a unified model. All three classes of glasses have freezing (glass transition) at T_f , below which the random order becomes static, and crossover temperature (Burns temperature), T_A , below which dynamic short-range order is observed. We showed earlier that in relaxor ferroelectrics dynamic local ferroelectric polarization appears below the Burns temperature [1]. In metallic liquids above the crossover temperature T_A phonons are overdamped and the elementary excitations are local topological excitations named ananeons [2,3]. Below T_A ananeons interact through local phonons described in terms of the Eshelby field (Fig. 1) [4,5], and dynamics becomes collective. Now the major difference among the three is that in relaxor ferroelectrics the Curie temperature, T_C , is clearly observed, although it is diffuse. Below T_C the polar nano-regions (PNRs) are observed [6]. On the other hand spin-glass does not have an equivalent, and in real glasses the corresponding phenomenon is controversial. It may correspond to the appearance of dynamic heterogeneity [7]. It is possible that dynamic short-range bond-orientational order induced by the Eshelby field produces an equivalent of the NPR. I discuss what the relaxor ferroelectrics can tell us about the physics of real glasses.

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Charge order, superconductivity and pseudogap physics in the cuprates



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Keywords: Cuprates, CDW order, superconductivity

Recently, it has become widely accepted that charge ordering is a universal property of hole doped high-temperature cuprate superconductors [1-6]. This talk gives an overview of the current experimental effort to reveal the nature of the charge density wave order. Special focus will be given to x-ray diffraction experiments. Implications for the Fermi surface reconstruction and superconductivity will be discussed along with possible connections to pseudogap physics.

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Nano phase separation in Cobaltates



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Keywords: Cobaltates, Hour-glass spectrum, Nano phase separation

The hour-glass magnetic excitation spectrum has fascinated physicists over years. This spectrum has been observed in high-temperature superconducting cuprates and it is widely believed that fluctuating charge stripes are involved in the physics of these intriguing materials. Besides charge stripes also Fermi surface effects are able to describe the emergence of these hour-glass spectra in cuprates. Recently, Boothroyd *et al.* found in $\text{La}_{2-x}\text{Sr}_x\text{CoO}_4$ also an hour-glass magnetic spectrum implying that Fermi surface effects are not needed for the emergence of hour-glass spectra since this material is insulating [1]. In our study we go one step further and show that besides Fermi surface effects also charge stripes are not needed for the emergence of hour-glass spectra [2,3]. Instead, we observe electronic and magnetic nano phase separation within the cobalt oxygen planes, see **Fig. 1**. Within our nano phase separation scenario the high energy excitations within the hour-glass spectrum are basically hosted in nano phase separated undoped islands whereas the remaining hole-rich regions can be excited only at lower energies such that the hour-glass spectrum consists of strongly decoupled excitations with distinct origin on the nano scale.

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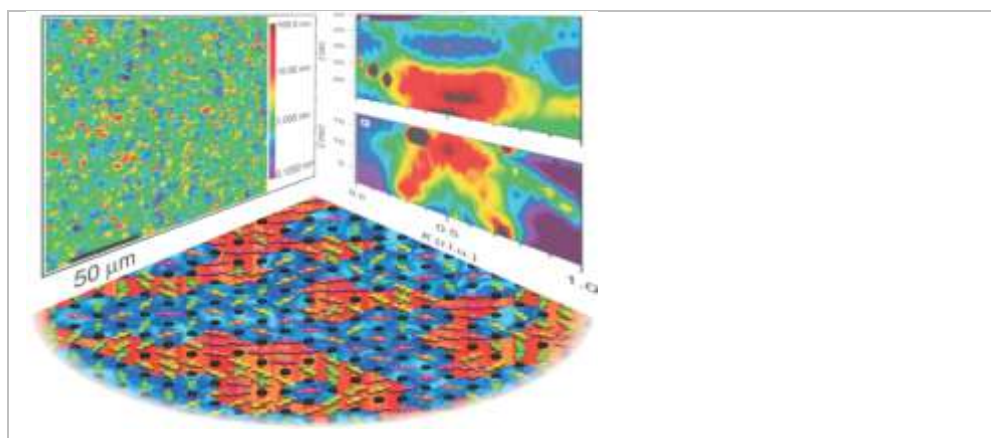


Figure 1: *Upper left:* Nano phase separation in $\text{La}_{2-x}\text{Sr}_x\text{CoO}_4$ revealed by microdiffraction. *Lower middle:* Schematic presentation of our novel electronic and magnetic nano phase separation scenario. Undoped islands (red areas) with large exchange interactions J and checkerboard charge ordered regions (blue areas) with small $J' \ll J$. *Upper right:* Our neutron measurements reveal an hour-glass magnetic excitation spectrum with an additional magnetic high-energy mode that could be expected from our new nano phase separation model but that has never been observed before in any hour-glass spectrum.

Looking at the mechanism for high critical temperature superconductivity through nanoscale YBCO devices



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Keywords: nanoscale high T_c superconductivity, mechanisms for high T_c , mesoscopic devices

The phase diagram of the high- T_c cuprate superconductors (HTS) is shaped by the spontaneous emergence of various ordered states, tuned by doping and driven by the many competing degree of freedom, where not only charge and spin are of relevance, but also lattice and orbitals have an active role in building up the ground state. The identification of all ordered states is crucial for understanding high-temperature superconductivity. In strongly correlated systems, the tendency of the valence electrons to segregate in periodically modulated structures can lead to the formation of a peculiar charge order. The evidences for a new charge state, ubiquitous in all cuprates families and with translational/rotational symmetry breaking have recently come from major developments of synchrotron based X-ray scattering [1,2]. This discovery has added considerable credibility to the suggestion that local order is an important bridge between the Mott insulator, representing the starting cuprate material at very low doping, and the more metallic state at heavy doping. However, while X-ray scattering experiments have clearly shown that the charge order competes with superconductivity, the consequences of such a local arrangements of charge carriers on the transport properties of HTS devices remain to be seen. In HTS devices at the nanoscale, like nanodots and nanowires, the locality of charge/spin arrangement is highly enhanced, which might lead to more dramatic effects on the transport properties of mesoscopic systems.

In this contribution I will review our recent experiments on High critical Temperature Superconductors (HTS) nanoscale devices showing how they can be decisive to get new insights into the microscopic mechanism leading to superconductivity in these materials.

I report on our progress in realizing a novel spectroscopic technique, based on an $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ (YBCO) underdoped nanoisland, that allows an unprecedented energy resolution, thanks to Coulomb blockade effects, a regime practically inaccessible up to now in these materials [3].

An all YBCO Single Electron Transistor (SET) has been fabricated by using biepitaxial grain boundaries as tunnel barriers. In such a devices we find that the energy required to add an extra electron to a nanometer size YBCO island depends on the parity (odd/even) of the excess electrons on the island itself and increases with magnetic field. This is inconsistent

with a pure d_{x-y}^2 -wave symmetry and demonstrates a complex order parameter component on the island that needs to be incorporated into any theoretical model of HTS. By using both a semiclassical and tight binding model calculation for the island I will also discuss the most probable symmetry for the subdominant imaginary order parameter.

I will also present unconventional transport properties in YBCO nanowires. We have been able to engineer pristine YBCO nanowires, with cross sections as small as $40 \times 50 \text{ nm}^2$, retaining the full superconductive properties with record values for the critical current density (Fig. 1a). Starting from untwinned thin YBCO films grown on MgO (110) close to the optimally doped regime, nanowires of the same length but different width, have been patterned at different angles (see Fig 1b). Preliminary measurements of the critical current density (Fig. 1c) have revealed an unconventional J_c angular dependence for nanowire's width below a certain threshold ($w \approx 80 \text{ nm}$), that cannot be accounted for by considering the anisotropy of the London penetration depth along a and b YBCO axis. This dependence indicates a new characteristic length scale, below 100 nm, which should correlate with the broken rotational/translation symmetry induced by charge order domains and/or the specific growth habits of YBCO films on substrates with a large mismatch.

In particular, the large mismatch of the YBCO lattice parameters with MgO (110), generates an out-of-plane waving of the YBCO atomic planes, confirmed by x-ray diffraction and TEM studies, which is more pronounced in very thin films while smearing out above 100 nm. To clarify the origin of the anisotropic J_c dependence and its possible correlation with the charge order it is important to study the transport properties on nanowires patterned on heavily underdoped films close to $p=1/8$ doping plateau where local charge order is enhanced. This work is in progress.

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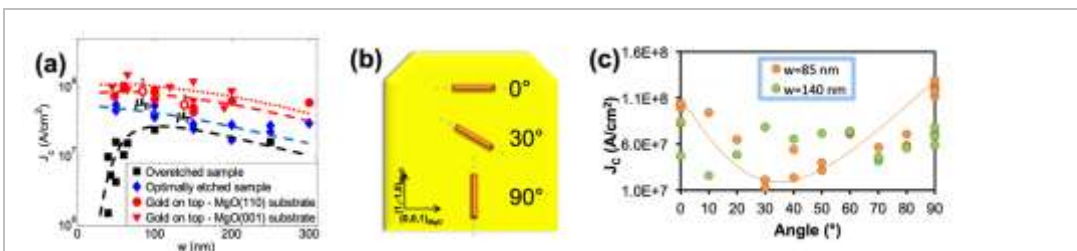


Figure 1: Width dependence of the critical current density J_c at $T = 4.2 \text{ K}$ for 200 nm long YBCO wires with and without a Gold capping layer [5]. (b) Orientation of the nanowires with respect to the in plane directions of the substrate. (c) Experimental J_c of 200 nm long wires as a function of the in-plane angle of the current transport with respect to the [001] MgO.

SESSION 43

NMR studies of charge order in $\text{YBa}_2\text{Cu}_3\text{O}_y$



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Keywords : cuprate – CDW – stripes

In 2011, the NMR discovery that superconductivity competes, and coexists, with charge-density-wave (CDW) order in $\text{YBa}_2\text{Cu}_3\text{O}_y$ was argued to strongly support the, hitherto controversial, view that underdoped cuprates are generically unstable towards CDW formation [1]. While this affirmation is now unanimously accepted, the exact nature of the CDW is not. In this talk, I will discuss insights into charge order from our NMR studies of $\text{YBa}_2\text{Cu}_3\text{O}_y$ [1-4], with emphasis on the possible effects of disorder as well as on the comparison between the normal state above T_c and the field-induced normal state at low temperature.

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Superconductivity and charge-density-wave state in the layered organic conductors α -(BEDT-TTF)₂MHg(SCN)₄



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Keywords : organic conductors, charge-density wave vs. superconductivity, magnetic field effects

Like many other materials of high current interest, crystalline organic conductors are “bad metals”, in which strong electronic correlations induce various competing instabilities of the normal metallic state. Their possible ground states range from charge- or/and spin-ordered or disordered (e.g. quantum spin-liquid) insulator to conventional or unconventional superconductor. Thanks to rather low relevant energy scales, a subtle balance between these ground states can easily be tuned by changing external parameters such as pressure or magnetic field, or by minor chemical substitutions [1]. Taking further into account the simplicity of the electronic band structure and typically very high crystal quality, one can consider organic conductors as perfect model objects for studying the physics of correlated electronic systems.

In this talk I will focus on one family of organic metals, α -(BEDT-TTF)₂MHg-(SCN)₄ with M = K, Tl, or Rb. The electronic band structure of these compounds is determined by layers of the organic donor BEDT-TTF alternated by insulating anionic MHg(SCN)₄⁻ layers. The Fermi surface consists of a cylindrical (quasi-two-dimensional, q2D) part and a pair of weakly warped open (quasi-one-dimensional, q1D) sheets, see Fig. 1(a). The compounds undergo a charge-density-wave (CDW) transition at a very low temperature, $T_{\text{CDW}} \approx 10$ K. At $T < T_{\text{CDW}}$ the q1D part of the Fermi surface is gapped, however the system remains metallic due to the remaining q2D band.

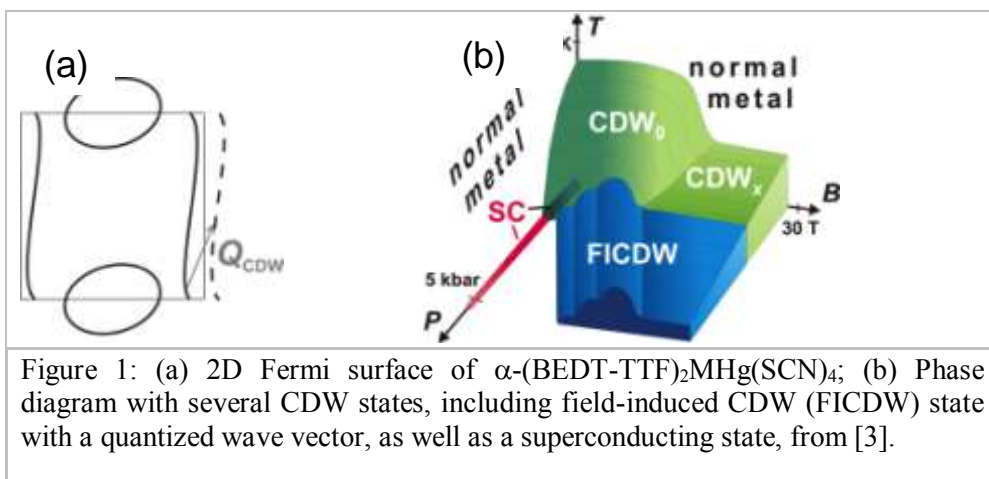
Interestingly, the CDW wave vector, which can be determined precisely by angle-dependent magneto-resistance measurements, appears to vary from sample to sample, although its x -component is always equal to $2k_{\text{F}}$. The magnificent “magnetic field – pressure – temperature” phase diagram [Fig. 1(b)] is determined by the interplay between

orbital and Zeeman coupling of the magnetic field to the CDW and the Landau quantization of the 2D band [2,3].

Under a hydrostatic pressure $P \geq P_c \sim 2.5$ kbar the CDW state is suppressed and the compounds become bulk superconductors with a very low $T_c \cong 0.1$ K [4]. The measured critical fields anisotropy appears to be by far the highest ever obtained on a layered superconductor. At $0 \leq P < P_c$ the superconducting and CDW phases coexist but are most likely spatially separated from each other. Remarkably, the onset temperature of the superconducting transition is found to increase dramatically upon entering the coexistence region of the phase diagram, suggesting a nontrivial interplay between the CDW and superconducting instabilities.

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Intertwining of charge and superconducting orders in cuprates above T_c



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Keywords : cuprates, superconducting fluctuations, charge order, muon spin rotation

The existence of short-range charge order (CO) in the pseudogap state of high- T_c cuprate superconductors is now well established. Recently it has been demonstrated that antiferromagnetic correlations can give rise to both the known d -wave superconductivity, and the d -wave form of the CO observed in non-lanthanum-based cuprates by scanning tunneling microscopy (STM) [1]. Hence there is good reason to believe that the superconducting and charge orders are intertwined.

Using muon spin rotation (μ SR) we have investigated CO and/or superconducting correlations above T_c in the low- T_c superconductor NbSe₂ and hole-doped high- T_c cuprates. I will summarize these results and discuss a phenomenological model based on charge inhomogeneity that describes the μ SR results on cuprates [2]. I will also discuss an extension of the model, which suggests that the spatially varying potential energy associated with CO provides the energy scale for the superconducting pairing potential.

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SESSION 44

Lifshitz transitions and quasiparticle de-renormalization in heavy fermion YbRh_2Si_2



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Keywords : heavy fermion metal – Lifshitz transition – Kondo effect

Hybridization is a fundamental concept in strongly correlated electron physics. In heavy fermion metals, it may result in the generation of low-energy scales that can give rise to interesting phenomena like quantum criticality and unconventional superconductivity. On the other hand, the strong correlations often complicate an adequate description of the interplay of such phenomena in these materials.

YbRh_2Si_2 has evolved as a prototypical heavy fermion compound in which signs of quantum criticality have been observed by numerous experimental methods. Here we focus on high-field magnetotransport measurements which show several anomalies at different characteristic fields. By comparison of our data to field-dependent renormalized band structure calculations we can identify three Lifshitz transitions associated with the heavy fermion bands [1]. Moreover, our Hall measurements indicate that the de-renormalization of the quasiparticles, i.e. the destruction of the local Kondo singlets, occurs rather smoothly while the Lifshitz transitions are confined to small regions of the magnetic field. The severe changes of the Fermi surface topology of the dominating bands vis-a-vis the shifting of the Zeeman-split Kondo resonance through the Fermi level will be discussed in detail. Our findings are augmented by recent thermodynamic [2] and STM measurements [3].

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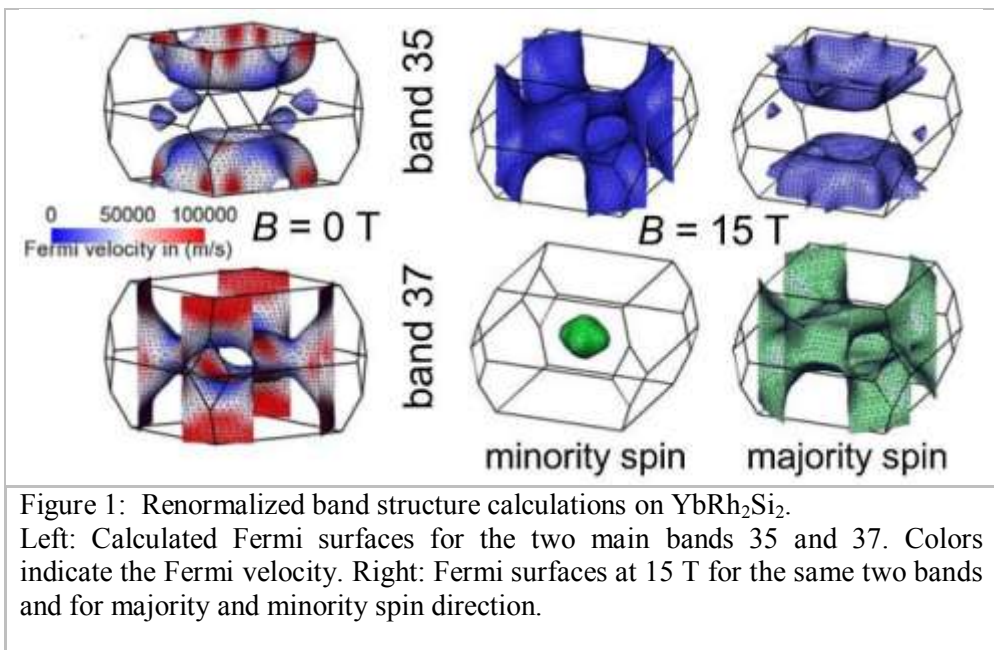


Figure 1: Renormalized band structure calculations on YbRh_2Si_2 .

Left: Calculated Fermi surfaces for the two main bands 35 and 37. Colors indicate the Fermi velocity. Right: Fermi surfaces at 15 T for the same two bands and for majority and minority spin direction.

Pressure-driven magnetic and structural transitions in the 122-pnictides



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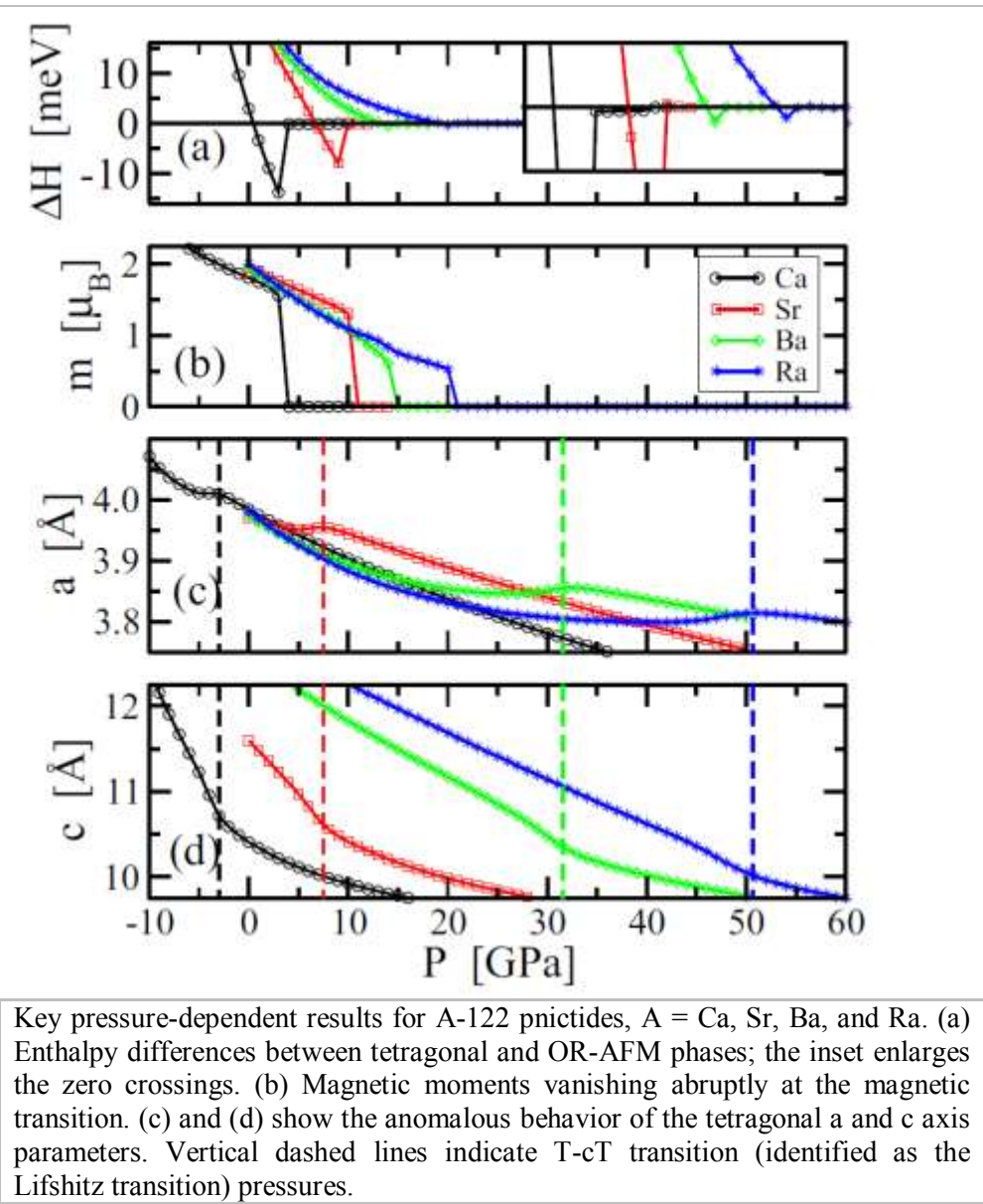
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Keywords : Structure collapse – soft mode – Lifshitz transition

Pnictides of the family AFe_2As_2 , where A is an alkali earth element, exhibit several phase transitions in their structure and magnetic order as functions of applied pressure. We employ density functional theory total energy calculations at $T=0\text{K}$ to model these transitions for the entire set of alkali earths ($\text{A}=\text{Ca}, \text{Sr}, \text{Ba}, \text{Ra}$) which form the 122 family. Three distinct types of transition occur: an enthalpic transition [1] in which the striped antiferromagnetic orthorhombic (OR-AFM) phase swaps thermodynamic stability with a competing tetragonal phase; a soft-mode transition through which the OR-AFM phase loses its magnetism and orthorhombicity; a lattice parameter anomaly in which the tetragonal c-axis collapses. We identify this last transition [2] as a "Lifshitz transition" caused by a change in Fermi surface topology. Depending on the element A, the tetragonal state exhibiting the Lifshitz transition might be metastable ($\text{A}=\text{Ca}$) or stable ($\text{A}=\text{Sr}, \text{Ba}$ and Ra).

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Lifshitz Transition in 122-Pnictides Under Pressure



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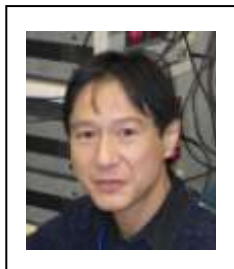
Keywords: Lifshitz Transition, Pnictides, collapsed tetragonal phase

Lifshitz transitions in solids occur due to topological change(s) of the Fermi surface caused by external pressure or chemical substitution. Resulting anomalies in lattice parameters, density of states near the Fermi energy, elastic properties, and electron dynamics manifest in thermodynamic and transport properties that may be observed experimentally. At sufficiently high pressures, the 122 pnictides, AFe_2As_2 ($A = \text{Ca, Sr, Ba}$), display transition from a tetragonal phase (T) to a "collapsed" phase (cT). Based on our $T = 0$ first principles total energy density functional theory calculations as a function of pressure, we propose that the observed T-cT transitions result from $T = 0$ K Lifshitz transitions. Our results [1,2] for energy band dispersions and spectra, c- and a-axis lattice parameters, and elastic constants over a wide range of hydrostatic pressure support our view

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Fermiology in iron-based superconductors via quantum oscillation measurements



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Keywords : Fermi surface – quantum oscillation – iron-based superconductors

Since superconducting pairing occurs on the Fermi surface, detailed knowledge of the Fermi surface is a prerequisite for the elucidation of pairing mechanisms in superconductors. We have been working on the fermiology of iron-based superconductors via quantum oscillation measurements [1-5]. In this talk, I will focus on two compounds, KFe_2As_2 and FeSe . Intriguingly, standard band structure calculations fail to give satisfactory description of the Fermi surface in both compounds.

KFe_2As_2 is the end member on the hole doped side of $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$ [6]. It becomes superconducting below $T_c \sim 3$ K. Because of overdoping, the Fermi surface consists solely of hole cylinders α , ζ , and β at the zone center and ε near the corner (Fig. 1) [1, 3]. The sizes of the observed cylinders and magnitudes of the k_z modulation (three dimensionality) are very different from those predicted by LDA calculations. The calculations give wrong crystal field splitting of the Fe 3d levels: They predict that the $d_{xz/yz}$ bands, which are degenerate in the absence of the spin-orbit coupling, are above the d_{xy} band at the zone center. However, the β cylinder is distinctly larger than $\alpha \square \square \square \zeta$, the sizes of which are not very much different, and hence it is more reasonable to attribute the β cylinder to the d_{xy} band. Namely, the d_{xy} band is higher than the $d_{xz/yz}$ bands at Γ in reality. Effective masses of holes on the β cylinder with the d_{xy} character are as large as $\sim 20 m_e$. These observations seem to be in line with orbital selective Mott scenarios [7], in which the d_{xy} band is most renormalized and tends to approach half-filling, i.e, the corresponding hole sheet gets larger. Pressure and/or Ba-substitution effects on the Fermi surface of KFe_2As_2 may also be presented in the talk [4].

FeSe is isoelectronic with FeAs^{-1} layers in BaFe_2As_2 . It has a tetragonal to orthorhombic structural transition caused by an electronic nematic order but no magnetic transition at ambient pressure. It becomes superconducting below $T_c \sim 9$ K [8]. It is a suitable compound to study influence of the nematic order in the absence of the antiferromagnetic order. The Fermi surface observed via SdH measurements is surprisingly different from that predicted by LDA calculations [5]. It most likely consists of one hole cylinder at the zone center and one electron cylinder at the corner, while the calculations predict three hole and two electron cylinders. Furthermore, the carrier number is one order-of-

magnitude smaller than calculated, as small as ~ 0.01 carriers/Fe. Clearly, these observations show the impact of the electronic nematicity on the electronic structure and the necessity of further investigations.

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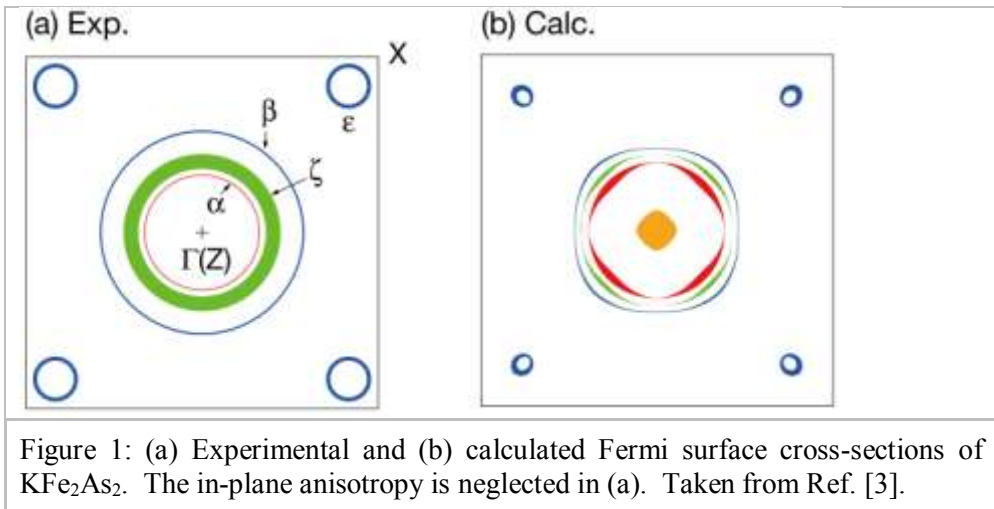


Figure 1: (a) Experimental and (b) calculated Fermi surface cross-sections of KFe₂As₂. The in-plane anisotropy is neglected in (a). Taken from Ref. [3].

SESSION 45

**Tuning electronic correlations in transition metal pnictides:
chemistry beyond the valence count**

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Keywords: correlation, high-T_c, iron pnictides, ARPES, orbital, band filling

The effects of electron-electron correlations on the low-energy electronic structure and their relationship with unconventional superconductivity are central aspects in the research on the iron-based pnictide superconductors. Here we use soft X-ray angle-resolved photoemission spectroscopy (SXARPES) to study how electronic correlations evolve in different chemically substituted iron pnictides. We reveal that correlations are intrinsically related to the effective filling of the correlated orbitals, rather than to the filling obtained by valence counting. Combined density functional theory (DFT) and dynamical mean-field theory (DMFT) calculations capture these effects, reproducing the experimentally observed trend in the correlation strength. The occupation-driven trend in the electronic correlation reported in our work supports the recently proposed connection between cuprate and pnictides phase diagrams. The high sensitivity of the correlations to small changes in the filling opens new ways of tuning the strength of electronic correlations in transition metal pnictide systems by systematic chemical substitutions, pressure or constraints.

Non-Fermi-liquid scattering rates and anomalous band dispersion in ferropnictides - an ARPES study [1]



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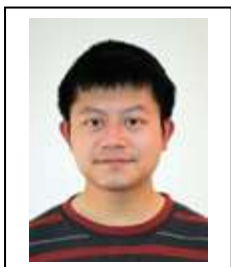
Keywords : electronic structure of ferropnictides

Unconventional/high temperature superconductivity (SC) is observed in heavy fermion systems, cuprates, molecular crystals, and ferropnictides close to a point in the phase diagram where, as a function of a control parameter such as pressure, chemical pressure, or doping, the antiferromagnetic order is suppressed. A widespread view is that at this point, which is called a quantum critical point, strong antiferromagnetic fluctuations are a candidate for the glue mediating superconductivity and that these fluctuations would also account for the normal state non-Fermi-liquid behavior as is visible in transport and thermal properties. Based on angle-resolved photoemission spectroscopy (ARPES) studies of the band dispersion and the quasiparticle scattering rates in ferropnictides, we establish here a different scenario: a co-action between a highly correlated electron liquid, which can be described by a marginal Fermi liquid *and* a crossing of a van Hove singularity, e.g. the top(bottom) of a hole(electron) pocket or a saddle point, through the chemical potential causes an anomalous band dispersion at the Fermi level which leads to a strong mass enhancement in the normal state and to a small effective Fermi energy favoring a Bardeen-Cooper-Schrieffer -Bose-Einstein crossover state in the superconducting phase. The results can be generalized to other unconventional superconductors.

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Lifshitz transitions in iron-based superconductors – our findings and current points of view



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Keywords: ARPES – Iron-based superconductors – Lifshitz transitions

The pairing mechanism for the iron-based high- T_c superconductors, like that for the cuprates, is currently subject to extensive investigation and heated debate. The first candidate pairing model, endorsed by many researchers in the beginning years of the iron pnictides, claims that these novel systems adopt an s^\pm -wave pairing mediated by spin-fluctuation modes (magnons), whose signature in the Fermi surface being the similarity in the sizes of the hole and electron Fermi pockets, i.e., the vicinity to a perfect nesting condition between the disconnected Fermi surfaces [1, 2]. As systematic studies on more iron-based systems are available, a new point of view is emerging that orbital fluctuations might play a more important role in forming the Cooper pairs than previously thought [3]. In the band structure point of view, this idea focuses on the conjecture that the highest T_c occurs when the system's chemical potential is put to the vicinity of a band edge, i.e., the system being on the verge of a “Lifshitz transition” – a change in the topology of the Fermi surfaces.

While evidences of this new pairing channel is gathered on the newly discovered pnictide systems such as LiFeAs [4], BaFe₂(As_{1-x}P_x)₂ [5], etc., we show in this talk that similar effects appear in the “traditional” electron-doped 122 systems. Our systematic ARPES studies on Ba(Fe_{1-x}Co_x)₂Fe₂ [6, 7] found that the superconducting region of this system is markedly bracketed by two sets of Lifshitz transitions. The low-doping onset of

superconductivity is pinpointed by the disappearance of the small Fermi dots near the M points, while the high-doping offset of superconductivity is close to the doping level where the innermost Γ hole pocket disappears at the Fermi energy. In other words, superconductivity is not supported in this system when either one set of the Fermi pockets (central or corner) vanishes, changes its carrier nature, or shows considerable reconstruction.

The current interpretation and outlook of these experiments will also be discussed in this talk. We will discuss to what extent our findings in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{Fe}_2$ can be applied to other pnictide systems, in particular the isovalent-doped 122 system $\text{Ba}(\text{Fe}_{1-x}\text{Ru}_x)_2\text{Fe}_2$, where the band structure as well as the Fermi level is found to be unchanged over the whole doping range, rendering the emergence and disappearance of superconductivity unrelated to the topology of the Fermi surfaces [8].

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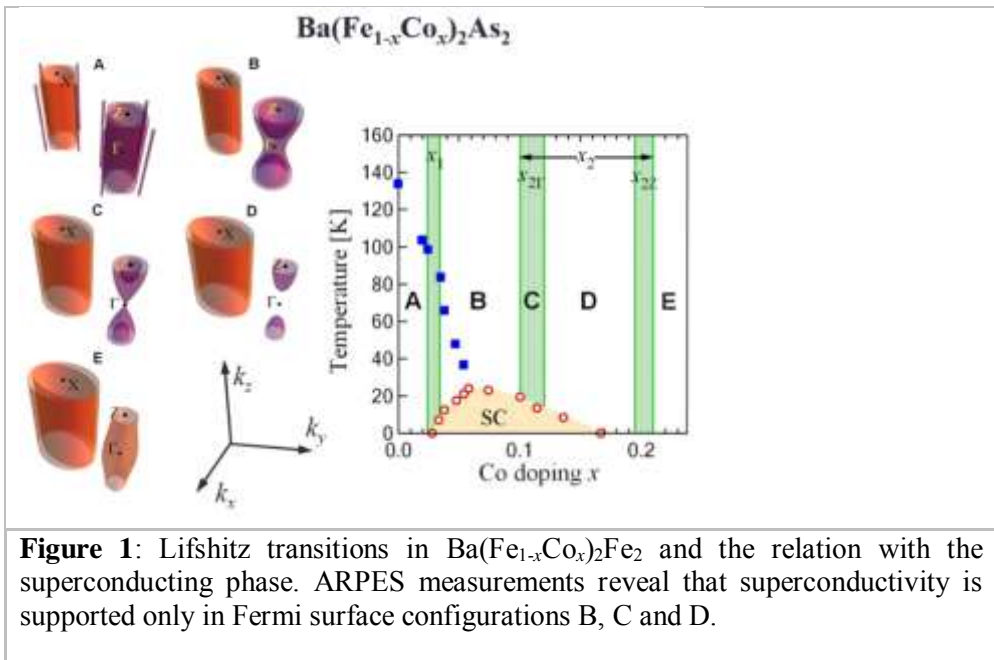


Figure 1: Lifshitz transitions in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{Fe}_2$ and the relation with the superconducting phase. ARPES measurements reveal that superconductivity is supported only in Fermi surface configurations B, C and D.

Conventional superconductivity at 203 K at high pressures



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The Bardeen–Cooper–Schrieffer (BCS) theory gives a guide for achieving high critical temperature of superconductivity (T_c): it should be a favorable combination of high frequency phonons, strong coupling between electrons and phonons, and high density of states, and puts no apparent bounds on T_c . These conditions can be fulfilled for metallic hydrogen and covalent hydrogen dominant compounds. We found that sulfur hydride transforms at pressure ~ 90 GPa to metal and superconductor with T_c of 203 K at pressure 140 GPa [1,2]. We have proved occurrence of superconductivity by the sharp drop of the resistivity to zero, the decrease of T_c with magnetic field; the pronounce isotope shift of T_c in D_2S which evidences of a major role of phonons in the superconductivity, and by magnetic susceptibility measurements.

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SESSION 46

Vortex Mott transitions: experiment and theory



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Keywords: Vortex Mott transition, phase transitions, critical behavior.

Mott metal-insulator transition and its relation to standard paradigms of phase transition and the nature of the resulting metallic state remain controversial. The challenge is that in experiment the Mott transition is often disguised by accompanying magnetic, charge, structural, or orbital orderings. Vortex system offers a tunable experimental playground for studying pure Mott physics. Investigating a square array of nano-patterned superconducting islands we find first experimental evidence for the dynamic Mott transitions of different universality classes corresponding to different commensurate fillings f_c . We observe both thermodynamic and dynamic (non-equilibrium) vortex Mott transition and demonstrate that at $f_c = 1$ both the non-equilibrium Mott transition and thermodynamic Mott transitions have the same quantum critical behavior. We propose a theory of the dynamic Mott transition based on the PT -symmetry breaking mechanism.

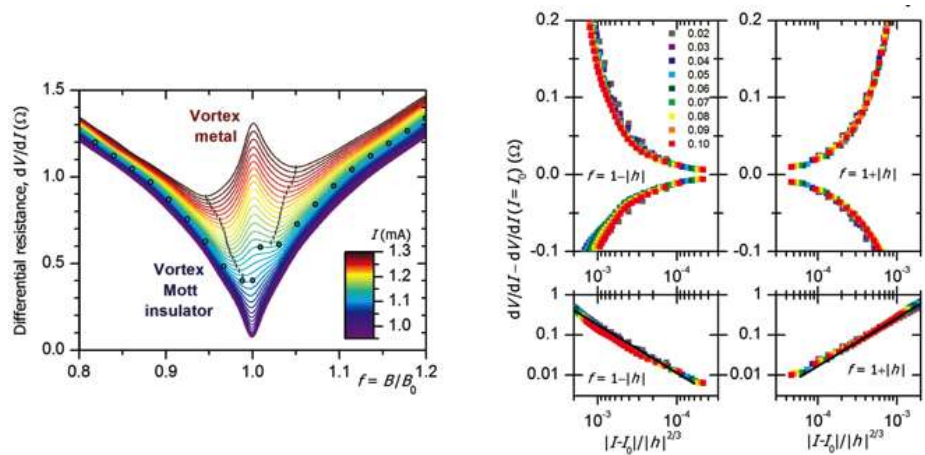


Figure 1.
Left panel: the representative differential resistance in the vicinity of filling $f_c=1$ taken at different currents.
Right panel: the corresponding scaling of the differential resistance as function of current and magnetic field.

Escape dynamics from Josephson to phase slip modes

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We have characterized the escape dynamics of different types of Josephson junctions also in unconventional regimes, through the measurement of switching current distributions (SCD). We have used SCD as a sophisticated detector at the same time of resistance and phase dynamics in an unprecedented energy range. We have used YBaCuO grain boundary Josephson junctions because of their wide tunability of the critical current density. A transition from classical Josephson phase dynamics, which takes place in junctions characterized by low values of critical current density J_c , to a regime in which dissipation is driven by local heating processes, for high values of J_c . These results point to a more articulate phase diagram of weak links in terms of electrodes coupling and dissipation. We speculate on possible intrinsic nanoscale ordering occurring in high critical temperature systems.

This transition is of relevance for all kinds of weak links including the emergent family of nano-hybrid junctions, including nanowires, two-dimensional graphene and topological insulator flakes as barriers. Information on the search of quantum phase slips can be also derived.

Quantum fluctuations in low-dimensional superconductors



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Keywords : mesoscopic superconductivity, quantum fluctuations, quantum phase slips

The topic of quantum fluctuations in quasi-1D superconductors, also called *quantum phase slips* (QPS), has recently attracted the significant attention. It has been shown that the phenomenon is capable to suppress the zero resistivity of ultra-narrow superconducting nanowires at low temperatures $T \ll T_c$ [1-3] and quench persistent currents in tiny nanorings [4]. The coherent QPS effect enables fabrication of the new generation of quantum logic devices – qubits [5]. It has been predicted that a superconducting nanowire in the regime of QPS is dual to a Josephson junction [6]. In particular case of an extremely narrow superconducting nanowire imbedded in high-impedance environment the duality leads to an intuitively controversial result: the superconductor should enter an insulating state. Here we experimentally demonstrate that the I-V characteristic of such a wire indeed shows Coulomb blockade which disappears with application of a critical magnetic field and/or above the critical temperature proving that the effect is related to superconductivity [7]. Such system can be considered as a junctionless single electron transistor (with charge $2e$), where the QPS provide the dynamic equivalent of weak links in conventional devices containing static (in space and time) tunnel junctions. Application of external RF radiation can be synchronized with the internal Bloch oscillations of charge. The phenomenon is dual to the well-known Shapiro effect: the voltage steps for a Josephson junction are substituted by the current steps for a QPS wire: the proof-of-principle demonstration of the long-awaited metrological application - the quantum standard of electric current [8]. We will also discuss our latest results demonstrating finite noise below the ‘residual’ critical current and temperature due to the same QPS effect. In ultra-narrow nanowires the quantum fluctuations of the amplitude of the order parameter result in smearing of the energy gap edge, which has been measured in tunneling experiments. **This study (research grant No 15-01-0153) was supported by The National Research University–Higher School of Economics’ Academic Fund Program in 2015-2016.**

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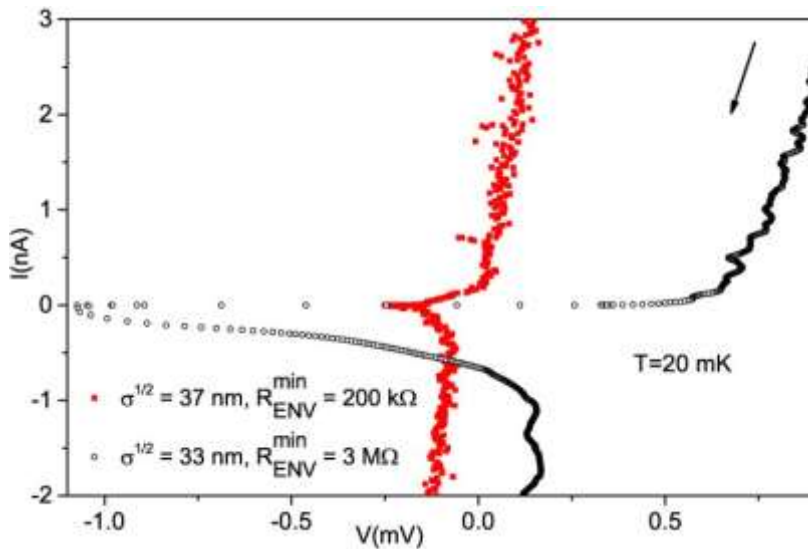


Figure 1: Coulomb blockade of two titanium nanowires with close values of cross section and significantly different impedance of the environment. Arrow indicates the direction of data recording.

SESSION 47

First order melting of a weak spin-orbit Mott insulator into a correlated metal



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Keywords metal insulator transitions – spin-orbit coupling

In this talk, I will present the results of our recent experimental exploration of the metal-insulator phase transition in the electron-doped spin-orbit Mott insulator $(\text{Sr}_{1-x}\text{La}_x)_3\text{Ir}_2\text{O}_7$. $\text{Sr}_3\text{Ir}_2\text{O}_7$ is the $n=2$ (bilayer) member of the strontium iridate Ruddlesden-Popper series and manifests a spin-orbit Mott (or $J_{\text{eff}}=1/2$) insulating ground state in the weak limit. This ground state has been the focus of increasing attention due to its predicted proximity to a number of other novel electronic ground states such as spin liquids, high temperature superconductivity, and new forms of symmetry-protected nonlocal order. Very little, however, remains understood regarding how competing symmetries affect the stability of the spin-orbit Mott state and, more broadly, the mechanism through which the $J_{\text{eff}}=1/2$ Mott phase transitions into the metallic regime upon carrier substitution. Understanding this information is critical for deciphering recent findings reporting anomalous metallic states, such as Fermi arcs [1] and negative electronic compressibility [2], in spin-orbit Mott systems once driven beyond the parent Mott state. Here I will present the results from transport, magnetization, neutron/x-ray scattering, and scanning tunneling microscopy measurements exploring the electronic and structural response of a canonical weak spin-orbit Mott state to electron doping. Our results demonstrate the first order melting of the insulating state under 2% electron substitution per Ir, and the emergence of a correlated metallic state beyond the phase boundary. The potential for an additional channel of symmetry breaking coincident with the onset of the metallic state will be discussed.

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Tiny cause with huge impact: polar instability through strong magneto-electric-elastic coupling in bulk EuTiO_3

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Keywords : multiferroics, polar instabilities, magnetic fluctuations

Multiferroic materials with combined polar, magnetic, and elastic orderings are at the forefront of scientific research in view of their multiple interactive couplings: magnetic order can be tuned by strain and an electric field, polar order can be triggered by a magnetic field and strain, and elastic properties are controlled by a magnetic and/or an electric field. Such materials are desirable for multiple applications. Even though the phenomenon of multiferroicity has been predicted long ago [1], its realization remains rare for rather simple reasons: typically polar order is achieved when a transition metal d^0 configuration is combined with highly polarizable anions, whereas magnetic order relies on a finite d^n configuration. Obviously these two requirements yield a certain incompatibility of the coexistence of the two phenomena which have been tried to overcome by combining magnetic layers with polar ones, by growing composites, and via strain engineering [2, 3]. Even though a rather large number of materials have been shown to exhibit the desired properties, the coupling between magnetic and polar order is either very weak, or the spontaneous polarization/magnetization appears at low temperature only and remains too small to be of technological interest. Here we propose a new strategy to achieve strong magnetic-polar coupling by deriving the soft mode frequency of EuTiO_3 as a function of its lattice parameters which exhibits unusual, yet very small temperature dependencies at high and low temperatures [4, 5]. Specifically we develop a route of how to induce ferroelectric order in *bulk* EuTiO_3 (ETO) by combining experimental results with theoretical concepts. We show that marginal changes in the lattice parameter of the order of 0.01% have a more than 1000% effect on the transverse optic soft mode of ETO and thus easily induce a ferroelectric instability. In combination with muon spin rotation data, where evidence for nanoscale magnetic domains was obtained [6], ETO appears to be the ideal candidate to achieve strong coupling magneto-electric properties at high temperatures.

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Induced Raman scattering in bulk EuTiO_3



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Keywords: EuTiO_3 , multiferroics, Raman spectroscopy, phase transitions

EuTiO_3 is a compound where its paraelectricity associated with the Ti^{4+} ions in the TiO_6 octahedra is coupled with the magnetic degrees of freedom from the Eu^{2+} ions. The structure characteristics of EuTiO_3 are very similar to SrTiO_3 ; both have a cubic structure at room temperature and adopt the tetragonal structure below 105K and $\sim 282\text{K}$ for SrTiO_3 and EuTiO_3 respectively. In both systems the ions are situated at sites with inversion symmetry and therefore, the associated phonons are Raman inactive in the electric-dipole approximation. In the cubic structure the three triply degenerate F_{1u} modes have been observed by IR spectroscopy. At low temperatures there are many more modes from the doubling of the unit cell and some of them are expected from group symmetry to be Raman active. In spite of that, no Raman active mode has been observed up to now at any temperature. In this work we have employed an external electric field in order to break the inversion symmetry and activate some of the modes to Raman scattering. Without any external effect, the Raman spectra were structureless with a strong continuum scattering. As a result of the field, the spectra have been considerably modified showing peaks that varied in intensity with the amount of applied voltage. In a cycle of applying voltage and letting the compound to relax, a clear hysteresis has been observed with the modified spectrum remaining for several days, but with a continuously reduced intensity. In a polished sample the effect was stronger, apparently related with the formation of strains and/or domains. All data indicate that we have broken the inversion symmetry activating Raman scattering in the paraelectric phase of this compound.

Dielectric properties of ferroelectric stripe domains



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Keywords : ultrathin ferroelectrics – stripe domains – oxide superlattices

Over the last decade, there have been a number of significant breakthroughs in our understanding of ferroelectric domains and domain walls [1]. The traditional view that ferroelectric domain walls are purely Ising-like has been challenged by recent high-resolution TEM data and theoretical calculations that predict a plethora of complex internal polarisation structures and even separate phase transitions within domain walls [2]. Perhaps even more exciting have been the numerous discoveries of unexpected emergent behaviour at domains walls, not intrinsic to the bulk of the material. Enhanced domain wall conductivity, large photovoltaic responses, domain wall magnetism and the appearance of polarisation in otherwise centrosymmetric materials are just a few of the phenomena that bring hope of new technologies and fuel the ever-growing interest in the newly emerged field of domain-wall nanoelectronics [1]. Collective responses of domain-walls are also being re-examined, particularly as research on nanoscale ferroelectrics has revealed that extremely dense, regular domain structures can be engineered in ultrathin films and heterostructures and are predicted to have interesting collective domain-wall dynamics [3,4]. We have investigated the dielectric properties PbTiO₃-based superlattices with such ultradense nanoscale ferroelectric stripe domains [5]. Dielectric impedance spectroscopy measurements in the 100 Hz–2MHz frequency range have been performed over a wide temperature range, from the cryogenic regime where domain walls are pinned to well above the Curie point where they no longer contribute to the dielectric response. We will discuss the effect of domain structures and domain-wall motion on the dielectric response of these artificially layered ferroelectrics, focusing in particular on the unusual behavior close to the ferroelectric-paraelectric phase transition.

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SESSION 48

Nanoscale fluctuations in electronic and atomic structure in strongly correlated electron and charge ordered systems



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Keywords: Pair distribution function, PDF, neutron diffraction, x-ray diffraction, diffuse scattering.

The observation of robust stripes of charge and spin in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_2$ superconductor was made as long ago as 1995, but after an initial flurry of excitement that high T_c superconductivity may be caused or enhanced by this phenomenon, interest has slowly waned with time. The reason first, is that it was found fairly quickly that the stripes tend to suppress superconducting T_c and so they compete with superconductivity. Second, the stripes were not found to be ubiquitous in all the cuprate superconductors, like antiferromagnetism or the observation of pseudogaps, for example. Stripes appeared to be an interesting side-show in a special class of materials. However, in the past 3-5 years or so, this has dramatically changed. Broken symmetry states have now been seen in a number of different cuprate systems, notably BSCCO and YBCO systems, using first scanning tunneling spectroscopy (STS) and later resonant elastic x-ray scattering (REXS). The phenomenon is therefore quite ubiquitous. Its role in the superconducting phenomenon is far from understood but quantum critical points between different broken symmetry orders are implicated under the superconducting dome of the cuprates. This is now a, if not the, forefront area of research in the cuprates.

As hard as it is to detect these broken symmetry phases in general, it is even more difficult to study them if and when they are short-range ordered and fluctuating. We have been using local structural probes augmented with inelastic scattering to study local symmetry breaking in the cuprates and related materials. A surprising picture emerges with locally symmetry broken states existing over fairly wide ranges of doping and temperature in a number of systems. We demonstrate a correlation between the observation of such features in the local structure and both transport and spectroscopic signatures.

Epitaxial growth and *in-situ* angle-resolved photoemission spectroscopy study on novel artificial iridates



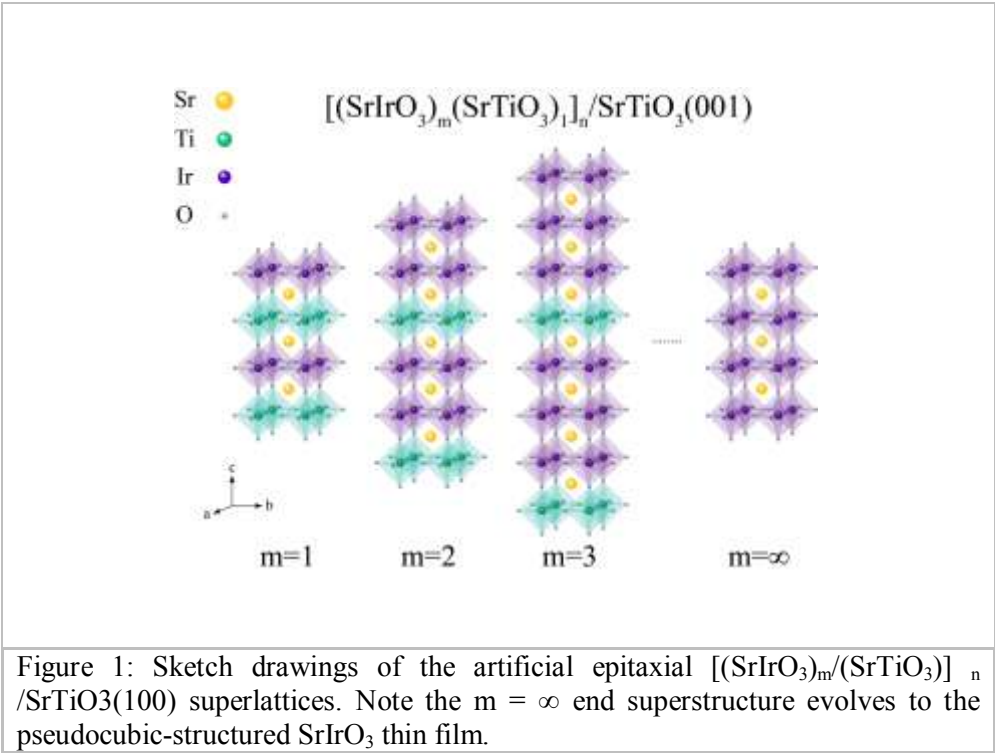
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Keywords: In-situ ARPES – Oxide MBE – Iridates

In this talk, we will introduce how to synthesize and study the artificial 5d iridate thin films by the combo of oxide molecular beam epitaxy (OMBE) and angle-resolved photoemission spectroscopy (ARPES) techniques. We will report the in-situ ARPES measurement on the electronic structure of epitaxial pseudocubic-structured SrIrO_3 thin films, in which the unique semi-metallic properties caused by the delicate interplay of spin-orbit coupling and electron correlations were comprehensively investigated. In addition, we successfully synthesized a series of high-quality $[(\text{SrIrO}_3)_m/(\text{SrTiO}_3)]_n/\text{SrTiO}_3(100)$ superlattices (as illustrated in Fig. 1) using OMBE, and then realized the metal-insulator transition (MIT) by artificial dimensionality control of iridates. The mechanism of this MIT was then investigated by both transports and our combined OMBE and ARPES system.



Fermi Pockets and Pseudogap in Lightly Doped Strontium Iridates



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Keywords : iridates, doped Mott insulators, ARPES, pseudogap, Fermi pockets

The insulating ground state of the layered perovskite iridates is often described in a single band pseudospin - 1/2 Hubbard model [1,2]. Iridates were thus proposed as analogues to the cuprates and as such, a potential platform for engineering high-temperature superconductivity under electron doping [2]. However, it proved difficult to dope iridates in the bulk and to date little is known about the evolution of their electronic structure with increasing carrier concentration.

Here we report first angle resolved photoemission data from La doped single crystals of the single and bilayer perovskites Sr_2IrO_4 and $\text{Sr}_3\text{Ir}_2\text{O}_7$. La^{3+} substitutes for Sr^{2+} on the B-site and dopes electrons in the IrO_2 plane with minimal disorder and without affecting the strong spin-orbit coupling on the Ir site that drives the antiferromagnetic insulating ground state of the parent compound.

In single layer $(\text{Sr}_{1-x}\text{La}_x)_2\text{IrO}_4$, we find a rapid collapse of the Mott gap with doping. At the highest doping level of $x=0.05$, quasiparticle like excitations forming a large circular Fermi surface centered at Γ emerge. As in cuprates, we find a strongly anisotropic quasiparticle residue and a momentum dependent pseudogap that increases in magnitude towards the antinode resulting in a Fermi arc-like contour. However, our data show significant weight on the backside of the arcs, which we attribute to backfolding due to the structural distortion of the IrO_2 plane. Intriguingly, the doping evolution of $(\text{Sr}_{1-x}\text{La}_x)_3\text{Ir}_2\text{O}_7$ is fundamentally different. In the bilayer iridate, we find highly coherent quasiparticle excitations, devoid of a pseudogap, that form a small Fermi surface obeying the Luttinger theorem. We conclude that lightly doped Sr_2IrO_4 does indeed share much of the electronic structure phenomenology with cuprates while $(\text{Sr}_{1-x}\text{La}_x)_3\text{Ir}_2\text{O}_7$ is more akin of a doped semimetal and can be described qualitatively by a rigid shift of the chemical potential into the unoccupied states of the parent compound.

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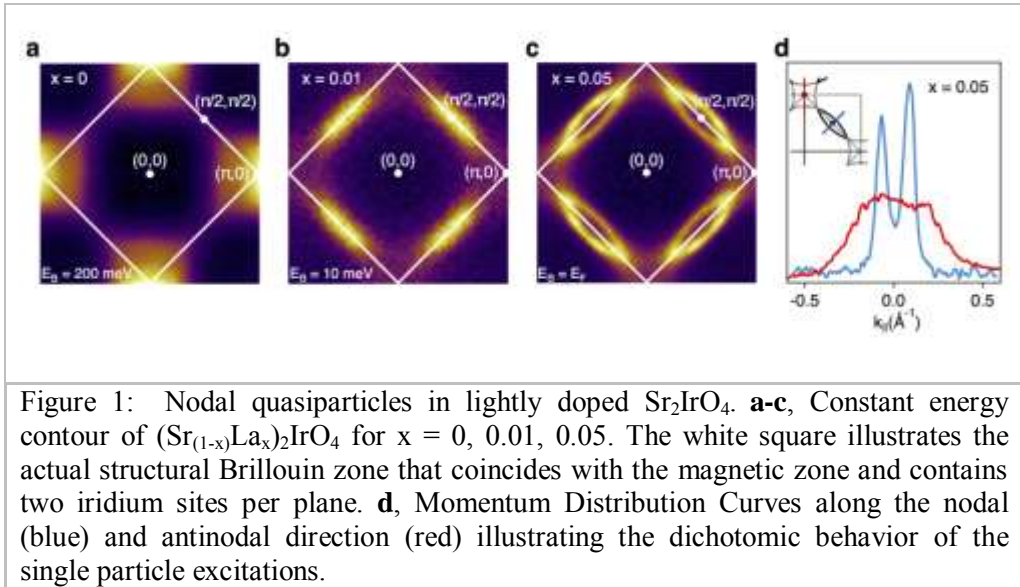


Figure 1: Nodal quasiparticles in lightly doped Sr_2IrO_4 . **a-c**, Constant energy contour of $(\text{Sr}_{1-x}\text{La}_x)_2\text{IrO}_4$ for $x = 0, 0.01, 0.05$. The white square illustrates the actual structural Brillouin zone that coincides with the magnetic zone and contains two iridium sites per plane. **d**, Momentum Distribution Curves along the nodal (blue) and antinodal direction (red) illustrating the dichotomic behavior of the single particle excitations.

SESSION 49

Emergent long-range magnetic ordering in manganite superlattices



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Keywords: magnetic ordering – oxide superlattices – X-ray Diffraction

The basic physical and chemical properties of transition-metal-oxides and their interfaces are of great importance as their correlated electronic structure induces a variety of phenomena like charge, spin and orbital orderings and they are the key to understand macroscopic properties like electrical- and thermal transport, magnetism, optical response, metal-insulator transitions and superconductivity of these materials.

In this work we focus on the magnetic configuration of superlattices of LaMnO_3 (LMO) and SrMnO_3 (SMO). Both are supposed to be antiferromagnetic insulators with a transition temperature well below 300K.

However, the combination of both oxides with stoichiometry $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ is a ferromagnetic metal at temperatures below 400K.

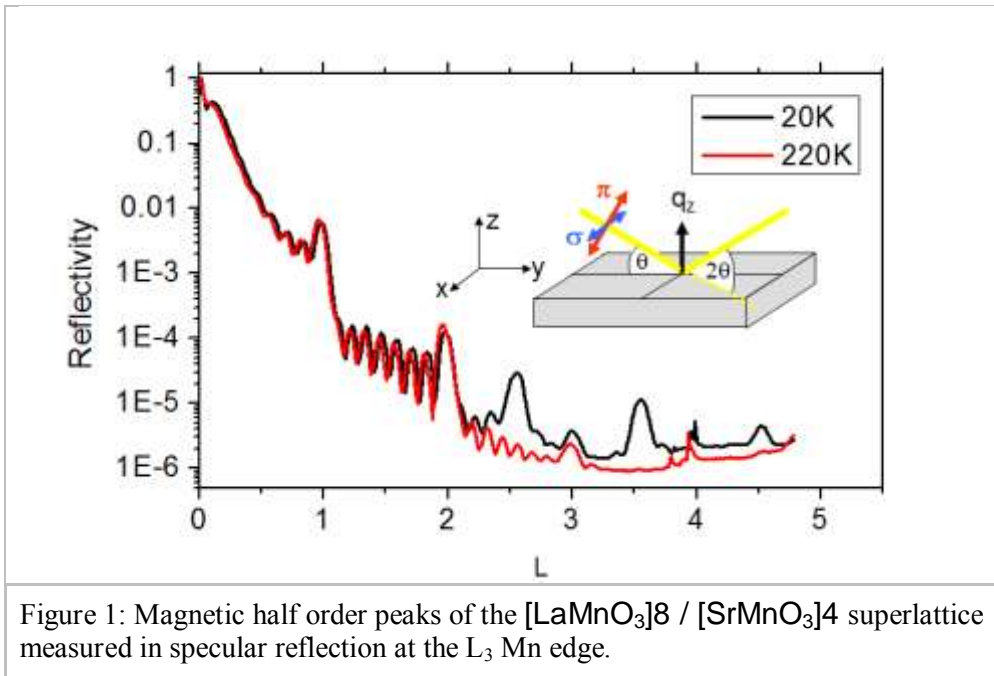
Hence, superlattices of LMO and SMO grown on SrTiO_3 potentially combines an A-type (layered) antiferromagnet with an G-type (checkerboard) antiferromagnet, but with a ferromagnetic interface [1-4].

In order to characterize the magnetic and orbital ordering, we measure resonant soft X-ray reflectometry (RSXR) on the Mn $L_{2,3}$ edge, which allows a non-destructive, element selective analysis of the magnetic profile [5].

An unexpected antiferromagnetic ordering is observed for the $[\text{LaMnO}_3]_8 / [\text{SrMnO}_3]_4$ superlattice with distinct half-order superstructure peaks as shown in Figure 1. This gives rise to a long range antiferromagnetic ordering with a period twice as large (24 unit cells) than the chemical period (12 unit cells). We will analyze the polarization dependence, as well as the temperature dependence, and will provide several models for this ordering.

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Emergence of an inhomogeneous state in a triangular antiferromagnet



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Keywords : geometrical frustration – phase separation – dynamics – DFT

The crystal structure of the Jahn-Teller distorted AMnO_2 ($\text{A} = \text{Na}, \text{Cu}, \text{Mn}^{3+}$ in $t_{2g}^3 e_g^1$) rock-salt derivatives maps out on a two-dimensional triangular spin lattice with anisotropic intra- and inter- chain exchange interactions ($J_1, J_2 < 0$). Since the ground-state degeneracy of these frustrated magnets serves as a source of phase competition, these materials offer a playground for testing exotic states of matter and serve as ideal candidates for previously unseen inhomogeneities.

The interplay between the structural and magnetic degrees of freedom in AMnO_2 has been studied by neutron powder diffraction and shows a monoclinic-to-triclinic phase transition with the simultaneous appearance of antiferromagnetic order. [1, 2] A-site cation interactions with the lattice are shown to play a significant role in the structural transition, reflected also in the increase of the Néel temperature from 45 K in Na- to 65 K in Cu-analogues and the modification of the interplane coupling (Figure 1). Our theoretical studies and experimental investigations postulate that the increase of the elastic energy due to the monoclinic-to-triclinic transformation is mainly balanced by the magnetic exchange; while the magnetic degeneracy is removed by the triclinic distortion the magnetoelastic contribution is minimal.

Surprisingly though, local probe $\mu^+\text{SR}$ and NMR in NaMnO_2 , complemented by synchrotron X-ray diffraction, point to spontaneous emergence of competing magnetostructural states at the nanoscale. [3] In order to fully understand this phenomenon it is highly desirable to use local probes and draw similarities to other isomorphous systems, such as the CuMnO_2 derivative. In the case of Cu-analogue we envisage the A-site as a parameter that controls the transition from a disordered to an ordered, less inhomogeneous ground state. [4] Our analysis shows that the two major opposing effects (elastic vs. magnetic exchange) of similar magnitude, lead to nearly equivalent crystal structures, which enables already infinitesimal quenched disorder to locally lift the inherent frustration of the parent monoclinic phase in either case. This previously unseen route provides a solid foundation for the realization of a multiple-minima free-energy landscape that is required for the formation of nanoscale domains in an insulating spin system where no active charge degrees of freedom are available.

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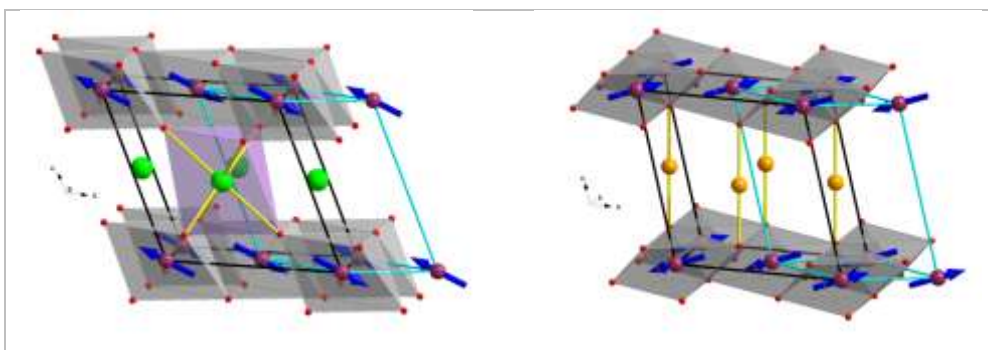


Figure 1: Interlayer-cation mediated relief of frustration in spin-2 triangular lattices, NaMnO₂ (left) and CuMnO₂ (right).

Character and dynamics of orbital order in magnetite



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Keywords : complex number orbital order – Verwey transition – laser-induced dynamics

Even though magnetite (Fe_3O_4) has been known for more than 75 years to exhibit a metal-to-insulator transition the character of that transition has remained elusive as of today. The so-called Verwey-transition involves an abrupt structural distortion from a cubic high-temperature phase to an - only recently determined - monoclinic low-temperature phase [1] as well as an increase of resistivity by about two orders of magnitude. That charge localization via charge and orbital ordering plays a role here has been put forward early, but the precise character of the order has been strongly disputed in particular since different experimental techniques apparently gave contradictory information.

We carried out resonant soft x-ray diffraction at the $\text{Fe } 2p \rightarrow 3d (L_{2,3})$ resonance from magnetite thin films and bulk samples [2,3]. The films were grown such that via strain crystalline twinning was largely suppressed. An analysis of the resonance spectra revealed a striking quantitative agreement with the Complex-number Orbital Order (COO) model for magnetite put forward recently [4]. This model, based on ab-initio calculations, predicts an unusual ground state where large orbital moments form spontaneously into a non-collinear pattern, which only weakly couples to the spin order. Charge order is only weakly developed in this model.

While our resonant diffraction data clearly rule out any real-number orbital order and charge order pattern based on earlier crystal structure models for magnetite, the most recent monoclinic crystal structure [1] does in principle allow for a real-number charge and orbital-order pattern with a symmetry as seen in our experiments. A clear contrast between real and complex-number order, however, is to be expected when the circular dichroism in resonant diffraction is being probed. Results from first corresponding experiments will be presented.

In a second line of research, we studied the dynamics of the Verwey transition when induced with a femtosecond laser pulse. Again using soft x-ray diffraction techniques, we could probe structural and electronic degrees of freedom separately. In a first experiment [5], we found the transition to occur in steps. After a first rapid local destruction of electronic superstructures as well as of the low-temperature crystalline phase, the actual phase transition occurs via spatial reorganization within a regime of phase coexistence of residual low-temperature and high-temperature phase patches (Fig. 1).

Very recently we were able to take a closer look into the fast initial processes. We found that electronic order is locally destroyed within a few femtoseconds. Consequently there is a realistic chance to observe a transient state where electronic order has been quenched while the lattice remains in the low-temperature structure.

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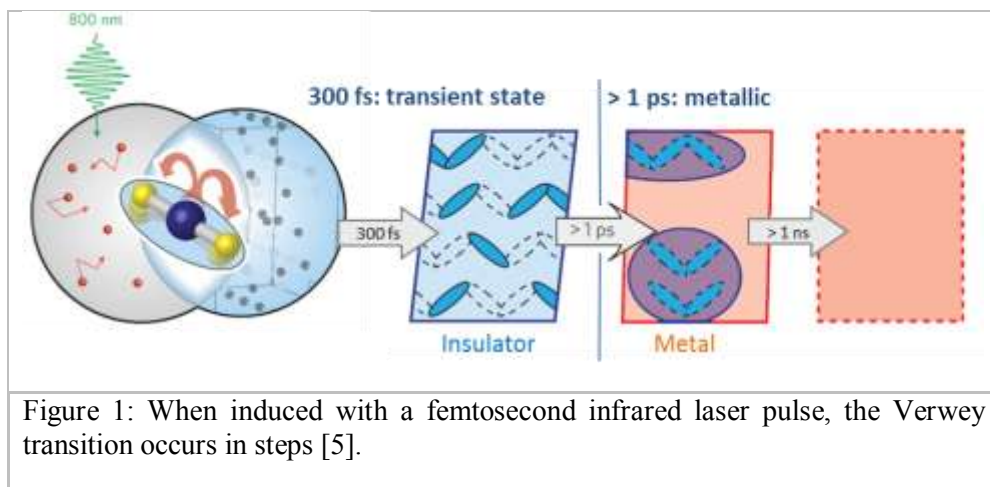


Figure 1: When induced with a femtosecond infrared laser pulse, the Verwey transition occurs in steps [5].

SESSION 50

Switching dynamics of Josephson junctions in a wide range of J_c values: crossover from Josephson to phase slip modes

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Studies of phase dynamics and macroscopic quantum phenomena have been recently extended to a large variety of unconventional Josephson junctions, such as high critical temperature superconductors [1] and novel types of hybrid systems [2]. Fundamental issues on coherence and dissipation have been raised, concerning the nature of the transition from the superconducting to the normal state in a wide class of devices, including nanoscale and hybrid structures [3].

We will report on measurements of switching current distributions (SCDs) in different types of junctions, including YBCO grain boundary junctions in a wide range of critical current density (J_c) values [4,5]. Josephson phase dynamics takes place in junctions characterized by lower values of J_c , while in high J_c junctions dissipation is driven by local heating processes as phase slip events. Numerical simulations confirm that a heat diffusion-like model breaking phase-coherent information is consistent with the data on high J_c junctions [5].

Different sources of dissipation can be detected by a comparative analysis of the SCDs, and fluctuations turn to be a powerful tool to analyze such different dynamical processes. These results are of relevance for all kinds of weak links. Every experiment using nanowires or more in general low dimensional barriers should be concerned about possible heating effects, leading to distorted phase information.

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Spintronics with magnetic nanomolecules and graphene flakes



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Keywords: magnetic nanomolecules – graphene flakes – spin dynamics

Techniques of regulating spin dynamics in magnetic nanomolecules and graphene flakes are theoretically studied. An efficient method is suggested allowing for fast spin reversal and for regulating the whole spin dynamics of separate nanomolecules and flakes as well as of the assemblies of many nanomolecules. The method is based on the use of the Purcell effect induced by a resonator. Spin dynamics is analyzed both analytically, by employing scale separation approach, and by numerical computer simulations.

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Probing the nature of high-T_c superconductivity using quantum nano devices



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Keywords: mechanisms for high T_c – nano devices – quantum devices – YBCO thin films

New insights into the coupling mechanism leading to High critical Temperature Superconductivity can be obtained by studying the superconductive state on the nanoscale and as a function of doping. The real issue is to go beyond the present state-of-the-art by realizing devices, which could probe the superconducting transport on length scales predicted by the various theories. Indeed, the correlation lengths of spin fluctuations or striped charge order are expected to be in the nanometer scale.

The recently discovered charge density wave (CDW) order in Y- [1] and Bi- [2] based HTSs clearly demonstrates that nano-scale ordering plays a major role in the doping dependence of the superconducting and normal state of the entire family of cuprate superconductors. Whereas X-ray scattering experiments point towards a competition between the CDW order and the superconducting state in underdoped HTSs, very little is known about the effect of nanoscale ordering on the electrical transport properties in the superconducting state of HTSs.

In this contribution we present measurements on YBCO nano devices in the form of wires and nano Superconducting QUantum Interference Devices (nanoSQUIDs), which could give insight into the microscopic mechanism of superconductivity in this class of strongly correlated electron materials. In order to understand the role of nanoscale ordering on electrical transport properties in the superconducting state it is imperative to master the nanofabrication of YBCO thin films down to a few ten nanometers (close the correlation length of CDWs). Our recent results on nanowires and nanoSQUIDs clearly show that our nano-patterning process retains pristine superconducting properties of as-grown films [3, 4] (see Fig.1). From the magnetic flux periodicity of the critical current of nanoSQUIDs and the voltage position of Shapiro-like steps in the current voltage characteristics of microwave irradiated nanowires one can obtain the fundamental charge of the superfluid. Indeed, in case of a (superconducting) pair density wave one would expect for the fundamental charge 4 times the elementary charge (4e) compared to the conventional 2e of a simple BCS superconductor [5]. Measurements performed in the optimal doping regime reveal a 2e charge in the full temperature range below T_c. The investigation of the

fundamental charge close to the $1/8$ anomaly doping, where CDW are more pronounced, are currently in progress.

Moreover, our nano-patterning process allows for new exciting developments towards quantum-limited sensors such as single photon detectors and nano Superconducting Quantum Interference Devices (nanoSQUIDs) with unprecedented sensitivity.

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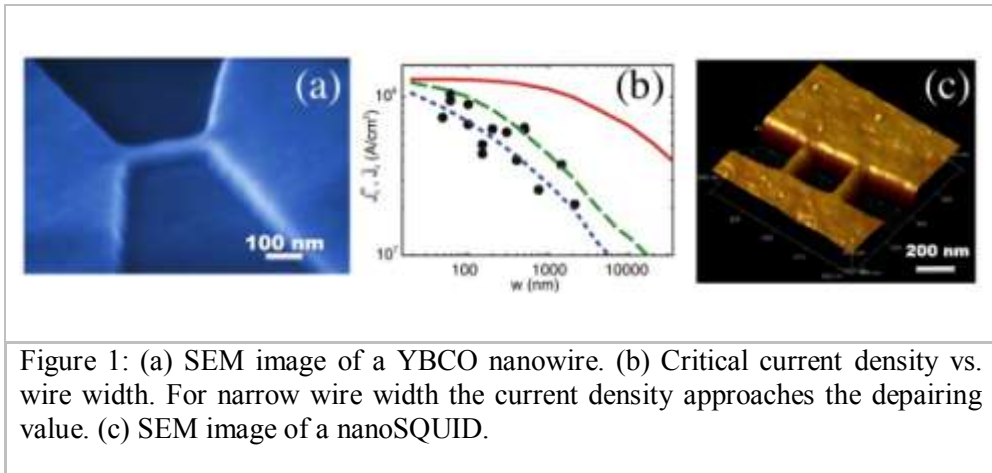


Figure 1: (a) SEM image of a YBCO nanowire. (b) Critical current density vs. wire width. For narrow wire width the current density approaches the depairing value. (c) SEM image of a nanoSQUID.

Infrared studies on the Collapsed Tetragonal phase of $\text{Ca}_{0.86}\text{Pr}_{0.14}\text{Fe}_2\text{As}_2$



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Keywords : Iron-based superconductor –Infrared spectroscopy

There is growing evidence that the covalent Fe-As bond plays an important role in the appearance of superconductivity in iron-pnictides [1]. Among the Fe-As based superconductors, CaFe_2As_2 is an excellent prototype material to explore the nature of superconducting mechanism due to its strong Fe-As bonding and large structural instability [2]. Upon doping or applying pressure, CaFe_2As_2 undergoes a remarkable structure transition from the orthorhombic phase directly into the so-called collapsed tetragonal phase in which the local Fe moment and spin fluctuation are quenched. Recent transport measurements further revealed that following the lattice-collapse transition, Fermi-liquid behavior abruptly recovers along with the disappearance of bulk superconductivity [3]. We have investigated the temperature dependence of in-plane optical conductivity in $\text{Ca}_{0.86}\text{Pr}_{0.14}\text{Fe}_2\text{As}_2$ which shows a structural transition from tetragonal (T) to collapsed tetragonal (cT) phase at T_{cT} of about 73 K. Upon entering the cT phase, drastic change characterized by the formation of a mid-infrared peak near 3200 cm^{-1} (0.4 eV) in the optical conductivity is observed. Analysis of the spectral weight reveals reduced electron correlation after the cT phase transition. Based on the calculated band structure and simulated optical conductivity, we attributed the new feature around 0.4 eV to the formation of interlayer As-As bond. The As-As bond strongly affect the Fe-As hybridizations, and in turn, drastically change the $\text{Ca}_{0.86}\text{Pr}_{0.14}\text{Fe}_2\text{As}_2$ into a nonmagnetic Fermi-liquid system without bulk superconductivity in the cT phase.

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SESSION 51

Dual Features of Spin and Charge Excitations in High- T_c Cuprates.



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Keywords: t-J-G model, collective excitations

The dynamical spin and charge susceptibilities in the t-J-G model combining the random phase approximation (RPA) and projection operator method are discussed [1,2].

First we focus on the mutual interplay between the local and the itinerant components of spin susceptibility. Near the antiferromagnetic wave vector the calculated dispersion of the spin excitations reproduces well the so-called hour-glass dispersion, characteristic for several layered cuprates. It is formed as a result of competition between the original spin-gap in magnon-like excitations spectrum and the superconducting gap, which affects the itinerant component of the susceptibility. Furthermore, the calculated collective spin excitations along $(0, 0)-(0, \pi)$ are in agreement with the positions of the absorption peaks in the inelastic X-ray scattering spectra. They refer to the paramagnon-like modes, characteristic to the itinerant spin system, rather than magnon-like excitations that originate from short range order effect in the system of local spins at Cu sites.

The dynamic charge susceptibility as a function of the wave vector and the frequency is discussed in the context of the existing experimental data on the plasmon frequencies and softening of the longitudinal phonon modes. It is emphasized that a set of all experimental data can be explained only under the assumption that the parameters of the electron-phonon coupling depend not only on the value of the momentum transfer \mathbf{q} but also on the wave vector \mathbf{k} .

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Effects of the proton irradiation on the microwave properties of the multiband system $Ba(Fe_{1-x}Co_x)_2As_2$ films. Theory vs experiment.



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Keywords : multiband model, impurities, microwave, irradiation

For iron pnictides, the symmetry of the superconducting order parameter is still under debate. It was suggested that only in the case of s_{\pm} symmetry, non-magnetic impurities can induce a crossover from s_{\pm} to s_{++} symmetry [1], meaning that the smaller superconducting gap Δ_1 first closes and then reopens. Terahertz (THz) spectroscopy is an ideal tool to investigate this process, as it allows us to extract model-independent the complex optical conductivity of thin films, providing the possibility to directly observe the superconducting energy gap [2].

Therefore, we have step-wise irradiated a $Ba(Fe_{0.9}Co_{0.1})_2As_2$ thin film (26K) with protons and measured its complex conductivity in the terahertz frequency range (0.5 - 4.3 meV). For the first irradiation steps, we find that the critical temperature of the film is decreased linearly with the irradiation dose, while Δ_1 gets suppressed faster. For higher irradiation doses, we observe a clear anomaly in the optical conductivity, consistent with the theoretical predictions for a crossover from s_{\pm} to s_{++} symmetry, solving the longstanding question of the iron pnictides in favor of s_{\pm} -symmetry.

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Nonlinear Response in the Cuprates



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Keywords: nonlinear response – stripe order dynamics – pseudogap

In this talk I will present insights into some of the important aspects of cuprate physics gained from measurements of nonlinear response to external fields. The experiments are made possible by a specially developed probe, which eliminates sample heating problems by using rapidly alternating (radio-frequency) fields and detecting the sample response at harmonics of the excitation frequency [1]. Although not a conventional method, nonlinear response can provide a wealth of information on electronic physics, and the conditions necessary for the occurrence of nonlinearities will be expounded. These include strongly nonlinear response close to the superconducting transition temperature of several cuprates [2,3], collective dynamics of charge order [4], and unconventional charge stripe precursor phases [5]. Also, some components of the nonlinear signal can be connected to broken symmetries in the sample – this will be discussed in the context of nematic order and pseudogap.

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SESSION 52

A new theoretical approach to macroscopic quantum coherence in high temperature superconductivity.



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Keywords : High temperature superconductivity – *p*-type cuprates – macroscopic quantum coherence – electron pairing – fractal networks.

We present a recently published theoretical approach to explain macroscopic quantum coherence and High Temperature Superconductivity (HTS) in the *p*-type cuprates [1].

We begin by identifying a number of key challenges, which we address within the context of the theory. These include:

Support or refute alternative e-pair coupling mechanisms that have been proposed in the literature to date.

Identify the role of dopants in HTS.

Resolve the proposed dual e-pair coupling mechanisms responsible for the Pseudo Gap (PG) and Super Conducting (SC) phase.

Identify the correct relations between the PG and SC phases highlighted by Huffner *et al* [2].

Identify the role of the PG in HTS.

Identify relations between the antiferromagnetic insulator and HTS [3].

Address e-pair localization theory in disordered networks [4].

Identify the mechanism whereby an expected diffusive process in a fractal network leads to macroscopic quantum coherence [5].

As a first step we consider electron pair (e-pair) coupling mechanisms in the SC and PG phase. Based on the evidence, we conclude that e-pair coupling in the SC phase is facilitated by dopant induced quantum potentials, whilst e-pair coupling in PG phase is facilitated by fractal spin waves (fractons).

On another level, the paper considers new insights into the emergence of a macroscopic quantum potential generated by a scale free (fractal) distribution of dopants reported by Fratini *et al* [6]. This in turn leads to the emergence of coherent, macroscopic spin waves and a second associated macroscopic quantum potential. These quantum potentials play two key roles. The first involves the transition of an expected diffusive process (normally

associated with Anderson localization) in fractal networks, into e-pair coherence through a mechanism directly analogous with Coherent Random Lasing. The second involves the facilitation of tunnelling between localized e-pairs. These combined effects (driven by dopant levels) explain observed phase relations in *p*-type cuprates [2], including the merger of the SC and PG phase into a single coherent condensate at optimal doping.

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Topological superconductivity with mixed chirality



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Keywords : topological superconductivity – chiral edge states – honeycomb lattice

Topological chiral superconductors have recently received a lot of attention. A primary example, with many material candidates proposed lately [1-8], is the chiral $d(x^2-y^2) + id(xy)$ -wave state in honeycomb materials with strong electron-electron interactions. This is a time-reversal symmetry breaking superconducting state with two co-propagating, i.e. chiral, edge states, see e.g. Ref. [9].

In this work [10] we find that a highly unconventional *mixed chirality d-wave* superconducting state likely also exists in these honeycomb materials. The lightly doped honeycomb lattice has two separate Fermi surfaces or valleys, at K and K' = -K. The mixed chirality state has $d+id'$ -wave symmetry in one valley, but $d-id'$ -wave symmetry in the other valley, and is thus a natural mix of the two chiralities, without invoking any domain structure or other real space variations. We find that this mixed chirality state is the ground state in a large part of the antiferromagnetic - superconducting coexistence region, which has been found to exist in honeycomb materials with electron-driven superconductivity [11, 12]. The antiferromagnetism is essential, since the d' component is odd under spatial inversion in the mixed chirality state and therefore necessarily in a spin-triplet configuration. The mechanism enabling the mixed chirality state is in fact closely related to previously discussed π -triplet superconducting states [13].

We also investigate the properties of the mixed chirality d -wave state. The state is topological on each Fermi surface, but the topological invariant cancels when summed over the whole Brillouin zone. This results in two counter-propagating edge states, which are only protected in the absence of intervalley scattering. Furthermore, we find that both the chiral and mixed chirality d -wave states are fully gapped and the two phases are separated by a first-order phase transition at a finite magnet moment M_c . This phase transition is thus a topological phase transition, but with no bulk gap closing, with is otherwise assumed to be a general prerequisite for changing topological order.

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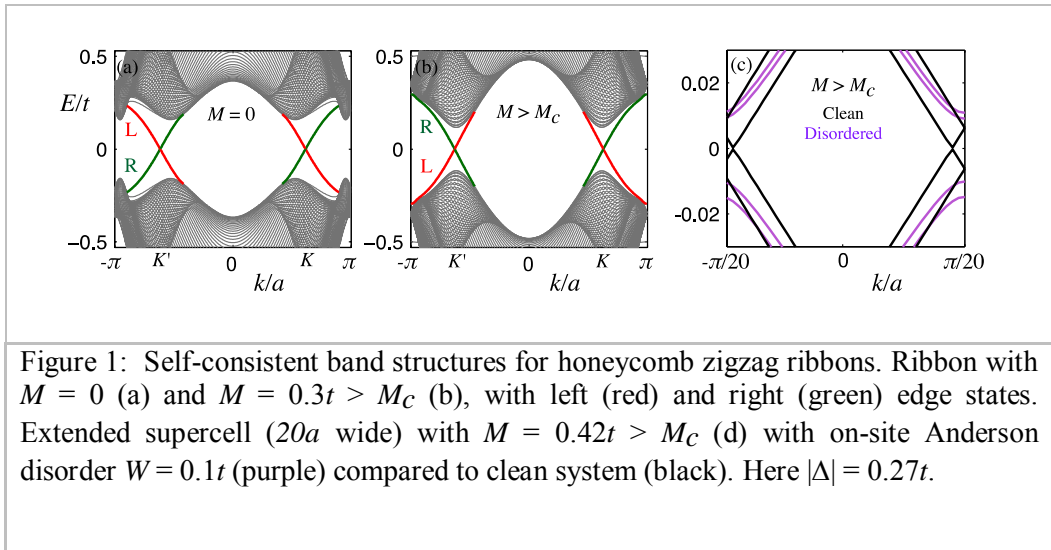


Figure 1: Self-consistent band structures for honeycomb zigzag ribbons. Ribbon with $M = 0$ (a) and $M = 0.3t > M_c$ (b), with left (red) and right (green) edge states. Extended supercell ($20a$ wide) with $M = 0.42t > M_c$ (d) with on-site Anderson disorder $W = 0.1t$ (purple) compared to clean system (black). Here $|\Delta| = 0.27t$.

Weber Blockade and Quantum Vortex Chains in Superconducting Nanowires



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Keywords : superconducting nanowires – vortices

Vortices in superconductors are topological excitations that carry quantized magnetic flux and can be viewed as basic degrees of freedom that describe the low-energy states of the system. Here we show that a short superconducting nanowire can behave as a quantum dot for vortices. In the range of magnetic fields in which vortices can enter the nanowire in a single row, we find regular oscillations of the critical current as a function of magnetic field, with each oscillation corresponding to the addition of a single vortex to the nanowire [1]. A charge-vortex dual of the Coulomb-blockaded quantum dot for electrons, the nanowire shows diamond-shaped regions of zero resistance as a function of current and magnetic field, in which the number of vortices is fixed. Besides demonstrating that macroscopic objects such as vortices can behave as fundamental particles, the fine control over critical currents and vortex configurations may prove useful for quantum devices that employ superconducting circuits.

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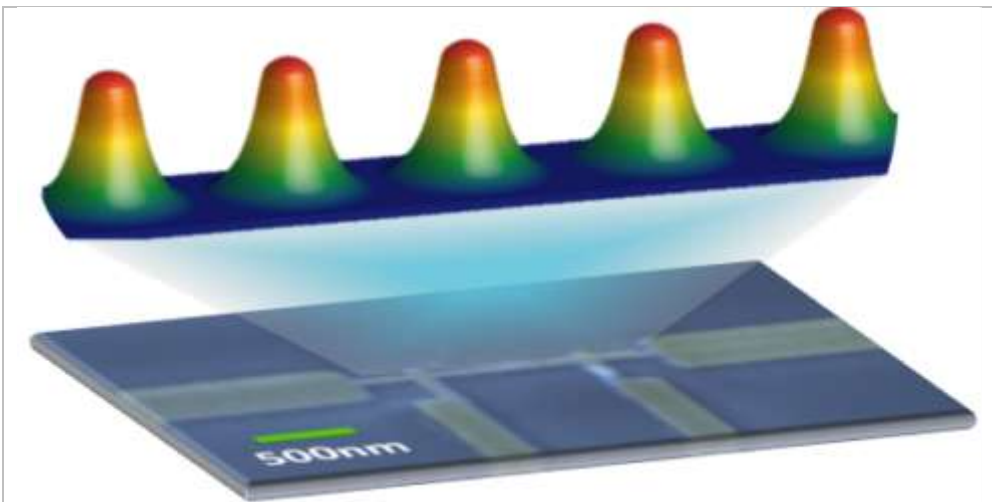


Figure 1: A scanning electron microscope image of an aluminum nanowire with a schematic of the vortex arrangement.

SESSION 53

Revised phase diagram of the cuprates



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Keywords: scattering rate, transport, magnetotransport, optical conductivity, Fermi liquid

The superconducting state of the cuprates evolves upon cooling from an enigmatic metallic phase that is characterized near optimal hole doping by a planar resistivity with large magnitude and extended linear temperature dependence. Below optimal doping, at temperatures below T^* , there exists an intermediate pseudogap phase with a partially gapped Fermi surface. These unusual properties have motivated proposals to consider unconventional electronic scattering mechanisms and even to abandon the Landau quasiparticle paradigm entirely.

HgBa₂CuO_{4+δ} (Hg1201) may be viewed a model cuprate system due to its relative structural simplicity, minimal disorder effects, and large optimal T_c of nearly 100 K (1). We have found that the planar resistivity of Hg1201 exhibits quadratic temperature dependence, the behavior characteristic of a Fermi liquid, at temperatures below T^{**} ($T^{**} < T^*$) (2). This result motivated optical conductivity measurements that yielded the quadratic frequency dependence and the temperature-frequency scaling of the optical scattering rate expected for a Fermi liquid (3). Furthermore, we demonstrated for Hg1201 (and for YBa₂Cu₃O_{6+δ}) that the magnetoresistance obeys Kohler's rule at temperatures below T^{**} (4). By combining our dc resistivity results for Hg1201 with published data for three structurally more complex cuprates, we obtained the universal sheet resistance throughout most of the temperature-doping phase diagram and arrived at the unexpected conclusion that Fermi-liquid behavior extends to very low doping, close to the Mott-insulating state (2). In contrast to previous approaches that extended ideas developed for the strange metal phase ($T > T^*$) to the pseudogap phase ($T < T^*$), we will discuss the former in the context of the now well-documented pseudogap Fermi-liquid state (5).

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Finite penetration depth above T_c in LSCO $x=1/8$.

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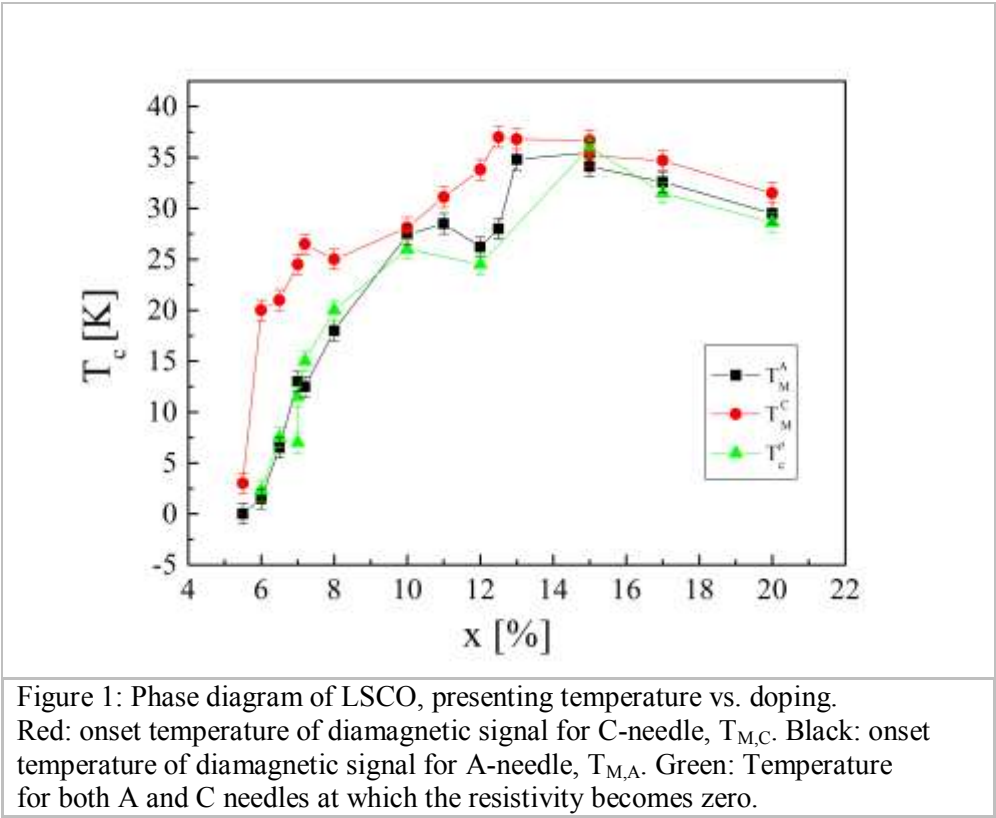
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Keywords : high T_c , cuprates, LSCO, susceptibility

Recently it was demonstrated that when measuring magnetization of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) single crystals, in the form of needles, the same compound becomes diamagnetic at two different temperatures, depending on the external magnetic field direction relative to the CuO_2 planes [1]. The transition temperature when the field is applied perpendicular to the planes, $T_{M,C}$, was found to be larger than the transition temperature when field is applied parallel to the planes, $T_{M,A}$. The resistivity falls to zero also at $T_c = T_{M,A}$. The difference between $T_{M,A}$ and $T_{M,C}$ is particularly large at the stripes phase with $x=12.5\%$ (see Fig. 1). One could argue that in this phase the transition from normal to superconducting state occurs in two steps. First, there is some kind of 2D superconductivity only in the CuO_2 planes, which starts at $T_{M,C}$, but there's no phase coherence between the planes. Upon further cooling, the correlation between the planes rises until at $T_{M,A}$, the whole sample becomes superconducting. In this work we report penetration depth measurements using low energy muon spin rotation (LEM) on LSCO $x=12.5\%$ samples, with external field parallel to the "c" direction. The measurements were done at $T_{\text{LEM}}=30\text{K}$ which satisfies $T_{M,A} < T_{\text{LEM}} < T_{M,C}$. A clear finite penetration depth was found in this sample, at the state which is associated with 2D superconductivity. This penetration depth will be compared with the BKT prediction.

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Theoretical Study of Phosphorene-based 2D Materials



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Keywords: 2D material, phosphorene.

In this talk, we will report the results of density functional theory calculations on phosphorene-based 2D materials including hybrid allotropes and extrinsic point defects of phosphorene, and phosphorene oxide. We will show that the electronic properties of phosphorene can be modified by the adatom functionalization. Additionally, the oxygen absorption may not degrade the phosphorene, and degree of the functionalization of phosphorene determines the electronic properties. This is reaffirmed by dependence of the diode-like asymmetric current-voltage response on the degree of stoichiometry for the phosphorene oxide.

(in collaboration with Gaoxue Wang and Shashi Karna)

Universal two superconducting domes in unconventional superconductors



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Keywords: New phase diagram of unconventional superconductivity, two superconducting domes, Quantum Critical point, Non-Fermi-liquid

Over the past few decades, several new classes of superconductors have been discovered hosting a superconducting (SC) dome when the pristine material is tuned towards a magnetic quantum critical point (QCP). This observation has led to a hypothesis that the formation of a SC dome in the vicinity of a QCP may be instrumental to the mechanism of unconventional superconductivity. In this talk, I will present a comprehensive analysis of the phase diagrams across several families of superconductors including copper-oxides, heavy-fermions, iron-pnictides and iron-chalcogenides, organics, and the recently discovered oxybismuthides.[1] Surprisingly, all these families inherently possess two distinct SC domes, which can be revealed using multiple control parameters, see attached figure. The SC dome at or near a possible QCP possesses a lower transition temperature (T_c) whereas the second SC dome, emerging nearer a non-Fermi liquid (NFL) state has a higher T_c and superfluid density. Comprehensive analysis reveals that the presence of two SC domes is a universal feature in unconventional superconductors. I will discuss the possible intimate relationship between NFL, electronic complexity and higher-temperature superconductivity.

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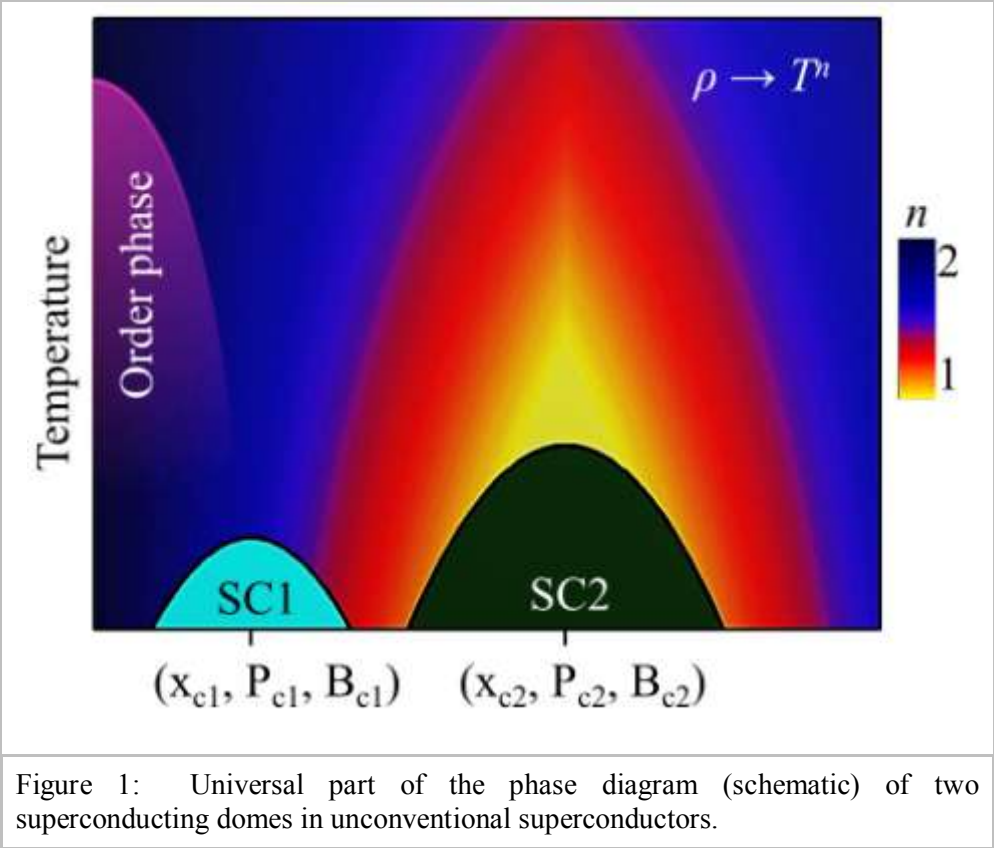


Figure 1: Universal part of the phase diagram (schematic) of two superconducting domes in unconventional superconductors.

SESSION 54

STM/STS study on electronic charge order and large pseudogap in Bi2212

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Keywords: high T_c cuprate – charge order – pseudogap

We performed scanning tunneling microscopy/spectroscopy (STM/STS) in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ (Bi2212) to investigate an electronic charge order (CO). In our previous works, we reported that the sample surface, where the CO appears very weak, the STS spectra are homogeneous spatially and their gap sizes are comparable to a pairing gap size Δ_0 . On the other hand, the STS spectra are very inhomogeneous spatially on the sample surface exhibiting the CO and the gap size of spatial averaged STS spectra Δ^* becomes larger than that of pairing gap Δ_0 . From these results, we pointed out that the appearance of large pseudogap links to the formation of CO. In the present study, we measured the STS spectra on the sample surface, where the areas of weak and strong CO's coexist. We find the CO is of a very short-range and inhomogeneous and confirm that in the region exhibiting the CO STS spectra are spatial inhomogeneous locally and their gap sizes become larger than that of pairing gap Δ_0 . In contrast, in the areas where the gap sizes are comparatively small, the STS spectra are spatially homogeneous and of a typical d -wave type. This result is similar to the previous report [1]. This result indicates that the formation of CO will be caused by the local development of large pseudogap, and also suggests that the CO will be directly linked to the large pseudogap. In this talk, on the basis of our recent results and the previous report [1], we will discuss the relationship between the CO and the large pseudogap as well as the origin of CO.

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Magnetic-field-induced Lifshitz transitions in heavy fermion materials



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Keywords: heavy-fermion materials – magnetic fields –Fermi surfaces

Recent results on the low-temperature phases of heavy-fermion materials are reported. The latter are usually inter-metallic compounds with lanthanide or actinide ions on regular lattice sites. At low temperatures, these materials exhibit complex phases and novel phenomena like metal-to-insulator transitions, heavy fermions, unconventional superconductivity and unusual magnetism. The quantum mechanical ground states are determined by subtle compromises between various interactions, and novel technical applications.

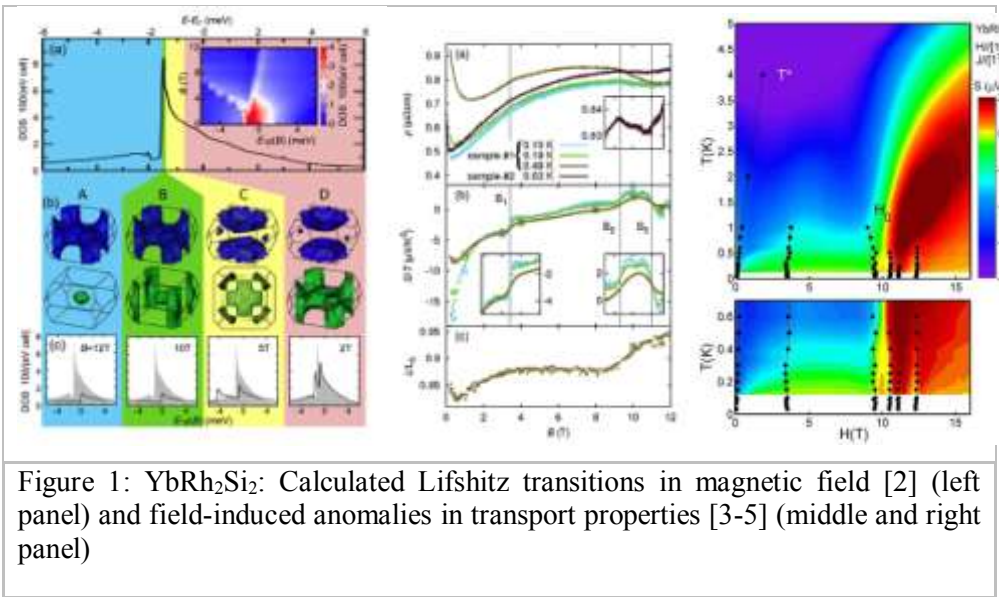
Of particular interest are Ce- or Yb-systems which can be tuned continuously from a magnetically ordered to a non-magnetic ground state. The anomalous behavior results from the degrees of freedom of the partially filled 4f shells. The non-magnetic state is a Fermi liquid which results from a Kondo effect. The strongly renormalized “heavy” quasi-particles can be viewed as composites involving the magnetic 4f degrees of freedom and the conduction electrons.

Magnetic fields lead to Zeeman splitting of the narrow quasi-particle bands and may concomitantly change the topology of the Fermi. An example is the transition into the B-phase in CeCu_2Si_2 [1] where the observed anomalies should result from a Lifshitz-transition.

Here I report recent theoretical results on the evolution with magnetic field of the Fermi surfaces in various Ce- and Yb-based heavy fermion compounds. The heavy quasi-particles are calculated by means of the Renormalized Band method. The field-dependent many-body effects like the g-factor enhancement and the quasi-particle mass in a Kondo system are explicitly accounted for [2]. The Zeeman splitting of the Kondo resonance induces a series of Lifshitz transitions. In YbRh_2Si_2 , the theoretically predicted critical magnetic fields were shown to agree quantitatively with the positions of anomalies in transport properties [3-5] (see Figure 1). Of particular interest is the influence of magnetic-field-induced Fermi surface transitions on Spin Density Wave instabilities as reflected in recent neutron scattering results.

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Fluctuating charge-density waves, stripes and associated origin of pseudogap and superconductivity



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Keywords : mechanisms for high T_c –superconductivity – stripes – pseudogap – CDW – holographic – Jahn-Teller polarons

Recent results show material and electronic complexity [1] in transition metal oxides. Doping of hole charge carriers induces a charge transfer leading to a creation of localized polarons and mobile Zhang-Rice holes. The latter are partially condensed into nearly mobile clusters, leading to a formation of electric dipolar moments and fluctuating stripes[2-5]. A single dipole moment is created by many-body interactions between the dopant ion outside and holes inside the CuO plane. In such a process Coulomb interacting holes[3,4] in the CuO plane are self-organised into 4-particle resonance valence bond plaquettes (RVBP) bound with dopants. RVBP may be ordered[5,6] into fluctuating spin- and charge-density waves(SDW and CDW), stripes and form a disordered state which configuration depends on the preparation of the sample. The lowest energy of the ordered system corresponds to a local anti-ferroelectric ordering. The mobility of individual disordered dipoles (or RVBP) is very low at low temperatures and they prefer first to bind into dipole-dipole pairs. Electromagnetic radiation interacts strongly with electric dipoles and when the sample is subjected to it the mobility changes significantly. This leads to a fractal growth of dipolar clusters. The existence of electric dipoles and CDW reveal a series of new phenomena such as anti-ferro-electricity, strong microwave absorption[7] as well as the field induced superconductivity. For free hole current carriers each dipole is a source of strong scattering that becomes even stronger when the doping increases and reaches its maximum at the optimal doping. RVBP is formed from four holes in the CuO planes due to the many-body over-screening of the Coulomb attraction[2,3,6] of Zhang-Rice holes to the charge fluctuations induced by dopant impurities or electron polarons which are created with the charge transfer in the LaO spacer layers. The RVBP-clusters are moving in a nearly flat band and form a state similar to 2D Luttinger [8] or orbital liquid[9,10].

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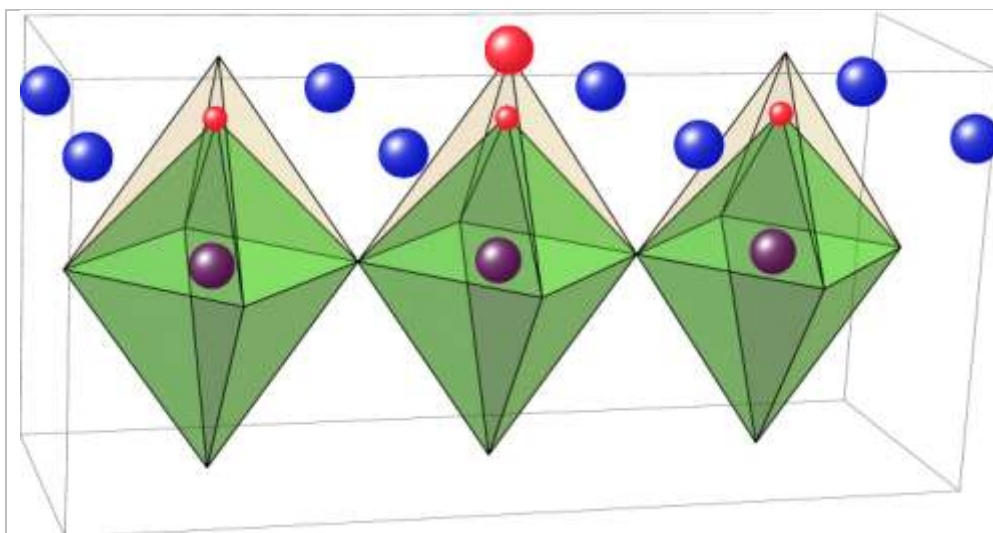


Figure 1: La_2CuO_4 crystal structure with one dopant impurity-topmost red sphere. Green octahedra have oxygens in all corners and Cu atom at the center -purple sphere. The apex oxygens - red spheres and La atoms-blue spheres form pacer layers, which separates the CuO planes. The dopant impurity atom with its negative charge pushes the apex oxygen down from the top of light red octahedron to the top of the green octahedron. This restores the e_g symmetry of the Cu orbitals (the anti-Jahn-Teller effect) and partially releases electrons from Cu atoms, forming the Zhang-Rice holes. Each Cu atom with surrounding oxygens can "loose" effectively one electron, forming Zhang-Rice singlet hole. The complex charge transfer involves five charges. The four holes form a dipolar cluster bound onto the impurity with charge 2- and one hole remains mobile.

SESSION 55

Effects of electronic doping and disorder on the upper phase transitions of pnictides: a numerical study



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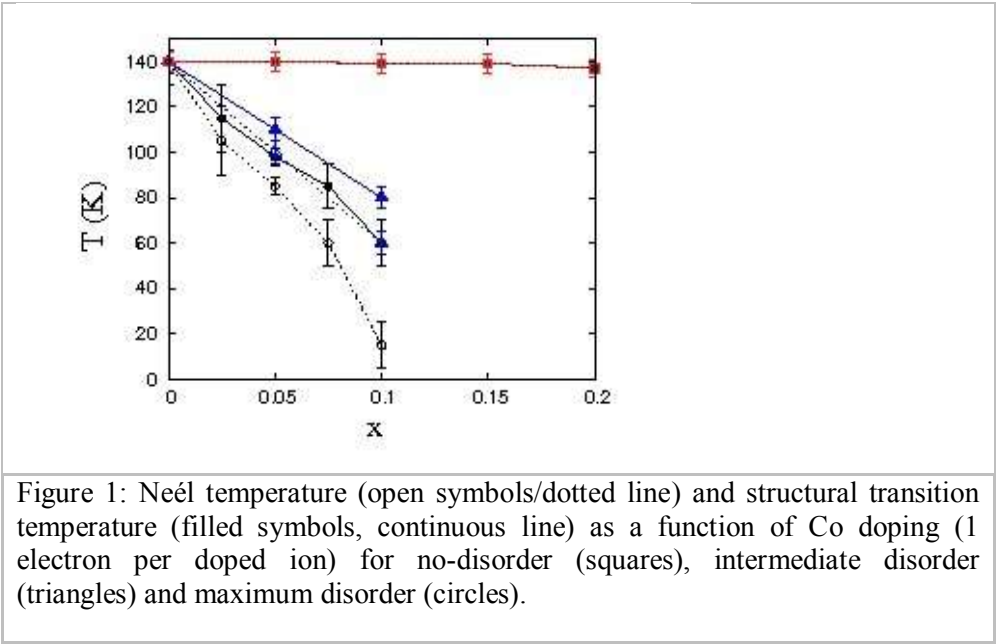
Keywords : pnictides superconductors – doping/disorder – nematic phase

The phase diagram for doped pnictides is studied as a function of temperature, electronic density, and disorder, applying numerical techniques to a three-orbital (xz, yz, xy) Spin-Fermion model with lattice degrees of freedom.[1,2,3] In experiments, chemical doping introduces disorder but the relationship between electronic doping and disorder is difficult to quantify. In the present study, since electronic doping is controlled by the chemical potential and disorder by modifying the model's parameters at randomly selected sites, it is possible to investigate the effects of electronic doping and impurity disorder in an independent way. Monte Carlo simulations unveil that the suppression of the Néel and the structural transition temperatures, T_N and T_S , observed upon electron doping of 122 materials, is controlled by the magnetic dilution caused by the in-plane disorder introduced by Fe substitution, while changes in the electronic density affect both temperatures only slightly. The separation between T_N and T_S leading to the stabilization of a nematic phase is also controlled by the disorder as shown in Fig.1 where the dependence of the two critical temperatures are shown as a function of Co doping, that introduces 1 electron per ion, for different degrees of disorder.

In the absence of disorder (red squares) the structural transition and the Néel transition occur at the same temperature. Results for Ru (0 electrons per ion) and Cu (3 electrons per ion) doping will also be presented and the effects of doping on the real space structure of the nematic phase, the lattice orthorhombicity, and the magnetic structure factor will be discussed.

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Glassy dynamics in geometrically frustrated Coulomb liquids without disorder



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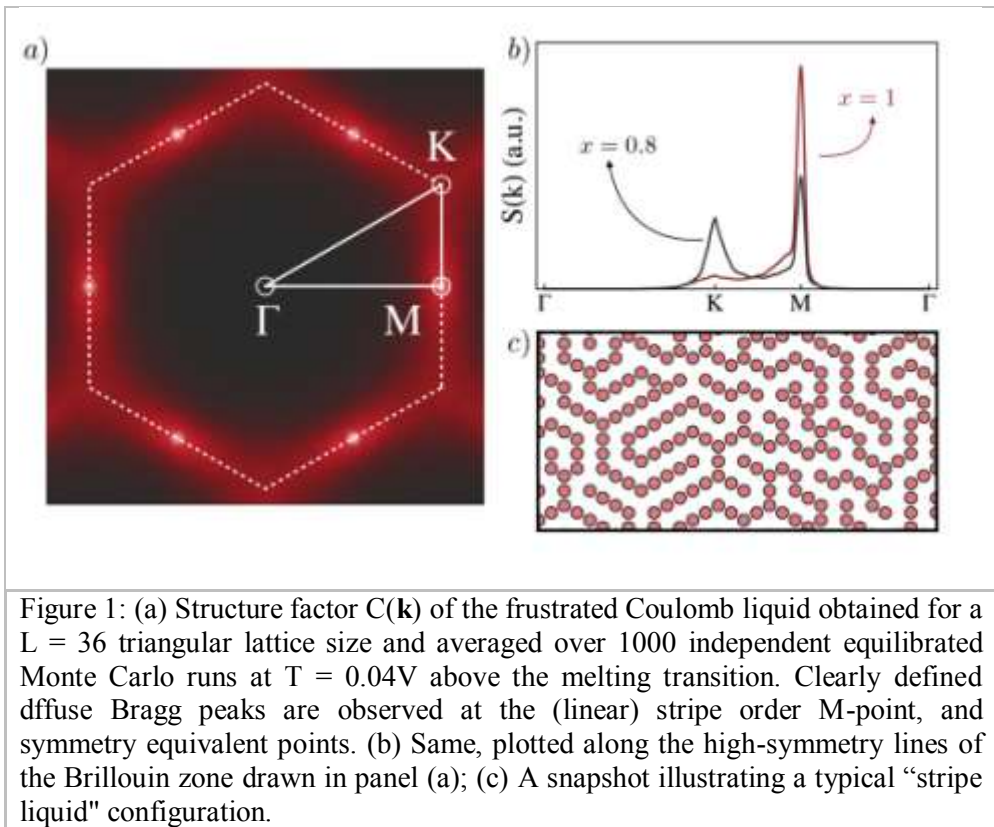
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Keywords : stripe glass, organic Mott systems

We show that introducing long-range Coulomb interactions immediately lifts the massive ground state degeneracy induced by geometric frustration for electrons on quarter-filled triangular lattices in the classical limit. Important consequences include the stabilization of a stripe-ordered crystalline (global) ground state, but also the emergence of very many low-lying metastable states with amorphous "stripe-glass" spatial structures¹. Melting of the stripe order thus leads to a frustrated Coulomb liquid at intermediate temperatures, showing remarkably slow (viscous) dynamics, with very long relaxation times growing in Arrhenius fashion upon cooling, as typical of strong glass formers. On shorter time scales, the system falls out of equilibrium and displays the aging phenomena characteristic of super-cooled liquids around the glass transition. Our results show remarkable similarity with the recent observations^{2,3} of charge-glass behavior in ultra-clean triangular organic materials of the θ -(BEDT-TTF) family.

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Magnetic and orbital ordering in the iron-based superconductors: role of spin-orbit coupling



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Keywords : COMPLEX FERMIOLGY OF SUPERCONDUCTORS

We analyze the magnetic ordering in the iron-based superconductors in presence of spin-orbit coupling. Based on several tight-binding parametrizations of the 3d electron states we show how the spin-orbit coupling introduces the anisotropy of the magnetization of the striped antiferromagnetic

state by lifting the degeneracy of all three components of the magnetization m_x , m_y and m_z . The orientation of the magnetic moment is determined by the contribution of the xy , xz , and yz orbitals to the electronic states near the Fermi level of the electron and hole bands and is determined by the electron filling. We find that within an itinerant approach the magnetic ordering is most favorable along the wavevector of the striped AF state. This appears to be a natural consequence of the spin-orbit coupling in the striped AF state where the ferro-orbital order of the xz and yz orbitals is only a consequence of the striped AF order. We further analyze the role of spin-orbit coupling for the C4 magnetic structure where SDW order parameters with both wavevectors, $Q_x = (\pi; 0)$ and $Q_y = (0; \pi)$, coexist.

Magnetic and superconducting phases and THz magnetoconductivity in δ -Sr-doped La_2CuO_4 superlattices



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Keywords : cuprate superconductors, magnetic and charge stripe order, delta-doping, phase separation, muon spin rotation, THz spectroscopy

One of the most striking manifestations of the complex interplay between superconducting and magnetic phases occurs in the La_2CuO_4 family of high-temperature superconductors (HTSC), where superconductivity and magnetism appear to have the same onset temperature [1-3]. Dopant disorder has a strong impact on the electronic properties and may lead to a nanoscale phase separation with the coexistence of magnetic and superconducting states [3-5].

Cation disorder adds a degree of complexity which makes it very hard to compare experimental results with theoretical models which typically ignore any form of disorder. To gain insight on the intimate connection between the superconducting and magnetic ground states, one needs to control the dopant distribution with atomic precision. Oxide Molecular Beam Epitaxy (MBE) provides thin films of HTSC which can be grown in a layer-by-layer fashion and doped with atomically controlled distribution of cations [6]. We investigate samples with the composition $[(\text{LaO-SrO-CuO}_2)+N\times(\text{LaO-LaO-CuO}_2)]\times M$ ($\delta\text{Sr-LCO}_N$), where $N = 3\ldots 12$ was chosen, and M was fixed such that the overall thickness of these superlattices (SLs) grown on (001) oriented SrLaAlO_4 substrates is ~ 50 nm. These asymmetrically δ -doped SLs have inherent broken inversion symmetry and substantially reduced Sr disorder, and hence could serve as the described HTSC model system.

We report low-energy muon-spin-rotation, magnetic susceptibility, and THz magnetoconductivity studies on $\delta\text{Sr-LCO}_N$ SLs, which are solely doped from a single layer of SrO within the structure and show superconductivity with T_c ranging from 18 to 29 K, and a London penetration depth of $\lambda \approx 220$ nm. The *SC-induced magnetism* is found right below T_c on the background of the AFM long-range order state (as in bulk La_2CuO_4) below $T_N \approx 150$ K. The upper critical field is significantly reduced compared to bulk $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, $H_{c2} \approx 1.5$ T. The SC gap measured by THz transmittance spectroscopy in the Faraday geometry closes at H_{C2} . Above H_{C2} , increasing field alters the scattering rate of the charge carriers in the SC layers. The negative magnetoconductivity is determined to be

of $\sim 15\%$ at 8T. An external magnetic field parallel to the SC layers is much less effective for pair breaking with only a half of the normal state spectral weight recovered within the SC gap. The paramagnetic Meissner effect is observed in this geometry. Our results show that the close proximity of the AFM and SC ground states in $\delta\text{Sr-LCO}_N$ is leading to a non-trivial interplay between the two orders.

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"Type-1.5" superconductivity: experimental evidence in Sr₂RuO₄ and possible occurrence in Ba_{1-x}K_xFe₂As₂



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Keywords : type-1.5 superconductivity, Sr₂RuO₄

I will present theoretical arguments and discuss experimental evidence that some of the newly discovered multicomponent materials should have several coherence lengths: some larger and some smaller than the magnetic field penetration length $\xi_1 < \xi_2 < \dots < \lambda < \xi_N < \dots$. As a consequence of this hierarchy of the length scales the type of superconductivity is realized which breaks the type-1/type-2 dichotomy [1,2,3]. This state was recently termed type-1.5 superconductivity[4]. This is a state where type-1 and type-2 supercurrent patterns are not antagonistic but coexistent, in particular resulting in long-range attractive, short-range repulsive intervortex interaction. I will focus on the recent substantial evidence that this kind of superconductivity is realized in Sr₂RuO₄ [5,6]. Also I will discuss that this state must be realized in Ba_{1-x}K_xFe₂As₂, if this material indeed exhibit s⁺is superconducting state at certain doping. This occurs as a consequence of the existence of divergent coherence length at the phase transition between s⁻ and s⁺is states [7].

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POSTER SESSION

Stripes in Cuprates as Polyominoes Tiling



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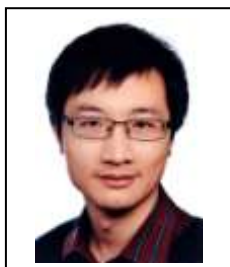
Keywords: mechanisms for high T_c – stripes – soliton.

Using quasi-1 D chains of bisoliton pairs. Leads to charged stripes in YBCO, Which are similar to tiling of Polyominoes in CuO_2 planes. We use the Fibonacci sequence properties to estimate the length of charged-stripes [1]. The smallest strip length is $26a$ (lattice constant of the CuO_2 planes), which equals, 100.1\AA for cuprate, and this is an accurate value by comparing with the experimental results [2].

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Incommensurate spin and charge correlations in the highly hole-doped $\text{La}_{2-x}\text{Sr}_x\text{CoO}_4$ and $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$



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Keywords: Cobaltates, Nickelates, Stripes, Hour-glass spectrum

The study of the layered cobaltates and nickelates has attracted considerable attention due to the charge correlations present in these systems that can be compared with the ones in the isostructural high transition temperature (high-T_c) superconducting cuprates [1-6]. Especially, stripe phases have become a strongly studied topic [1]. Another very interesting discovery was the observation of the universal hour-glass shaped magnetic excitations in a large family of high-T_c cuprates [2]. It has been suggested that the hour-glass spectrum might arise from the stripe-like correlations in these materials. This was further supported by the recent observation of hour-glass shaped magnetic excitation spectra in the insulating cobaltates [3,4]. However, our recent findings [5,6] question these interpretations and we propose a novel “nano phase separation” scenario for the hour-glass spectrum in cobaltates. For both - cobaltates and nickelates - the study of spin excitation spectra have been focusing mainly on the lower doped regime ($x \leq 0.5$). Very few is known for the highly oxidized materials which might be owed to the availability of sizeable single crystals for such high oxidation states of the Co and Ni ions. Using novel high pressure floating zone image furnaces we have succeeded in growing large crystals of highly hole-doped cobaltates and nickelates compounds with Co^{3+} and Ni^{3+} oxidation states. In this work, we present our elastic and inelastic neutron scattering studies on these materials and compare our results with the lower doped regime.

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Simultaneous action of intra- and interband pair channels in multiband superconductivity



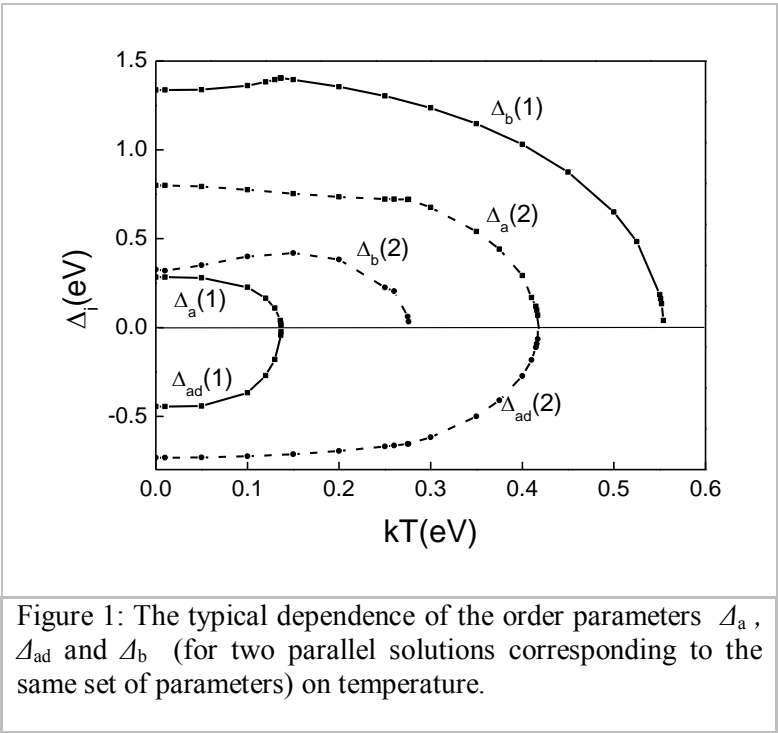
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Keywords : multiband superconductivity, intra- and interband pairs

Interband superconductivity channels with pairs formed from the same (a) and different (b) bands are compared in common action. A simple multiband model is inspected. It includes an itinerant band (d) coupled to two similar bands with creation of intraband – and interband pairs. The corresponding mean-field Hamiltonian containing three order parameters Δ_a , Δ_{ad} and Δ_b has been diagonalized. Two interaction constants W_a and W_b are leading for these quantities correspondingly ($\text{sign}(\Delta_a/\Delta_{ad}) = -\text{sign}(W_a)$ and $\text{sign}(\Delta_{1b}/\Delta_{2b}) = -W_b$). Complicated quasiparticle energies of the bands follow. The calculated necessary operator averages lead to a coupled nonlinear equation system for the order parameters. Illustrative calculations of them vs temperature have been made. Simple band dispersions bearing the chemical potential have been used. The (a-d) and (a-b) channels work with bands overlap. A novel circumstance has been found that at a fixed parameter set the system of basic equations has two independent parallel solutions. It means that the free energy has a complicated structure by the simultaneous action of two interaction channels. The obtained solutions correspond to stable and metastable extrema (states). Real minima define superconducting transition temperature for Δ vanishing at highest T . Both channels with different nature of pair constituents compete in simultaneous work. Correspondingly the phenomenon of the effective logout of one of the channels can be traced in various realizations. Starting from the temperature where Δ_i (a or b) reached zero, the solutions induced by W_j follow the results as W_i were zero, and define T_{cj} . The gaps Δ_a and Δ_{ad} appear as a pair with common vanishing temperature. The general image of gaps behavior is very sensible to of $|W_b|$. With rise of $|W_b|$, i.e. Δ_b , the $\Delta_{a,ad}$ complex becomes suppressed with more influence on Δ_{ad} . The reduction of $|W_b|$ stimulate the formation of closed “bubbles” built up by Δ_a , Δ_b and Δ_{ad} belonging to different solutions. These characterize the minimum and barrier of a metastable state which will be washed out when the bubble closes. Such bubbles are created as critical event on $|W_b|$. The results with changed chemical potential position reflect besides the change in bands density overlap also the alterations in the momentum space crossings.



The common case of two condensates in diborides and iron superconductors

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Keywords: neck disrupting Lifshitz transitions; shape resonance between superconducting condensates; weak interband pairing limit, multi-condensates

Cuprates [1-3], diborides [4,5] iron based superconductors [6,7] share the common physics of multi-condensates superconductivity. Multi-condensates superconductivity was considered impossible before having been proposed for cuprates and diborides [8]. Now it is an active field of research in many body quantum theory [9-14]. After 10 years of research in superconductivity in diborides, experimental data became available to test the predictions of the theory of shape resonances between a BEC-BCS condensate at a neck disrupting Lifshitz transition and multiple BCS condensates [5]. After 7 years from the discovery of high temperature superconductivity in iron based superconductors data are available [15-18] to test the shape resonance predictions in iron based superconductors. The key experimental data are the plots of the gap ratio toward the critical temperature as it was done in (Mg/Al)B₂ [5] while the chemical potential is tuned around a neck disrupting topological Lifshitz transition. It was noticed that the “universal correlation between the gap ratio and T_c in cuprates and iron based superconductors, which is not found in conventional superconductors, supports a common unconventional pairing mechanism in both families” [16]. In this work we have tested the well established shape resonance theory on recently collected data on oxypnictides and FeSe [17,18]. The results in Figure 1a show that the universal correlation between the gap ratio and T_c in iron based superconductors as a function of doping is well predicted by the theory of shape resonances in multi-condensates. The outcome of this work is that the high temperature superconductivity is achieved by nature by a small but essential exchange-like pair transfer terms c_{nm} and a very strong intraband pair coupling c_{nn} in the d_{xz} - d_{yz} Fermi surface at a neck disrupting Lifshitz transition with a transversal dispersion, due to interlayer hopping integral of the order of 23 meV as the related phonon frequency. The huge coupling in the hot spot is in agreement with observed effective mass renormalization and strong

polaronic behavior involving a very few electrons number at the hot spot at the Fermi level.

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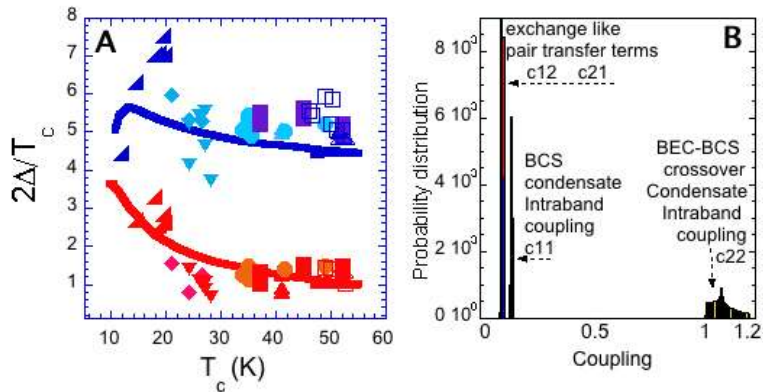


Fig. 1 (Panel A right side) The experimental large gap ratio $2\Delta/T_c$ at the hot spot in the k -space on the small Fermi surface at the gamma point with d_{xz} - d_{yz} orbital symmetry, where the chemical potential is tuned near the neck disrupting Lifshitz transition (blue symbols) and the small gap ratio $2\Delta/T_c$ in the large tubular Fermi surfaces (red symbols) in oxypnictides and FeSe iron based superconductors with variable doping. Solid lines are the theoretical behavior predicted by the theory of shape resonance in multi-condensates between a condensate at the BEC-BCS crossover with a large pair intraband coupling strength c_{22} (see panel B) right side and a weak coupling c_{11} BCS condensate (see panel B). The regime of multi-condensates is indicated by the small pair exchange interaction (see panel B) obtained by direct calculations of the overlap integrals.

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