

SUPERSTRIPES 2014

edited by
Antonio Bianconi and Giorgio Benedek

superstripes press



science series

Abstracts of the lectures given at the the International conference
SUPERSTRIPES 2014

Erice, Italy
July 19 – 25, 2014

64° course of the International School of Solid State Physics
directed by Giorgio Benedek

Organized by
Rome International Center for Materials Science Superstripes - RICMASS
of the non profit organization for scientific research Superstripes onlus

In collaboration with:
Ettore Majorana Foundation and Centre for Scientific Culture

Chairmen:
Antonio Bianconi, RICMASS, Roma, Italy
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Milano, Italy

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Cover project by Paolo Alberti

ISBN: 978-88-6683-029-X

Published by
Superstripes Press
Via dei Sabelli 119A
00185 Roma, Italy

www.superstripes.net
science@superstripes.net

The image on the book cover shows the nanoscale phase separation in a layered cuprate perovskite, a heterostructure at atomic limit, $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$, at 1/8 doping, where the basal plane is made of nanoscale puddles of ordered oxygen ions with a size ranging from 3 to 8 nanometers, from A. Ricci, N. Poccia, G. Campi, F. Coneri, A.S. Caporale, D. Innocenti, M. Burghammer, M. v. Zimmermann, A. Bianconi "Multiscale distribution of oxygen puddles in 1/8 doped $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$ " Scientific Reports 3, 2383 (2013).

PREFACE

The aim of this course is to promote discussion looking to a unifying scenario for high temperature superconductivity.

The discussion will be focused on understanding the mechanisms for evading temperature decoherence effects in quantum condensates.

A large number of experimental results have been accumulated on different aspects of the high temperature superconductors cuprates, diborides, FeAs layered superconductors and other systems with the competing electronic degrees of freedom and showing nanoscale phase separation.

The approach will be to direct future research in the field to search new materials with unique properties and to identify materials parameters for controlling and manipulating the superconducting phase for opening new perspectives in this field.

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Fermi liquid behaviour in strongly correlated metals

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A reference point for research on a wider range of correlated behaviour is provided by the so-called Fermi-liquids, characterized by a relaxation rate $\omega^2 + (p k_B T)^2$. The theoretical prediction for the relaxation rate appearing in the optical conductivity is $p=2$ when considering the experimentally most accessible range $\omega > k_B T$. A number of recent optical studies have addressed the issue of Fermi-liquid characteristics, reporting indeed ω^2 and T^2 for the optical scattering rate of a number different materials. However, a perfect match to the prediction $p=2$ has not been observed. One possible scenario that has been proposed to explain this discrepancy is the presence of magnetic impurities. In a recent study we have investigated Sr₂RuO₄, a material which can be synthesized in very pure form, with well established T^2 resistivity below 25 K. Here we observe a perfect scaling collapse of $1/\tau$ as a function of $\omega^2 + (p \pi k_B T)^2$ for with $\omega < 36$ meV, and temperature below 40K, with $p=2$. We also observe features in the spectrum at higher energy, which are manifestly beyond the Fermi-liquid model. The sign and size of these features agree quantitatively with the notion of resilient quasiparticles predicted by dynamical mean field theoretical calculations for this compound.

Acknowledgements: This work was supported by the Swiss National Science Foundation (SNSF) through grants 200020-140761 and 200021-146586, by the Slovenian research agency program P1-0044, by FP7/2007-2013 through grant 264098-MAMA, and by the ERC through grant 319-286 (QMAC). Computing time was provided by IDRIS-GENCI and the Swiss CSCS under project S404.

Unconventional strong spin-lattice coupling at high temperatures in almost multiferroic EuTiO₃

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EuTiO₃ (ETO) has long been ignored in research activities, since opposite to many other perovskite titanites no ferroelectric activity was detected in this compound. Also its transition to an antiferromagnetic state at $T_N=5.5\text{K}$ did not contribute to any increased scientific attention. This changed with the discovery of a substantial influence of the AFM transition on the dielectric constant which exhibits an unusual drop at T_N suggesting strong spin-lattice coupling. The temperature dependence of the dielectric constant has been related to the softening of a long wave length transverse optic mode reminiscent of a polar instability. However, the complete softening is suppressed rather analogous to SrTiO₃ (STO) where quantum fluctuations have been induce a plateau like temperature independent behavior. Recently, further similarities between ETO and STO have been reported, namely an oxygen octahedral rotational instability at $T_S=282\text{K}$, much higher than in STO with $T_S=105\text{K}$. This structural instability has been related to strong paramagnon-phonon coupling with the consequence that T_S can be tuned by a magnetic field. This strong coupling has more important and novel consequences, namely an unusual magnetoresistance, fluctuating ferromagnetism at high temperatures, and unconventional magnetostriction at low temperatures. Furthermore the phase diagram of the mixed crystal series $\text{Eu}_{1-x}\text{Sr}_x\text{TiO}_3$ has been investigated in detail and its properties will be discussed.

Evolution of the energy spectrum of underdoped cuprates in the pseudogap phase

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We focus on data for the Fermi Arcs (FAs) from ARPES, quantum oscillation and on the Fermi liquid resistivity regime in underdoped (UD) cuprates to explore evolution of their electronic spectrum with temperature and dopants' concentration x . Analysis of resistivity and of the Hall data proves that umklapp scattering between FAs prevails as main relaxation mechanism in the kinetics of UD cuprates, extending the FAs concept even above PG (pseudogap) temperature $T^*(x)$. We show that *single* electronic pocket appears not due to the Fermi surface reconstruction at the charge order (CO) transition with $T_{CO} \sim 50$ K, but grows gradually at the Γ -point of the Brillouin zone with developing of the PG order parameter below $T^*(x)$ and manifests itself as a shallow maximum of the Hall coefficient (HC) at temperatures where fluctuations of unidirectional CO are weak ($T < T_{CDW} \sim 150-170$ K). As in case of 1/8 doped LBCO [1] sizes of FAs shrink below CO transition at $T_{CO} \sim 50$ K and their contributions into HC correspondingly diminish giving way to that one from the electronic pocket. We argue that namely this effect causes change of sign in the Seebeck and Hall coefficients for UD YBCO and single layer Hg1201 in high magnetic fields at $T < T_{CO} \sim 50$ K [2]. In addition we discuss changes in superconducting pairing in the CO phase.

The work of L.P.G. was supported by NHMFL through NSF Grant No. DMR-1157490, the State of Florida and the U.S. Department of Energy; that of G.B.T. through RAS under Grants No. P20; No. OF03.

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Keywords: cuprates, pseudogap, electron spectrum

Competing charge, spin, and superconducting orders in underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$

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The discovery of charge density wave (CDW) order in $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ in 2012, triggered a tremendous renewed interest in this system. $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ was only the second cuprate member – other than charge and spin stripe order in La-based cuprates such as $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ – to show a static charge order in diffraction experiments on samples close to the famous 1/8-doping. Here we present a summary of our recent high-energy X-ray diffraction studies, which includes new data for a heavily underdoped ortho-II $\text{YBa}_2\text{Cu}_3\text{O}_{6.44}$ crystal. We find that CDW order exists at least for charge carrier concentrations (p) in the CuO_2 planes of $0.078 \leq p \leq 0.132$. This implies that CDW order exists even in close vicinity to the quantum critical point for spin density wave order in the lightly doped compounds. Although the CDW in $\text{YBa}_2\text{Cu}_3\text{O}_{6.44}$ is weaker and its onset temperature lower than for higher dopings, it still shows the same type of competition with superconductivity, and a similar magnetic field dependence. The incommensurability of the CDW order continues the linear growing trend with underdoping. Surprisingly, the correlation length of the CDW order is approximately constant at $\sim 60 \text{ \AA}$ in the entire doping range, independent of the type and correlation length of the oxygen order. This may indicate a coupling between the in-plane CDW order and local chain states. Finally, CDW order sets in remarkably close to the spin-pseudo-gap temperature observed with nuclear resonance techniques. Our discussion of these findings includes a detailed comparison with the charge stripe phase in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$.

The work at Brookhaven was supported by the Office of Science, U.S. Department of Energy, under Contract No. DE-AC02-98CH10886.

keywords: cuprates, charge density wave order, charge stripe order

Investigation of charge density wave order in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ using resonant soft x-ray scattering

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Charge density wave (CDW) order has recently been established as a generic feature of underdoped cuprates and it is now clear that understanding CDW order and its competition with superconductivity is a key component to elucidating the pseudogap phase. In this talk I will present resonant soft x-ray scattering (RSXS) measurements of CDW order in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ (LBCO) and $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ (YBCO) at the Cu L and O K absorption edges. Using RSXS we address a number of pertinent issues regarding CDW order in the cuprates, including the effect of oxygen disorder on CDW order in YBCO, the doping dependence of CDW order in YBCO, the microscopic character and orbital symmetry of CDW order in LBCO and YBCO, and the competition of CDW order and superconductivity, aspects of which we show can be understood in terms of thermal angular fluctuations of a multi-component order parameter.

Keywords: Cuprate superconductors, Charge density wave order, Resonant x-ray scattering, Disorder X-r

Dipolar clusters and ferroelectricity in high temperature superconductors

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In this paper we show that strong electronic correlations together with the local Jahn-Teller lattice distortions locally lead to formation Charge Density Wave(CDW) order originated from the bound states of four holes in conducting CuO planes. They are bound into doped, additional negative charges in the spacer (LaO) layer. This separation of bound charges induces the dipolar field. The four holes clusters could be called resonance valence plaquettes although they are different from resonance valence bonds suggested by Phil Andersen long ago despite the fact that in both cases correlations are responsible of their formation.

In the paper we consider the properties of these plaquettes as a function of doping and temperature. They coexist with free charge carrying holes, but are localized and deeply bound in the underdoped phase and their number is exactly equal to the number of free holes. The pseudogap temperature is defined as the temperature when all four holes are released from a plaquette.

We also show that the resonance plaquettes are responsible for critical fluctuations in the region of the optimal doping of cuprates, i.e. for the quantum critical point (QCP) where the dipolar field disappears. In this region the resonance plaquettes become mobile and produce the major contribution into the linear dependence of the resistivity and entropy on the temperature observed in many experiments. Based on our microscopic calculations we argue that cuprates belong to a novel class of holographic superconductors.

Our microscopic many-body calculations show that these four holes bound states in the quantum fluid of holes can exist only when the correlations are important, that is when $r_s > 2.5$, and they disappear in the strongly overdoped region. All results are in excellent agreement with numerous experimental data including pseudogap dependence on doping which is extracted from ARPES, transport, Hall effect data and many others. In the paper we present the comparison with all these data and also estimate and compare our results with the linear dependence of resistivity on temperature.

Moreover, we show that these bound states may lead to the anti-ferroelectric short range order in cuprates, which exists in the underdoped region and vanishes at optimal doping. We show that this predicted order is related to recent experimental observation by Bianconi et al. of oxygen ordering induced by X-rays as well as the ferroelectric order in much underdoped LSCO recently discovered.

Coulomb effects of Sr doping on the Fermi surface of LSCO

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Ionic effects on the metal in the CuO_2 planes are investigated in the specific framework of Sr doping in La_2CuO_4 by a bulk DFT+U calculation. We confirm earlier calculations finding that the Sr charge remains highly localized. Only a small part of the charge of each introduced strontium atom arrives in the CuO_2 plane, by a cascade of inter-orbital charge transfers, amounting to dielectric screening by the ionic orbitals, in which lanthanum barely participates. The bulk of the charge observed in the plane is delocalized between Cu and O atoms in the plane. The Sr dopands provoke this delocalization similarly to a gating potential, which we can also simulate. The net effect of doping on the emergent metallic states is a highly selective movement of the vH singularity towards and through the Fermi energy, accounting for the well-known fact that the Fermi surface evolution cannot be modeled in a rigid-band picture. We pinpoint the reason in a change of band symmetry along the various directions in the zone and in function of energy. Overlaps between the La/Sr site and antinodal states are significant, while the nodal (arc) states are orthogonal to out-of-plane atoms. This difference identifies the selective vH shift with doping as a background dielectric effect, and also accounts for the arc-protection phenomenon. Rapid change of orbital symmetry along the Fermi surface emerges as a qualitative physical criterion for the validity of rigid-band implementations of the tight-binding model, without invalidating the latter, or the Fermi liquid paradigm itself.

Arcs and pockets in the underdoped cuprate superconductors

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We have shown that, in the pseudogap state, the model cuprate $\text{HgBa}_2\text{CuO}_{4+\delta}$ (Hg1201) exhibits a clear quadratic temperature dependence of the planar resistivity, the characteristic behavior of Fermi liquids [1]. This finding was corroborated by optical conductivity measurements that yielded the quadratic frequency scattering rate and temperature-frequency scaling expected for a Fermi liquid [2]. Most recently, we demonstrated that Kohler's rule for the low-field magnetoresistance is obeyed in moderately-doped Hg1201 [3]. By combining our dc resistivity results with published data for three structurally more complex cuprates, we arrived at the unexpected conclusion that this Fermi-liquid behavior extends to very low doping, close to the Mott-insulating state [1]. We furthermore obtained the universal sheet resistance throughout most of the temperature-doping phase diagram [1], consistent with photoemission results that indicate a doping-independent nodal Fermi velocity [4]. The observation for underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ (Y123) [5] and $\text{YBa}_2\text{Cu}_4\text{O}_{8+\delta}$ (Y124) [6,7] of very small Fermi-surface (FS) pockets via quantum oscillations (QO) is in stark contrast to the situation at high hole concentrations, where a large FS is observed. However, it has remained an open question whether the apparent FS reconstruction has anything to do with aspects of the unidirectional structures of Y123 and Y124, or if it is a universal property. We have settled this issue through the observation of QO in the magnetoresistivity of simple tetragonal Hg1201 (hole concentration $p \approx 0.09$) [8]. This eliminates chains as the source of the FS pockets. Finally, we have demonstrated that the pristine zero-field transport properties of Hg1201 are compatible with (short-range) charge-density-wave order [9]. We will discuss the relation between the FS pockets, observed at low temperatures in high magnetic fields, and the zero-field normal state.

Key words: Cuprates, Quantum oscillations, Arcs, Fermi Liquid, Normal state properties

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Numerical modeling of tunneling conductance spectroscopic maps in high T_c cuprate superconductors

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Scanning tunnelling spectroscopy is known to be an efficient technique to probe in real space the local electronic density of states of the materials. What is a less known is that the tunnelling spectra can be very accurately modelled, providing additional physical quantities of relevance to investigate the microscopic mechanisms triggering high temperature superconductivity (HTS).

We present here STS measurements performed on single crystals of Bi-based cuprates (Bi-2201 Bi-2212 and Bi-2223). These materials typically present inhomogeneous surfaces, attributed to local variations of the charge carrier doping level, clearly evidenced in spectroscopic maps. We show that by fitting all individual spectra of a map, it is possible to quantify relevant microscopic parameters and to establish the links between them *at the local scale*. We can gain access to the band structure of the compound and correlate it with other parameters like the superconducting pairing strength or the coupling of the quasiparticles with the collective bosonic excitations, possible candidates to be the mysterious “pairing glue” of HTS.

Key words : Scanning Tunneling Spectroscopy, High T_c superconductivity, Strong-coupling analysis

Rotation symmetry breaking in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ revealed by ARPES

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Since the discovery of high-temperature cuprate superconductors, the study of various instabilities (e.g. magnetic and charge order) emerging in close proximity to superconductivity has attracted much attention. Significant efforts have been devoted to reveal other instabilities than superconducting one, as a function of doping and temperature, and how they are intertwined with the superconductivity. Using angle-resolved photoemission spectroscopy (ARPES) we revealed that in the vicinity of optimal doping the electronic structure of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ cuprate is reconstructed along the Cu-O bond direction associated with a wave vector $\mathbf{q}_a = (\pi, 0)$. The reconstructed Fermi surface and folded band are distinct to the shadow bands observed in BSCCO cuprates and in underdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ with $x \leq 0.12$, which shift the primary band along the zone diagonal direction. Furthermore the folded bands appear only with $\mathbf{q}_a = (\pi, 0)$ vector, but not with $\mathbf{q}_b = (0, \pi)$. We demonstrate that the absence of \mathbf{q}_b reconstruction is not due to the matrix-element effects in the photoemission process, which indicates the four-fold symmetry in the system is broken and reduced to two-fold symmetry. The $\mathbf{q}_a = (\pi, 0)$ wave vector could be related to the second harmonic of an incipient CDW in the region of optimal doping, which is the smooth continuation of the incipient CDW with doping as observed recently in other cuprates, or points to a new instability in the system.

Key words: superconducting cuprate, CDW, ARPES

SDW-CDW nanoscale phase separation and complex dynamics in $\text{La}_{1.72}\text{Sr}_{0.28}\text{NiO}_4$

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The problem of charge-spin-lattice interaction in cuprates High Temperature Superconductors (HTS) and in strongly correlated systems is still on the center of a big discussion. Recently, new techniques like scanning micro X-ray diffraction (mXRD) and X-ray Photon Correlation Spectroscopy (XPCS) have been used to evidence high spatial inhomogeneous properties and the dynamics of these functional materials [1-7]. In this work we provide a direct visualization of the nanoscale phase separation of the SDW and CDW domains organization in $\text{La}_{1.72}\text{Sr}_{0.28}\text{NiO}_4$ using mXRD. Moreover by the use of resonant XPCS at ALS (Berkeley) has been possible to observe an interesting complex behavior in the SDW-CDW domains walls fluctuations. SDW and CDW show multiscale phase separation and describe a complex “Superstripes” scenario where multiple networks of CDW-SDW and lattice stripes coexist [8].

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Local properties of impure superconductors

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The modern imaging techniques allow the systematic studies of local properties of superconductors. These show a large degree of inhomogeneities. Assuming the existence of local disorder, we theoretically study the properties of superconductors by solving the Bogolubov-de Gennes equations in the real space. We shall present the results obtained for two different models: (i) the two component model also known as the boson-fermion (BF) model and (ii) two band model with inter- and/or intraband effective interactions. The first model has been shown to lead to the description of local properties of cuprate superconductors, while the other model has been proposed for effective description of iron based superconductors. The strong on-site electron-electron repulsion U treated with help of Gutzwiller approximation has been shown to change the local properties of the models. *Inter alia* the electron correlations change the size of the local gap making it larger near the impurity sites, contrary to the results for the same model but without U . The system with interband only pairing interactions

Tuning order-by-disorder multiferroicity in CuO by doping

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The high Curie temperature multiferroic compound, CuO, has a quasidegenerate magnetic ground state that makes it prone to manipulation by the so called "order-by-disorder" mechanism.[1]

First principle computations supplemented with Monte Carlo simulations and experiments show that isovalent doping allows to stabilize the multiferroic phase in non-ferroelectric regions of the pristine material phase-diagram with experiments reaching a 250% widening of the ferroelectric temperature window with 5% of Zn doping. Our results[2] allow to validate the importance of a quasidegenerate ground state on promoting multiferroicity on CuO at high temperatures and open a path to the material engineering of new multiferroic materials.

Work done in collaboration with: G. Giovannetti, S. Kumar, A. Stroppa, J. van den Brink, S. Picozzi, J. Hellsvik., M. Balestieri, T. Usui, A. Bergman, L. Bergqvist, D. Prabhakaran, O. Eriksson, T. Kimura

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Spin-driven Ferroelectricity in Two-dimensional Manganites

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Electronic phase separation in chemically homogeneous systems is a fascinating effect often requiring active charge degrees of freedom, as in high- T_c cuprates and CMR manganites. Conversely, nanoscale inhomogeneities in insulating spin systems are rare. They have been predicted to arise, even in the dopant-free limit, from geometrical frustration as a source of phase competition. NaMnO_2 layered rock-salt-type oxides are appealing in this respect, as they provide a paradigm where polymorphism and lattice topology have remarkable implications on their properties. The magnetic ground state of a quasi-1D spin system in the geometrically frustrated α -polymorph [1] goes through complex modulated structures to a quasi-2D magnet for the β -polymorph [2]. Fingerprints of a unique magnetostructurally inhomogeneous ground state are identified in α - NaMnO_2 by synchrotron X-ray diffraction complemented by local-probe NMR and muon-spin relaxation (μ^+ SR) measurements, and further supported by *ab initio* calculations [3]. We demonstrate the unique potential of such manganite lattices to generate nanoscale domains with symmetry-breaking pinning sites that allow coupled electric and magnetic dipole orders. We argue that their frustration-mediated structural complexity goes beyond the limitations of the bulk symmetry and magnetoelectricity is unveiled in otherwise collinear magnetic systems.

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Nanodomains in Artificially Layered Ferroelectrics

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The static and dynamic properties of ferroelectric domains have long been a subject of intense studies due to their overwhelming influence on the functional properties of these technologically important materials. As the dimensions of ferroelectric components are reduced, domain structures become progressively denser and the properties of domains and domain walls begin to dominate the overall behaviour of the material. In the ultrathin limit, where domain periodicities are of the order of a few nanometres, domain-wall motion has an enormous effect on the dielectric, piezoelectric and switching characteristics of ferroelectrics. We have studied in detail the static and dynamic properties of nanodomains in artificially layered superlattices composed of ferroelectric and dielectric oxides. Using a combination of X-ray diffraction and dielectric impedance spectroscopy over a broad range of temperatures, allows us to probe nanoscopic domain-wall displacements and relate them to the macroscopic dielectric and switching properties. Electrostatic interactions between ferroelectric layers, as well as domain periodicity and morphology, can be efficiently controlled by changing the superlattice composition, leading to a number of interesting properties.

Keywords: ferroelectricity, nanodomains, oxide superlattices,

The superconducting dome in the cuprates from the strong binding description

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We demonstrate that the superconducting dome in the cuprates can be understood quantitatively from the strong binding description, *without use of any free parameter*. In the underdoped side, the suppression of the superconductivity, and the shorter-range pairing correlation measured by the Nernst effect, is shown to originate from the mass divergence of preformed pairs of doped holes, corresponding to a local level crossing into incoherent p-wave. This naturally explains the very soft phase in the entire superconducting dome, as well as the glassy electronic structure below 5.2%. We then show that the kinetic energy (phase stiffness) of the pairs starts to suffer from the bosonic Mottness of the extended-hardcore at ~15% and is nearly completely suppressed at ~25%. This new paradigm of superconducting dome invokes no amplitude fluctuation like the BCS theory or the RVB theory.

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[2] [arXiv:1302.7317](https://arxiv.org/abs/1302.7317)

SQUID-on-tip with two axis magnetic field sensitivity for study of nanoscale superconductivity and magnetism

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In recent years, nanoSQUIDs residing on the apex of a quartz tip, suitable for scanning probe microscopy with record size, spin sensitivity, and operating magnetic fields, were developed. The SQUID-on-tip (SOT) is fabricated by pulling a quartz tube into a sharp pipette, followed by three thermal evaporation steps of a thin superconducting film onto the sides and the apex of the pipette. This self-aligned fabrication method requires no additional lithographic processing. A limitation which is common to all scanning SQUID systems is their sensitivity to only one component of the magnetic field.

A new device that is fabricated by pulling a quartz tube with a “ θ ” shaped cross section overcomes this limitation. This geometry gives rise to two parallel SQUID loops sharing a common branch. Using a focused ion beam, we then etch the tip so that the two SQUID loops become oblique with respect to each other. In this structure, the quantum interference pattern is periodic in both the sum (Φ^+) and the difference (Φ^-) of the magnetic flux in the two SQUID loops. As a result of the 3D structure, a field in the z direction generates a Φ^+ signal and a field in the x direction generates a Φ^- signal, allowing tuning the sensitivity of the device to each of the two components of the magnetic field. This θ SOT can be fabricated as small as 200 nm in diameter and can measure magnetic dipoles with spin sensitivity of $10 \mu_B/\text{Hz}^{1/2}$. This device is a powerful tool to probe local current distribution in nanostructures down to 25 nA.

A magnetic analogue to the isotope effect demonstrated by Raman and ARPES in the $(\text{CaLa})(\text{BaLa})_2\text{Cu}_3\text{O}_y$ cuprate

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We present Raman scattering and Angle-Resolved Photoemission Spectroscopy (ARPES) investigations of the charge compensated cuprate superconductor $(\text{Ca}_x\text{La}_{1-x})(\text{Ba}_{1.75-x}\text{La}_{0.25+x})\text{Cu}_3\text{O}_y$. In this system x controls the interactions and y the doping. We focus on two extreme families with $x=0.4$ and $x=0.1$. For each family we determine the two-magnon Raman peak position E_{max} for different oxygen concentration y . In the absence of doping E_{max} is directly proportional to the superexchange strength J . We find that both x and y affect E_{max} considerably. The Raman measurements are accompanied by a muon spin rotation determination of the Néel temperature on the same samples, which confirm independently the strong dependence of the magnetic interaction on x and y . The Raman data reinforce the relation $T_c^{max}(x) \propto J(x)$, where $T_c^{max}(x)$ is the maximum superconducting transition temperature for a given x . ARPES experiments are done on overdoped surfaces. We determine the electrons velocity in the nodal direction below and above the "kink" energy. The velocity below the "kink" is proportional to the hopping parameter t . We find that $T_c^{max}(x) \propto t^2(x)$. These results demonstrate the importance of orbital overlap to cuprate superconductivity in the same way that changing isotopes clarified the importance of atomic mass to metallic superconductivity.

Key words: Magnetism, Superconductivity, Cuprates, Raman, ARPES

Ultrafast Photoinduced Electron Dynamics in Correlated Cuprate Systems

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Ultrafast carrier dynamics in strongly correlated electron systems have significantly attracted much attention, because a number of time-resolved experimental techniques 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.

1) Transient dynamics of hole carriers injected into a Mott insulator with antiferromagnetic long range order is studied based on the two dimensional t-J model. Time dependences of the optical conductivity spectra and the one-particle excitation spectra are calculated based on the Keldysh Green's function formalism. We show that at early stage after dynamical hole doping, the Drude component appears, and then incoherent components originating from hole-magnon scatterings start to grow. Time profiles are interpreted as that doped bare holes are dressed by magnon clouds, and are relaxed into spin polaron quasi-particle states.

2) The photo-excited states in the two-leg ladder Hubbard model are studied. Real-time evolutions of photoexcited electronic states are calculated by the exact-diagonalization method in finite size cluster. It is shown that the low-energy optical response reflecting a doped metallic state is remarkably suppressed just after the photoexcitation, in contrast to the half filled case. The results are interpreted from the view point of the electron pair correlation changed by photoirradiation.

[1] E. Iyoda and S. Ishihara, Phys. Rev. B (to be published), and arXiv:1312.1077.

[2] H. Hashimoto and S. Ishihara, (in preparation).

key words: Ultrafast dynamics, Cuprates, Theory

Dynamics of broken symmetry in cuprate superconductors

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“Cosmic quench” experiments are specially designed to investigate the nonergodic evolution of systems through symmetry-breaking transitions. By carefully choosing optical pump and probe geometry in femtosecond spectroscopy experiments, excitations which indicate broken spatial symmetry can be detected. Unlike many other probes used to investigate symmetry breaking, these experiments are not surface-sensitive, so they probe the dynamics of the bulk. Presently we report experiments on the BiSCO 2212 system. As the system evolves in time, it undergoes a series of symmetry breaking events. First, starting from the high symmetry state, spatial rotational symmetry is broken, which can be associated with the formation of the pseudogap (PG) state on a timescale of ~ 0.5 ps. Importantly, with our experimental setup we can investigate the presence of critical behaviour in the single particle relaxation dynamics associated with the transition to the PG state. This can show unambiguously for the first time whether the N-PG transition is cooperative in nature, thus distinguishing “stripe physics” from “CDW physics”. Thereafter, on a timescale of a 3-5 ps, gauge symmetry is broken as the superconducting state appears, with the presence of a clear divergence of the SP excitations at the critical time of the transition indicating unambiguously cooperative behaviour and the onset of long range order. The formation of the SC state appears to be preceded by coherent fluctuations of the SC order parameter. The new experimental data are consistent with the notion that the PG state is a nano-textured broken symmetry state, with inhomogeneity on the length scale of a few nanometers. No additional symmetry breaking is detected at the superconducting transition in these experiments.

**Boson-mediated effects following ultrafast pumping of strongly correlated materials:
thermal and non-thermal response.**

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The paradigm of time domain studies of complex materials is that different degrees of freedom interact on different timescales. In this framework, borrowed from semiconductor physics, the details of the photo-excitation processes are often disregarded and simply treated as an impulsive injection of electronic energy that subsequently thermalizes with vibrations and other degrees of freedom. Here, 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

Magnetic-field-tuned superconductor-insulator transition in underdoped La_{2-x}Sr_xCuO₄

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In the underdoped pseudogap regime of cuprate superconductors, the normal state is commonly probed by applying a perpendicular magnetic field (H). However, the nature of the H -induced resistive state remains a subject of long-term debate, and clear evidence for the zero-temperature ($T=0$) magnetic-field-tuned superconductor-insulator transition (SIT) has proved elusive. We present a study of magnetoresistance in underdoped La_{2-x}Sr_xCuO₄, which provides striking evidence for the quantum critical behavior of the resistivity, a signature of the H -field driven SIT. We also clarify the interplay of the vortex line physics and quantum criticality, the key question in the H -field-tuned SIT that had remained largely unexplored so far. Importantly, our finding of a two-stage H -field-driven SIT goes beyond the conventional scenario in which a single quantum critical point separates the superconductor and the insulator in the presence of a perpendicular H . Similar two-stage field-driven SIT, in which both disorder and quantum phase fluctuations play an important role, may be expected also in other copper-oxide high-temperature superconductors.

**In collaboration with X. Shi, P.V. Lin, T. Sasagawa and V. Dobrosavljević*

Keywords: cuprates, superconductor-insulator transition, quantum criticality, magnetotransport

Generic Features of an Electron Injected into the Luttinger Liquid

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It is well known that the one-electron spectral function of one-dimensional (1D) interacting electrons $A(p,\omega)$ is featured by the spinon and holon structures. We have carefully studied $A(p,\omega)$ in the whole region of p and ω to find an electron-like excitation structure in addition to those bosonic ones. This electron-like excitation has interesting properties reflecting a non-perturbative aspect of the 1D system which is treated by mapping our problem to that of obtaining $A(p,\omega)$ for an impurity electron injected into the Luttinger liquid. In particular, for 1D interacting electron gas with quadratic dispersion at zero temperature, the results are summarised as follows [1]: When p is close to the Fermi one p_F , the electron-like excitation provides a peak-like cusp in $A(p,\omega)$ as a correction to the spin-charge separation. As p goes away from p_F , the excitation spectrum gets broader and difficult to be detected because it is sandwiched between the spinon and holon divergent peaks, although we do not expect that its total contribution to the spectral weight is negligible. With the further increase of p , it becomes less broad and eventually for p far away from p_F , it evolves as a main and divergent peak in $A(p,\omega)$.

In our talk, we present results not only for the electron gas but also for the lattice model to extract generic features of the electron-like excitation in 1D correlated electron systems.

[1] H. Maebashi and Y. Takada, arXiv: 1307.1399.

Key words: One-dimensional electron systems, Luttinger liquid, Spin-charge separation, One-electron spectral function

Hunting down pairing bosons in a cuprate high temperature superconductors

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Superconductivity is caused by pairing of electrons resulting from virtual exchange of bosons. In low-temperature superconductors Cooper pairing is mediated by phonons, but for high-temperature superconductors the pairing interaction is not yet confidently known. Here I overview our recent experimental study [1] which sheds light on this problem by performing a new type of non-equilibrium boson generation-detection spectroscopy. In contrast to the conventional tunneling spectroscopy we probe not the single electron current into the sample, but directly hunt down the emission of nonequilibrium bosons that are responsible for Cooper pairing. When non-equilibrium electrons recombine into Cooper pairs, the binding energy is carried away by recombination bosons that are mediating in pairing. Identification of such bosons provides a direct clue about the pairing "glue". We employ intrinsic Josephson junctions, built in the crystalline structure of a layered $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+d}$ cuprate for generation and detection of recombination bosons. We observe that bosons are well defined and carry clear spectroscopic information about the superconducting energy gap. Bosons decay at a $\sim\mu\text{m}$ distance, which together with a $\sim\text{ps}$ decay time yields the boson propagation speed of 10^6 m/s. This is more than two orders of magnitude larger than the phononic (sound) velocity and is close to the electronic Fermi velocity. This provides a direct and unambiguous evidence for involvement of an unconventional electron-electron pairing mechanism in cuprates.

[1] V.M.Krasnov, S.O. Katterwe and A.Rydh, *Nature Commun.* 4, 2970 (2013).

Keywords: Hole doped cuprates, pairing mechanism, nonequilibrium phenomena.

Superconductivity, magnetism, charge orderings, and phase separation in a lattice model of superconductor with short coherence length

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The phase separation phenomenon involving superconductivity is a very current topic, because it can play a crucial role in determining behaviour in many real compounds [1] and fermions on optical lattices [2]. In our work we have studied a model which is a simple generalization of the standard model of a local pair superconductor with on-site pairing (i. e. the model of hard core bosons on a lattice) to the case of finite pair binding energy [3-8]. We have analysed the extended Hubbard models with pair hopping in the atomic limit and focused on phase separation [4-8] and paramagnetic effects of the external magnetic field [5,8]. The phase diagrams and thermodynamic properties of this model have been determined within the variational approach (VA), which treats the on-site interaction term exactly and the intersite interactions within the mean-field approximation (exact in $d \rightarrow +\infty$). Moreover, the exact results derived for $d = 1$ and approximated results for various lattices at $d < +\infty$ beyond VA are also presented [4,5,8]. We analysed mutual stability of the superconducting (SS) phase and charge (CO) or magnetic (F/AF) orderings as well as homogeneous mixed phases [6-8]. Our investigation of the general case shows that the system can exhibit not only the homogeneous phases: superconducting (SS) and non-ordered (NO), but also the phase separated states (PS: SS/NO, PS:SS/CO, PS:SS/F). The superconductivity can coexist with the CO or F orderings only in states with electron phase separation. Moreover, depending on the values of interaction parameters, the PS:SS/NO state can occur in higher fields than the homogeneous SS phase (field induced PS).

The work has been financed by National Science Center (NCN, Poland) as a project No. 2011/01/N/ST3/00413 in years 2011-2013 and as the doctoral scholarship No. DEC-2013/08/T/ST3/00012, as well as ESF - OP "Human Capital" – No. POKL.04.01.01-00-133/09-00.

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keywords: superconductivity, phase separation, complexity, extended Hubbard model, local pairing

On Strain, Doping and Ionic Liquid Gating Field Effect Studies in High-T_c and Novel Correlated Electron Materials

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Following systematic studies of the role of strain in high-T_c cuprates, we have performed experiments with ionic liquid gating and developed a laboratory method of sample sandwich preparation, as well as materials characterisation and transport measurements. We have studied the electric field effect on heteroepitaxial cuprate structures within electric double layer transistor (EDLT) geometry [1] and were able to substantially vary T_c with the applied electric field. We have observed striking quantum phase transition in LSCO films and are currently exploring the emergence of (super-)conductivity in other quasi-two-dimensional materials, like WO₃, or magnetic chain compounds. We present a brief progress overview of our ongoing studies and provide a critical discussion of the emerging underlying physics.

[1] Guy Dubuy, EPFL doctoral Thesis (2014)

Keywords : Superconductivity, Cuprates, Heteroepitaxy, Electron Transport, ARPES, Field effect, Pulsed laser deposition, EDLT, Quasi-two-dimensional electronic (q2D) materials.

Fano Resonances in Geometrically Frustrated Hyperkagome Iridates

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One of the most striking manifestations of the electron-phonon interaction is the quantum interference between discrete phonons and the continuum of electron-hole excitations. Drawing on a spectroscopic ellipsometry study, we report evidence that conditions favorable for Fano interference are met in the three-dimensional hyperkagome lattice of $\text{Na}_3\text{Ir}_3\text{O}_8$ [1], the semimetallic counterpart of Mott-insulating $\text{Na}_4\text{Ir}_3\text{O}_8$, one of the best candidates for a three-dimensional (3D) spin-liquid state [2]. The entire set of well-defined phonon modes in the ellipsometric IR spectra of $\text{Na}_3\text{Ir}_3\text{O}_8$ single crystals exhibit highly asymmetric line shapes characteristic of Fano resonances. With decreasing temperature, we observe a sharp increase of the infrared intensity of the resonances followed by concomitant changes in the underlying electronic background, formed by electronic transitions between Ir 5d t_{2g} bands of a mostly $J_{\text{eff}} = 1/2$ character. Because of the lack of inversion symmetry the four $J_{\text{eff}} = 1/2$ bands have linear Rashba-type dispersion in the vicinity of the Γ point. These bands originate from strong spin-orbit coupling and intersect near the Fermi level, resembling the Dirac cone in graphene. An analysis of dipole matrix elements has shown that interband transitions between these partially filled bands have a high probability. This provides high density of electron-hole excitations which interfere with superimposed discrete phonon states, in a similar manner as discussed for graphene.

[1] Y. Okamoto *et al.*, Phys. Rev. Lett., **99**, 137207 (2007)

[2] D. Pröpper *et al.*, Phys. Rev. Lett., **112**, 087401 (2014)

Key words: iridate, Fano resonance, spin-orbit coupling

Multiscale phase separation revealed by scanning nano x-ray diffraction: Five essential ingredients for materials design of high temperature superconductors

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High Temperature superconductivity emerges in functional "heterostructures at atomic limit" made of atomic units where five essential ingredients are well tuned. 1) Two or more electronic components give multiple Fermi surface spots with different symmetry so that a) single electron inter-band hopping is forbidden while b) inter-band exchange-like pair transfer is allowed. 2) The Fermi energy of one of the components is close to the band edge so the system is close to the 2.5 Lifshitz transition at a metal-to-metal transition. 3) The lattice and electronic structure shows the complex granular "superstripes" matter: a nanoscale phase separation made of superconducting puddles coexisting with normal stripes with charge order (CDW) and/or magnetic puddles with spin order (SDW) which does not suppress but enhances the stability of quantum coherence. 4) Intra-grain High temperature superconductivity is controlled by the "shape resonance" in the puddles with multicondensates superconductivity and Percolation Superconductivity in scale free networks establish long range coherence (Bianconi, G. EPL (Europhysics Letters) 101, 26003+ (2013); Physical Review E 85, 061113+ (2012)) 5) the optimum T_c is reached tuning the inter-layers charge transfer and the lattice misfit-strain.

New Stripe-Domain Phenomena in Nano-Ferroelectrics

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Several new effects have been observed recently in the study of ferroelectric domains in small-area thin films: (1) Disk-shaped samples facet spontaneously, usually into hexagons but also into pentagons or rectangles, accompanied by stripe domain realignment parallel or perpendicular to the faceted edges; (2) Under HRTEM electron beams this faceting oscillates, typically with 10-20 s periods, which is probably due to charge sevcumulation not heating; (3) multiferroic materials (ferromagnetic ferroelectrics) exhibit domains within domains and unusual dynamics, including switching of ferroelectric domains with modest (0.3-1.8 T) magnetic fields; (4) For submicron diameter samples many ferroelectrics violate the Kittel Law that requires stripe domain width proportional to the square root of film thickness, and a theory is presented that shows this can arise from cylinder "hoop" stress, ignored in earlier work.

High-throughput synthesis of oxide thin films

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Interest in thin film transition metal oxides is driven in part by the potential technological application of devices exploiting intriguing phenomena, i.e. oxide electronics, and in part by the novel structures and properties observed in epitaxial oxide films, using phase, strain, and interfacial engineering. However, in spite of the large number of observations and promise of epitaxial oxide thin films, most of the investigations have been focused on films on low-index commercially-available single-crystal substrates, which have limited the scope of the study.

Here, we develop a high-throughput synthesis process (called combinatorial substrate epitaxy) where an oxide film is grown epitaxially on a polycrystalline substrate. Based on few well-known examples like BiFeO_3 or Sr_2MnO_2 , we will show how functional properties could be investigated across the entirety of epitaxial orientation space, and provide a library of physical property observations. Ultimately, it will expand our understanding of engineering function into transition metal oxides.

D. Pravarthana et al., Appl. Phys Lett. 104, 082914 (2014)

D. Pravarthana et al., Appl. Phys Lett. 103, 143123 (2013).

Partial support from the MEET project is acknowledged.

Investigation of helix-chirality due to spin and quadrupole orientations in magnetoelectrics by resonant x-ray diffraction

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Resonant x-ray scattering is known as powerful technique to study symmetry breakings by orderings of various multipole moments, such as spin and orbital. This technique is recently applied to verify symmetry breakings by the development of the chirality which is determined as an asymmetry of the object upon its mirroring in crystallography and magnetism, and which plays a crucial role in various materials' functionality such as piezoelectricity and multiferroicity. With the help of the resonant x-ray scattering technique using circularly-polarized and highly-focused x-ray beam, we investigated the helix-chiral domains of magnetic dipole and electric quadrupole moments in some magnetoelectrics with right-handed and left-handed helical structures.

Key words: helix-chirality, resonant x-ray diffraction, magnetoelectrics

Ferroelectricity and Magnetoelectric Coupling in Cuprates and Related Striped Perovskites

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We have investigated the ground state properties of insulating lanthanum-based 214 cuprates and related layered perovskite materials using measurements of the electrical polarization and the dielectric constant. Tracing the effect of dopant atoms we find electronic heterogeneity and charge fluctuations result in switchable spontaneous polarization. In addition, the polarization can be tuned with an external magnetic field, a consequence of strong magnetoelectric coupling. Both the magnitude of the polarization and its magnetic field dependence are strongly anisotropic, consistent with the crystal symmetry and electronic structure of the materials. Our results, valid for a variety of dopants and doping levels point towards a spin-charge coupling mechanism that is tuneable by charge carrier concentration and may be universal to 214-type compounds. Compared to other perovskites these findings may suggest paraelectric fluctuations in ferroelectric materials supporting mobile charge carriers in an electronic heterogeneous environment may encourage interactions towards novel electronic states.

Key words: electronic heterogeneity, ferroelectricity, magnetoelectric coupling, stripes

Model of the inhomogeneous magnetic response of cuprate superconductors above T_c

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We present a theoretical framework for understanding recent transverse field muon spin rotation (TF- μ SR) experiments on cuprate superconductors in terms of localized regions of phase-coherent pairing correlations above the bulk superconducting transition temperature T_c . The local regions of phase coherence are associated with a tendency for charge segregation. We simulate the appearance of these regions by a conserved order parameter dynamics, and perform self-consistent superconducting calculations using the Bogoliubov-deGennes method. Within this context we explore two possible scenarios: (i) The magnetic field is diamagnetically screened by the sum of all varying shielding currents inside each small-sized superconducting domains. (ii) These domains are isolated entities that become increasingly correlated by Josephson coupling as the temperature is lowered and the main response to the applied magnetic field is from the sum of all varying tunneling currents. The results indicate that these two approaches may be used to simulate the TF- μ SR data but case (ii) yields a better agreement.

Key words: Disordered Superconductors, Muon Spin Relaxation, Bogoliubov-deGennes theory

Bound clusters and pseudogap transitions in layered high Tc superconductors

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We show that the extra negative charge of dopant atoms in layered superconductors induces small bound clusters of four holes in CuO layers. This phenomenon requires double degeneracy of the hole bands and low density. The degeneracy is provided by the anti Jahn-Teller effect, which pushes apical oxygens into their symmetry positions when hole carriers are released. In underdoped region below the pseudogap the density and temperature are low enough for bound states, seen experimentally as nanoscale inhomogeneity of the spatial distribution of density of states. In very recent scanning tunneling microscopy measurements[1] with $\text{Bi}_{2+y}\text{Sr}_{2-y}\text{CaCu}_2\text{O}_{8+x}$ this inhomogeneity is clearly correlated with interstitial dopant oxygen atoms located near apical oxygens.

The broad pseudogap transition as a function of temperature has been recently split into two transitions. At higher temperature experiments[2] show a weak but sharp phase transition, which does not break the translational symmetry and at lower temperature a broader transition, where directional order is formed, is seen in Kerr rotation experiments and as a strong Nernst effect. The higher temperature transition could be connected to unbinding of clustered holes out of the singlet s-state in the CuO plane. The lower temperature transition removes directional order of clusters. That order is caused by the dipolar structure of separated charges. Dopant atoms are located in interstitial layers whereas holes bound with them are in the CuO plane. With increasing temperature directional order disappears before clusters unbind. Ordered structures are seen in many experiments and they can be even organized by fast X-ray radiation [3].

In this work we report results on the energetics of the cluster formation and fit the density parameter r_s and dielectric constant to Hall measurements. Our model leads to the quantum critical point at doping 0.2 where bound clusters disappear at zero temperature. We also calculate energetics of the ordered phase and connect that to the Nernst effect.

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[3] N. Poccia, M. Fratini, A. Ricci, G. Campi, L. Barba, A. Vittorini-Orgeas, G. Bianconi, G. Aeppli and A. Bianconi, *Nature Materials*, 10, 733 (2011).

Electronic structure and properties of superconducting materials Titolo

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The electronic structures of the ground state for several different superconducting materials, such as cuprates, conventional 3-dimensional superconductors, doped semiconductors and low-dimensional systems, are presented. In some cases it has been useful to calculate the electronic structure for non-equilibrium states through consideration of lattice distortions and magnetic fields. Properties like the Fermi-surface (FS) topology, density-of-states (DOS), stripes, electron-phonon coupling (λ_{ep}) and spin fluctuations (λ_{sf}) are analyzed in order to find clues to what might be important for the mechanism of superconductivity. A high DOS at EF is important for standard estimates of λ 's, but it is suggested that superconductivity can survive a low DOS if the FS is simple enough. The latter is more realistic in low-dimensional systems as in some layered materials.

Key words: Band structure, electron-phonon coupling, spin-phonon coupling, cuprates, doped semiconductors.

Dynamics of fermions in a vicinity of a magnetic quantum critical point

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It has been established recently, both theoretically and experimentally, that cuprates have a Magnetic Quantum Critical Point (MQCP) at doping about 10%. Nature of the criticality is pretty complex and is related to the incommensurate spin ordering. In the present work we argue that the criticality dramatically influences properties of fermions.

To address the problem we consider a simplified model of MQCP, the standard O(3) MQCP in a two-dimensional system. Within the model we demonstrate the following:

- (i) The Fermi surface topology can change in a vicinity of the MQCP.
- (ii) Fermion spin and charge become separated at approaching the MQCP, the spin-charge separation.
- (iii) Critical magnetic fluctuations result in a non-BCS mechanism of pairing of fermions.
- (iv) The pairing is due to critical magnon Casimir effect.

The abstract is based on the following publications/results.

- [1] M. Holt, J. Oitmaa, Wei Chen, O. P. Sushkov, *Phys. Rev. Lett.* **109**, 037001 (2011).
- [2] M. Holt, J. Oitmaa, Wei Chen, O. P. Sushkov, *Phys. Rev. B* **87**, 075109 (2013).
- [3] Y. Kharkov and O. P. Sushkov, to be published.

Universal inhomogeneous magnetic response in hole-doped cuprates above T_c

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Charge-ordering that competes with superconductivity has now been established as a common phenomenon of hole-underdoped high- T_c cuprates. A notable feature of the charge order is that it is short range, and likely pinned by lattice defects. Above T_c where there is no longer a competition with superconductivity, one may ask whether elucidating the regions in between the short-range charge order is more relevant to understanding high- T_c superconductivity? To date there is ample experimental evidence for superconducting correlations persisting above T_c , but disagreement on the range of temperature over which they persist. Recently, we have used high-field μ SR in a comprehensive study of $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and $\text{Bi}_{2+x}\text{Sr}_{2-x}\text{CaCu}_2\text{O}_{8+\delta}$ to show that there is a universal inhomogeneous magnetic response in superconducting hole-doped cuprates that continues well above T_c . I will explain how the findings are indicative of diamagnetic patches of short-range phase-coherent Cooper pairs, and how μ SR can probe such superconducting correlations beyond the limitations of other spectroscopic, thermodynamic and transport techniques.

Key words: cuprates, normal state, phase separation

**The influence of impurity on the superconducting gap and the pseudogap of
 $\text{Bi}_2\text{Sr}_2\text{CaCu}_{2-x}\text{Fe}_x\text{O}_{8+y}$ and $\text{Bi}_2\text{Sr}_{2-x}\text{Eu}_x\text{CuO}_{6+y}$**

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One of the main challenges in understanding high- T_c cuprate superconductors lies in understanding the pseudogap. This pseudogap coexists with the superconducting gap below the superconducting transition temperature (T_c). The impurity effects in both the pseudogap and the superconducting state have been intensively studied so far. Concerning Bi2201, it was reported by ARPES experiments that out-of-plane impurities cause an enhancement of the pseudogap near the antinodes. In Bi2212, it was reported by STM/STS experiments that in-plane impurities such as Zn-doping causes strong pair-breaking on a local level. The energy gap around the Fermi level is strongly suppressed around the Zn sites. It is important to elucidate the effects caused by in-plane and the out-of-plane impurities to clarify the origin of the pseudogap.

In the present study, we report on effects resulting from in-plane and out-of-plane impurities determined by STM/STS and low-temperature specific heat measurements on Fe-doped Bi2212 and Eu-doped Bi2201. The out-of-plane impurities cause the suppression of the spectral weight around the off-nodes, but almost no effects on the superconducting gap around the nodes, which is in sharp contrast to the in-plane impurities.

key words: impurity effects, pseudogap, STM/STS

High pressure Raman study of underdoped cuprates

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Intense scientific effort has been devoted in understanding the complex phase diagram of copper oxide superconductors. Modifications of the chemical doping and/or application of external pressure allow us to explore and disentangle its various competing phases, as well as to directly compare the impact of carrier concentration to that of lattice distortions in mediating them. The recent discovery of a charge density wave (CDW) competing with superconductivity at low doping levels has provided new perspectives and stimulated further investigations [1].

Signatures of the CDW have been detected in the inelastic Raman spectra of underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$: we observe new Raman active phonon modes whose doping and temperature dependence unambiguously relates them with the charge ordering [2]. Exploiting the versatility of the Raman technique, we have investigated the new Raman modes under high pressure conditions, probing thus indirectly the effect of pressure on the CDW instability.

Additional measurements have been performed on stoichiometric underdoped $\text{YBa}_2\text{Cu}_4\text{O}_8$, for which no CDW-induced phonon modes like the ones of underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ were observed under ambient or high pressure conditions, in line with the results of x-rays scattering [1]. A pressure-induced structural phase transition is clearly reflected in our Raman data, which moreover reveal significantly different phononic behavior in the new high pressure phase compared to the original one. Our Raman data in combination with lattice dynamics calculations and measurements of the pressure dependence of T_c offer further insights in the emergence of superconductivity in the system.

[1] G. Ghiringhelli et al., *Science* 337, 821 (2012)

[2] M. Bakr et al., *Phys. Rev. B* 88, 214517 (2013)

Keywords: cuprates, charge density wave, pressure

High- pressure studies for iron-based spin-ladder compound BaFe₂S₃

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Iron-based superconductor has a two-dimensional (2D) iron lattice as a common feature and exhibits characteristic magnetic phases next to the superconducting phase. A striped magnetic order is observed in the 1111, 122, 111 and 11 type, and a block type magnetic order is observed in 245 type iron-based superconductor. Such a variety is valuable for understanding the interplay between magnetism and superconductivity.

Recently, a quasi-one-dimensional iron-based spin-ladder compound BaFe₂Se₃ [1] has attracted much attention. This compound exhibits the magnetic order, in which the magnetic moments form an Fe₄ ferromagnetic unit and it stacks antiferromagnetically along the leg direction. It is a one-dimensional analog of the block magnetism. CsFe₂Se₃ and BaFe₂S₃ is another example of the iron-based spin-ladder compound which has the same crystal motif as BaFe₂Se₃[2]. However, the magnetic structure is stripe type, with magnetic moments coupled ferromagnetically along the rung and antiferromagnetically along the leg direction. Thus, these compounds have both stripe and block type magnetic ordering phases, which is similar to the magnetism of the iron-based superconductors. In this study, we report that the magnetic and electronic properties of the iron-based spin-ladder compound BaFe₂S₃ under high pressure.

[1] Y. Nambu et al., Phys. Rev. **B85**, 064413 (2012).

[2] F. Du et al., Phys. Rev. **B85**, 214436 (2012).

Overall magnetic excitation in overdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ studied by neutron and x-ray

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Magnetic excitations in the high- T_c cuprates show “hour-glass” type magnetic excitation, whose origin is under debate. The hour-glass dispersion consists of two energy scales, below the saddle point energy E_r of the hour-glass, the excitation stands at incommensurate position around (π, π) with incommensurability δ , and above E_r the excitation shows apparently spin-wave-like dispersion. We have performed neutron and synchrotron x-ray scattering to observe magnetic excitations of heavily overdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) with $x=0.25$ and 0.30 in a wide energy range to elucidate the relation between magnetic excitation and the superconductivity.

Neutron study using triple-axis and time-of-flight technique up to 100 meV energy transfer revealed that the spectral weight of the lower part of hour-glass dispersion decreases with superconducting transition temperature T_c . On the other hand, the high energy part (> 100 meV) observed by neutron and resonant inelastic x-ray scattering (RIXS) at Cu-L_3 edge was found to have a dispersion relation similar to the spin-wave dispersion of non-doped La_2CuO_4 although the excitation in the overdoped sample is damped. Thus, the magnetic excitation of LSCO can be distinguished into two regions: low energy part which is highly sensitive to the doping, and the high energy part which is only weakly doping-dependent. We will report details of the above experimental results and discuss the origin of this phenomenon.

Lattice instability and superconductivity in $\text{LaO}_{1-x}\text{F}_x\text{BiS}_2$

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$\text{LaO}_{1-x}\text{F}_x\text{BiS}_2$ is a disordered, non-magnetic superconductor belonging to the novel family of BiS_2 layered superconductors. The parent phase is a band insulator with a layered tetragonal symmetry ($P4/nmm$) and with buckled BiS layers. The highest T_c (~ 11 K) is attained at $x = 0.5$ with F doping as in $\text{LaO}_{1-x}\text{F}_x\text{BiS}_2$. The mechanism of the superconducting transition is not well understood at present. Even though it is presumed to be a BCS-type superconductor, upon F doping or temperature change, little or no change is observed in the low-energy portion of the phonon spectrum and the question whether $\text{LaO}_{1-x}\text{F}_x\text{BiS}_2$ is a BCS superconductor or not remains. The local atomic structures of LaOBiS_2 and $\text{LaO}_{0.5}\text{F}_{0.5}\text{BiS}_2$ were investigated as a function of temperature by using neutron scattering and the pair density function analysis. In the parent compound, in-plane sulfur (S) in the BiS_2 layers is displaced from its average position and creates two Bi-S bonds locally that are not detected in the average structure. This produces two distinct types of Bi-S plaquettes, with long Bi-S bonds (expanded plaquette) and short Bi-S bonds (contracted plaquette) that can affect the Bi-S hybridization. With doping, the in-plane S displacement is reduced but still present. Moreover, the out-of-plane S is displaced along the z -axis, moving closer to the superconducting planes with F doping. The *axial* motion of the out-of-plane S and the in-plane S distortions in the y -direction can be reproduced by lowering the symmetry from the $P4/nmm$ to $P222_1$. The onset of the z -motion of the out-of-plane S suggests a charge transfer mechanism is most likely in place from the donor La-O/F planes to the superconducting Bi-S planes.

Pressure and disorder effects on the static stripe phase in cuprates

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The fascinating issue of charge and spin stripes in cuprate superconductors has attracted a lot of attention for many years. The mechanism of stripe formation and whether stripes promote or suppress superconductivity is still under debate. Therefore, it is important to find an external control parameter to tune structural and electronic properties of the cuprates and study the relation between superconductivity and stripe order.

We have studied pressure and disorder effects on static stripe phase in cuprates at 1/8 doping by means of muon-spin rotation experiments. It was found that the magnetic volume fraction of the static stripe phase decreases linearly with pressure, while the superconducting volume fraction increases by the same amount. This indicates that the magnetic fraction in the sample is directly converted to the superconducting fraction with increasing pressure. The mechanism of this transformation, however, is not clear at present and requires further studies.

We also studied effects of disorder on stripe phase by doping impurities in the CuO₂ planes. It was found that impurities strongly suppress stripe formation. Such a strong effect of in-plane impurities on stripe order might provide important clue for better understanding of stripes formation and their influence on superconductivity in cuprates.

Novel coexistence of superconductivity with short-range magnetic order in high- T_c T'-cuprates observed by muon spin relaxation

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In order to investigate the relationship between the Cu-spin correlation and the Ce-non-doped superconductivity in the parent compound of electron-doped high- T_c cuprates with the so-called T' structure [1,2], we have performed muon-spin-relaxation (μ SR) measurements of T'-Pr_{1.3-x}La_{0.7}Ce_xCuO_{4+ δ} (PLCCO) single crystals and Ce-non-doped T'-La_{1.8}Eu_{0.2}CuO_{4+ δ} (LECO) polycrystals. Zero-field and longitudinal-field μ SR spectra of $x = 0.10$ in PLCCO with $T_c = 27$ K has suggested that a short-range magnetic order of Cu spins with the volume fraction of $\sim 80\%$ and slowly fluctuating Cu spins with the volume fraction of $\sim 20\%$ coexist in the SC crystal in the ground state. Moreover, the SC volume fraction in this crystal has been estimated to be more than 60% from the electronic specific heat at low temperatures. The μ SR spectra in the ground state of LECO with $T_c = 18$ K have revealed that a short-range magnetic order with the volume fraction of 100% is formed. These results suggest that in the T'-cuprates including the parent compound, the coexistence of the superconductivity and the short-range magnetic order is an intrinsic feature. These results can be explained in terms of the band picture based on the strong electron correlation [3].

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Keywords: Electron-doped T'-cuprates, Muon spin relaxation, Ce-non-doped superconductivity

Collapse of superconductivity in Graphene decorated by diluted triangular arrays of superconducting dots

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The easily accessible 2D electron gas offered by graphene provides an ideal platform on which to tune, via application of an electrostatic gate, the coupling between adsorbates deposited on its surface. This situation is particularly interesting when the network of adsorbates can induce some electronic order within the underlying graphene substrate, such as magnetic or superconducting correlations [1]. We have experimentally studied the case of macroscopic graphene decorated with an array of superconducting tin clusters [2], which induce via percolation of proximity effect a global but tunable 2D superconducting state. By adjusting the graphene disorder and its charge carrier density on one side, the geometry and size of the superconducting dot network on the other side, the superconducting state can exhibit very different behaviors, allowing to test different regimes and quantum phase transition from a granular superconductor to either metallic or insulating states [3]. We will show recent experimental results involving set of triangular arrays sparsely distributed on graphene, in which superconductivity is suddenly destroyed for a critical gate value due to quantum fluctuations of the phase, giving rise to an intermediate metallic state at the zero temperature limit [4].

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Superconducting networks of two dimensional clusters

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The physical realization of complex networks as the underlying structure where condensed matter processes take place, poses many questions. Here, we show the experimental realization through electron beam lithography and standard nanotechnologies tools, of the model of a 2d pattern of superconducting materials as a network formed by interacting superconducting clusters. This model is inspired by recent experimental data using scanning nano x-ray diffraction, scanning micro XANES, time resolved x-ray diffraction and continuous X-ray irradiation on the structure of high temperature superconductors and two dimensional electron gas materials.

Key words: Intrinsic inhomogeneity, josephson junctions, non-equilibrium thermodynamics, Mott insulator.

Inhomogeneous Current Distribution at Oxide interface

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At the non-equilibrium interface between metal and oxide, free enthalpy of oxygen segregation is often close to free reaction enthalpy of oxide precipitation [1], resulting in the interface inhomogeneity. Then, the local current concentration accompanied with oxygen and/or cation electromigration induces local chemical reactions such as electro-oxidation and electro-reduction. They are further accelerated by local Joule heating and thermal diffusion. Drastic resistance change known as ReRAM or memristor are caused by them, demonstrating how serious the defect formation is in oxides.

Strong electron correlations give rise to many interesting phenomena which can be utilised in the future electronics. However, the charge localisation makes the system behave as an ionic crystal, thus again defects are formed easily; a formidable difficulty for the future electronics using correlated oxides.

In this talk, a successful method to suppress the defect formation is shown. The method, however, has eventually revealed an intrinsic inhomogeneous current distribution on the defect-free SrTiO₃ surface [2]. Interesting comparison of this intrinsic inhomogeneity with the filament formation discussed in Mott insulators [3] is given. Superconductivity of this defect-free SrTiO₃ surface is also compared with those of LaTiO₃/SrTiO₃ and EDL/SrTiO₃ interfaces.

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key words: Inhomogeneity, Oxide, Interface

Phase separation in complex oxides: RTiO₃

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It has been reported by Komarek et al [1] that the calcium doped rare earth titanium oxides usually show charge and orbital ordering (CO/OO) during temperature-driven metal-insulator transitions (T-driven MIT). By tuning hole-doping level (valence 2+ calcium ion replacing valence 3+ rare-earth ion), the transport behaviours can differ several magnitudes, which is similar to the magnetic-field-driven colossal magnetoresistance (CMR) effect. In such a system, we believe that the phase separation mechanics is responsible for the characteristic transport behaviours [2]. It is a nice analogy material for better understanding the HTC superconductors and CMR manganites, which shares the comparable underline physics, but eliminates the irrelevant complexities to unveil the long puzzled questions in complex oxides. In this talk, I will present our recent observation on phase separation dynamics during T-driven MIT in titanates at LCLS. It is the first time that the single crystal coherent x-ray diffraction patterns have been recorded in a time domain of 120Hz, which serves a huge leap in understanding the intrinsic mechanics of phase separation.

Key words: titanates, phase separation, dynamics, LCLS

Search for hidden broken local symmetry states in correlated electron systems

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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 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, 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. 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.

Possible Bose-Einstein-Hubbard Condensate-Type Behaviour Via a Novel Mechanism in the f Electron Mott Insulator $\text{UO}_2(+x)$

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The requirement for coherence among its constituent particles renders condensation an ultralow temperature phenomenon in systems comprised of atoms. It is possible that a mechanism that could give some of the unique properties of condensates at higher temperatures, involving a specific collective excitation, occurs in a quantum phase composed of carriers in the Mott insulator UO_2 . Differences between the structures of doped UO_{2+x} determined by neutron scattering vs. x-ray scattering and absorption demonstrate that this system exhibits intrinsic dynamics analogous to this property in cuprates. They also show a much more complicated excitation that includes charge transfer between U(IV) and (VI) states with the accompanying atom displacements far too large for the tunnelling polaron process. Accompanying O XAS measurements support this interpretation, showing the broadening of the electronic states expected with intrinsic dynamics. Magnetic susceptibility and epr measurements demonstrate that the spins as well as the charges display unusual behaviour, with a flip in the direction of the magnetization across the AFM transition and transitions between several states. The properties of unpinned carriers were examined with optical pump-optical/THz probe spectroscopy. These experiments show that the photoinduced charged quasiparticles created by relaxation from the $5f$ portion of the UHB aggregate and organize to form their own quantum phase separate from the UO_2 host that undergoes a gap opening phase transition at 50–60 K. The THZ probe also is consistent with quasiparticle condensation. The best and perhaps only explanation for these properties is that the domains containing the charges and spins are droplets of superfluid formed by the U(V)-U(IV/VI) charge transfer excitation made coherent within these domains by its coupling to a (111)-oriented phonon that changes the spacing between the U planes and the relative stability of these two forms of the material.

Keywords: condensate, urania, superfluid

Understanding and Manipulating Domain Configurations in Ferroelectrics

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The advent of conducting atomic force microscopy, and its use in mapping ferroelectric thin films, has reignited the notion that the functional properties of domain walls can be very different from the domains that they delineate [1-5]. Successive studies have shown that walls may be conducting or even superconducting, while domains themselves are insulating. Such discoveries have prompted new forms of devices to be envisioned, in which domain walls define functional operation: for example, transistors in which low and high resistance states would be realised through the presence or absence of conducting domain wall channels between electrodes. Success in “Domain Wall Electronics” [6] requires control and manipulation of domain patterns, as well as domain wall functionality.

In this talk, experimental research will be presented in which both morphology-driven surface depolarizing fields [7] and deliberately engineered field heterogeneity in capacitor structures [8] have been used to control domain microstructures in ferroelectrics. In addition, the factors controlling conductivity in domain walls in improper ferroelectrics, such as boracites and rare-earth manganites, will be discussed.

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Keywords: Ferroelectric; Domains; Domain Walls

Multi-probe characterization of coexisting antiferromagnetic and superconducting orders in Ba(Fe,Ni)2As2 near the phase boundary

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In unconventional superconductors, such as high-Tc cuprate, FeAs and heavy fermion systems, superconducting (SC) phase appears adjacent to the parent antiferromagnetic (AF) phase. In understanding interplay of these two orders, it is important to determine whether they are overlapping in real space or intertwined with microscopic phase separation, and whether the same electrons are involved in both orders. Experimental studies on these questions have, however, often been limited because different probes have different sensitivities, sometimes detecting only one of the two orders and/or providing only volume-integrated information. To overcome this feature, we have performed neutron scattering, muon spin relaxation (MuSR), Moessbauer effect, specific heat and scanning tunneling microprobe (STM) measurements using the same single crystal specimens near the AF-SC border region of Ba(Fe,Ni)₂As₂. The combined results with multiple probes demonstrate a clear overlap of AF and SC order in real space in majority of volume fraction. These results indicate s⁺- symmetry of superconducting order parameter, and put strong constraints on theories for superconducting mechanisms.

Interplay with magnetism has been an important issue in studies of superconductivity. In Chevrel phase compounds, boro-carbides and some cuprate superconductors including rare-earth elements, such as (Nd,Ce)₂CuO₄, antiferromagnetic (AF) order coexists with superconductivity, however, residing on a sub-lattice different from the superconducting (SC) network. In Sr₂RuO₄, a high sensitivity of SC order to extremely small amount of (Ru,Ti) substitution was taken as a strong signature of non-s-wave pairing. In many unconventional superconductors, including high-Tc cuprate, FeAs, organic BEDT, alkali-doped C60, as well

as heavy fermion systems CeRhIn_5 and CeCu_2Si_2 , SC phase appears adjacent to the parent AF phase. Elucidating their border region will provide important information on the role of magnetism in superconductivity,

In $(\text{La},\text{Eu},\text{Sr})_2\text{CuO}_4$, microscopic phase separation between superconducting volume and remaining volume with AF order was previously indicated by the trade-off of AF and SC volume fractions [Kojima], consistent with a competing nature of the two ground states. In CeCu_2Si_2 , the volume fraction of the “A-phase” region decreases with the onset of superconductivity, suggesting microscopic phase separation. In CeRhIn_5 near the AF-SC phase boundary tuned with applied pressure, some signatures of overlap of superconductivity in the volume with AF order have been reported. These studies are limited, however, since they usually reflect information of a single (or at most two) different experimental probes and are often based on volume-integrated information, such as the superfluid density in [Kojima], and/or gathering measurements on specimens with nominally different doping or pressure tuning levels.

Here we report a comprehensive study of the SC-AF border region in $\text{Ba}(\text{Fe},\text{Ni})_2\text{As}_2$ by applying five different experimental methods, i.e., neutron scattering, muon spin relaxation (MuSR), Moessbauer effect, specific heat and scanning tunneling microprobe (STM), on the same single crystal specimens. The crystals were prepared at the University of Tennessee Knoxville and the Institute of Physics in Beijing, using growth methods described elsewhere. The Ni concentration $x = 0.085$ in $\text{Ba}(\text{Fe}_{2-x}\text{Ni}_x)\text{As}_2$, indicated by the red arrow, was measured by all the five techniques, and some other samples with different Ni concentrations (indicated by black arrows) were checked with several different methods. The intensity decreases rapidly with increasing x , and a clear reduction of was found below the onset of superconductivity for the $x = 0.085$ and 0.092 samples.

Muon spin relaxation measurements have been performed at TRIUMF, Vancouver, on single crystal specimens with $x = 0.065, 0.085, 0.092, 0.10$ and 0.12 . For general aspects of MuSR method. A rapid relaxation sets in below about $T \sim 40\text{K}$, corresponding to an onset of static magnetic order. The spectra exhibits two distinct components of the asymmetry, having about a half of the full amplitude each, with a rapid and relatively slow relaxation, respectively. Magnitude of the static random local field causing the fast relaxation is $70/\gamma\mu \sim 840\text{ G}$ at $T = 2\text{ K}$, where $\gamma\mu$ is the gyromagnetic ratio of positive muon $2\pi \times 13.554\text{ x /kG } \mu\text{s}$. This internal field is compared with the muon precession frequency in ZF observed in parent AF compounds of various FeAs systems. The ordered Fe moment size is linearly proportional to the Neel temperature T_N , and the magnetism in the “fast relaxing” volume can be regarded as a direct continuation from the parent AF systems. Since 2/3 of the total asymmetry is expected to show fast relaxation in ZF-MuSR, the volume fraction of the “high-field region” is about 50-60% of the total volume.

Magnitude of the static random field for muons landed in the remaining volume with smaller relaxation rate is about an order of magnitude smaller, and is comparable to the field found by muons in dilute alloy spin glasses CuMn (1%) or AuFe (1%) suggesting that the field may originate from dilute frozen Fe moments in the “low-field volume”. The doping

evolution of the ZF time spectra at $T = 2$ K in Fig. 2(d) shows that a decent static magnetism remains up to $x = 0.10$, and nearly full volume becomes free from static magnetism at $x = 0.12$.

Measurements of ^{57}Fe Moessbauer effect have been performed at CBPF in Rio de Janeiro on the single crystal specimens with $x = 0.065, 0.075$ and 0.085 . Some spectra from the $x = 0.085$ sample is shown in Fig. 3(a). By fitting the results with paramagnetic or non-magnetic response (green line) plus response from static Fe (blue line), we derived the hyperfine field and the volume fraction of magnetically ordered region (Fig. 3(c)). The ordered volume fraction for $x = 0.085$ is about 50%, corresponding to the “high-field” volume fraction detected by MuSR. The magnitude of the observed hyperfine field scales linearly with the Neel temperature, consistent with MuSR results. The “low-field volume” cannot be distinguished from the “para- or non-magnetic” volume, due to limited resolution of Moessbauer effect for detecting small hyperfine fields. It is also conceivable that the “dilute-alloy” like situation reduced the number of Fe atoms with static moments in this volume.

The neutron Bragg-peak intensity IB for long-range ordered systems is proportional to the ordered moment squared multiplied by the volume fraction of the ordered region. Figure 1(d) compares IB with the corresponding values estimated from the results of MuSR and Moessbauer effect, by using a point for the $x = 0.065$ for normalization. With increasing Ni doping x , the neutron intensity is decreased much more rapidly as compared to MuSR and Moessbauer results. This indicates increasingly short-ranged nature of spatial spin correlations with increasing x . In the $x = 0.085$ sample, IB exhibits much more pronounced reduction with decreasing temperature below the superconducting T_c , as compared to the behaviors found by MuSR and Moessbauer effect. These results suggest that the change at T_c is due primarily to change of the correlation length (from longer range above T_c to shorter range below T_c) rather than the ordered moment size.

Coexistence of Magnetism and Superconductivity in Iron Pnictide Single Crystals Studied by Local Probe Techniques

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We have studied the coexistence of magnetism and superconductivity in selected single crystals of Fe-pnictide compounds using ¹⁵¹Eu and ⁵⁷Fe Mössbauer Spectroscopy (MS). Neutron diffraction studies on Ba_{1-x}K_xFe₂As₂ single crystal revealed a decrease in the Bragg peak intensity below TC that can be due to a reduction of iron moments or magnetic volume fraction, since this method can determine only the product of these two quantities. Detailed ⁵⁷Fe Mössbauer measurements on Ba_{0.75}K_{0.25}Fe₂As₂ single crystal mosaics were performed below TN and TC. The spectra analysis reveals an unusual decrease in the magnetic hyperfine field below Tc without change in the magnetic volume fraction. This indicates a reduction of Fe magnetic moment that occurs at Tc explaining also the neutron diffraction results. Mössbauer spectra obtained from Ni-doped BaFe₂As₂ also revealed a decrease of the hyperfine field below TC, and a correlation between nonmagnetic volume fraction, the variation of the magnetic hyperfine field and Ni-doping. These results confirm the coexistence and competition between magnetism and superconductivity, if we assume a phase separation whose dimension is smaller than the coherence length. Finally, another example of coexistence of magnetism and superconductivity is given by the EuFe₂As_{1.4}P_{0.6} compound, where the magnetism comes from the Eu²⁺ moments. All MS spectra reveal magnetic hyperfine fields below the magnetic ordering temperature TM = 18 K of the Eu²⁺ moments. The analysis of the data also shows that there is a coexistence of ferromagnetism, resulting from Eu²⁺ moments ordered along the crystallographic c-axis, and superconductivity below TSC ~ 15 K. We find indications for a change in the dynamics of the small Fe magnetic moments (~0.07 μB) at the onset of superconductivity: below TSC the Fe magnetic moments seem to be “frozen” within the a,b-plane. In all the studied compounds we were able to show a change in the Fe magnetic moment state when entering the SC state. This indicates coexistence of magnetism and superconductivity in these compounds.

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Hysteretic behavior in the optical response of the underdoped Fe-arsenide $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ in the electronic nematic phase

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The tetragonal-to-orthorhombic structural phase transition at T_S , coincident or preceding the onset of an antiferromagnetic ground state at T_N , in the underdoped regime of quite all families of iron-pnictide and chalcogenide superconductors breaks the four-fold rotational symmetry of the tetragonal phase, implying the onset of a nematic phase. The relevance of nematicity, either electronic in nature or spin-induced, in shaping their phase diagram is certainly one of the most debated issue nowadays. We report on an optical reflectivity study of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ with $x = 0$ and 2.5%, detwinned by uniaxial and *in-situ* tunable pressure acting as an external symmetry-breaking field. We discover a remarkable optical anisotropy as a function of the applied pressure, very much reminiscent of a hysteretic-like behavior. Its temperature dependence supports the analogy between pressure and external magnetic field with respect to the electronic anisotropy in iron-pnictides and magnetization in ferromagnets, respectively. We estimate the nematic susceptibility, which is Curie-like at temperatures close to and above T_S and which may hint to a ferro-orbital ordering as driving mechanism for both structural and magnetic transitions.

Work in collaboration with: A. Dusza, C. Mirri, S. Bastelberger, A. Lucarelli

Beyond quasiharmonic approximation: local structure of materials with negative thermal expansion

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Synchrotron radiation X-ray absorption techniques (XAFS) have undergone remarkable developments. In my talk a description will be made of the most important achievements. In parallel with the experimental techniques, XAFS theory and data analysis have made considerable progress. **Femtometer** accuracy in the determination of interatomic distances is now attainable [1]. In my talk the XAFS studies with femtometer accuracy will be discussed:

- isotopic effects on XAFS and the lattice dynamics of Ge⁷⁰, Ge⁷⁶ and SrTiO₃ (see [1,2] and Highlight ESRF 2008);
- materials with negative thermal expansion as ReO₃, ScF₃, AgO₂, etc. (see [3], Highlight ESRF 2006);
- materials with Jahn-Teller (JT) effect and solid solutions SrFe_xTi_{1-x}O₃ ([4], Highlight ESRF 2007), comparison with EPR data.

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Dynamic Vortex Mott Transition in a Proximity Array of Superconducting Islands

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We present the results of transport measurements on a square array of superconducting islands placed on a normal metal. This array provides a unique laboratory for study vortex states and dynamics, in particular, formation of a vortex Mott insulating states, allowing as well for the direct access to its out-of-equilibrium behaviour. A varying magnetic field tunes the on-site vortex repulsion-to-tunneling ratio while a current bias applied to the superconducting array implements an unprecedented degree of control over the Mott insulator dynamics.

We reveal vortex Mott insulating states at integer fillings and fractional Mott insulating states at partial filling of pinning sites, dual to fractional quantum Hall electronic states. We find dynamic phase transitions from Mott insulating to a metallic state and demonstrate critical behaviour of differential resistivity near the Mott critical points as function of the applied current and magnetic field. The experimentally determined critical exponents are in excellent agreement with the values expected from out-of-equilibrium mean field considerations.

This work was supported by the Dutch FOM foundation, the Russian Academy of Sciences, the Russian Foundation for Basic Research (Grant No. 12-02-00152), the Ministry of Education and Science of the Russian Federation, and by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division. N.P acknowledges for financial support the Marie Curie IEF project FP7-PEOPLE-2012-IEF-327711-IMAX.

The zero magneto resistance of low dimensional nanostructures at high electric field: polyacetylene nanofibers and MoS₂

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The zero magneto resistance (ZMR) observed in polyacetylene nanofibers¹ in high electric field is explained with the de-confined conduction of spinless charged solitons akin to a Majorana fermion state as 1-D topological insulator. Similar ZMR is also observed in MoS₂² in high electric field. The ZMR in MoS₂ in high electric field is compared with the reduction of MR induced by electric field in NbSe₃, which was suggested not to be correlated with de-pinning of CDW³.

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(key words) zero magneto resistance, polyacetylene nanofibers, MoS₂

Co-existence of Magnetism and Superconductivity in Granular Aluminum Films

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Granular Aluminum films consist of nano-scale metallic Al grains of about 1000 atoms each, separated by thin amorphous Al oxide tunnel barriers. The metallic grains are too small to be superconducting by themselves, yet the films have an enhanced superconducting critical temperature. In addition, it was found that the resistance of these films displays a Kondo behavior at low temperatures and a negative magneto-resistance at high temperatures, which were interpreted as resulting from the presence of free spins (1). Very recently muon spin rotation experiments were performed on these films at the Paul Sherrer Institute. It was found that the muon spin relaxation rate has a temperature dependence that directly point out to the presence of free electronic spins (2), at a concentration of the order of several hundred ppm. We will discuss the possibility that an unconventional pairing mechanism operating through local spin fluctuations is responsible for the enhanced superconductivity of the granular films, the spins being possibly located at the interface between the metallic grains and the oxide.

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Spontaneous formation of silicene on ZrB₂(0001) buffer layers

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Silicene, the Si-counterpart of graphene, is now uncontroversially demonstrated to be stable in epitaxy on different substrates [1-3], giving a clear evidence that silicon can crystallize in an unexpected graphene-like form possessing physical and chemical properties different from those of bulk silicon. In particular, the existence of a π electronic system, together with the two-dimension character of silicene is expected to offer new functionalities to silicon-based technologies.

A silicene sheet with a single orientation forms spontaneously on the surface of ZrB₂(0001) buffer layers grown on Si(111). The very high reproducibility of its preparation and its high stability make this epitaxial form of silicene a perfect test bench for the exploration of the properties of the two-dimensional allotrope of silicon [3].

In this talk, I will present an overview of the recent progress of our experimental and theoretical study of the properties of epitaxial silicene on ZrB₂(0001) and their evolution upon adsorption of atoms or as a function of the temperature.

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Silicene and Germanene: possible two-dimensional elemental high T_c superconductors

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Silicene [1-3] and germanene [4] are graphene's young cousins [5]. They combine its extraordinary electronic properties associated with quasiparticles behaving as massless Dirac fermions, yielding extremely high mobilities of the charge carriers, to a behavior of two-dimensional topological insulators, nearly up to room temperature for germanene. Both of them are possibly high temperature superconductors [6].

In my talk, I will present fundamental results on these novel synthetic silicon and germanium two-dimensional allotropes, which do not exist in nature, emphasizing superconductivity aspects.

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Keywords : silicene, germanene, superconductivity, topological insulators

Initial growth behavior, substrate interaction, and defect effects of silicene

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Using *ab initio* methods, we have investigated the growth behavior of silicon clusters on Ag(111) surface [1, 2]. Due to p-d hybridization, silicene clusters on Ag surface are more energetically favorable than the three-dimensional silicon clusters. Compared to Rh(111) surface, the lower diffusion barrier for silicon atom and the higher stability of silicene monolayer on Ag(111) demonstrate the superiority of Ag substrate for silicene growth. Three types of silicene superstructures on Ag(111) surface are investigated. We have examined the electronic properties of silicene sheets on two kinds of representative inert substrates, i.e., *h*-BN monolayer and 4H-SiC(0001) surface [3]. The Dirac cone is nearly preserved for silicene sheet on *h*-BN or hydrogenated Si-terminated SiC(0001), whereas the silicene sheet becomes metallic on a hydrogenated C-terminated SiC(0001) surface. We also systemically investigated the structures, formation energies, migration behaviors and electronic/magnetic properties of typical point defects in silicene, including the Stone-Wales defect, single and double vacancies, and adatoms [4]. Especially, Si adatoms as self-dopants in silicene sheets induce long-range spin polarization as well as a remarkable band gap.

Keywords: growth, substrate, defect

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Polaronic excitations and anomalous Isotopic Effects in the Pseudogap Region

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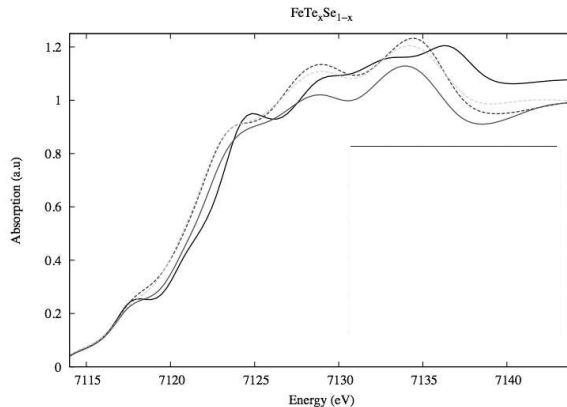
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Evidence for the existence of local dynamical lattice distortions in cuprates in the pseudogap region of the phase diagram is reviewed. The presence of these distortions is related to polaronic excitations. Using a simple three-site Peierls-Hubbard Hamiltonian, we show that for intermediate values of the electron-lattice coupling, the real space representation of the first excited state reproduces the observed local lattice distortions below the pseudogap appearance temperature, T^* . The excited state energies predicted by the model exhibit very different isotopic effects, depending on the nature of the particular excited state. These differences can explain conflicting results obtained with different techniques, as these are probing different excitations of the pseudogap phase. The plausibility of interpreting the pseudogap ground state as an inhomogeneous mixture of nanoscale regions of bipolaronic carriers and quasi-free fermion like particles from which the superconducting state arises at T_c is discussed.

Keywords: Polaronic Effects, Anomalous Isotopic Effects, Two-component superconductivity



Calculation of XANES of FeTe_xSe_{1-x} using the average crystallographic structure. The calculated spectra are inconsistent with the experiment, suggesting an inhomogeneous electronic structure.

Overview of contemporary superconductors grown under high pressure

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In order to get intrinsic and directionally dependent properties of the materials it is desired to find a way to make them in single crystalline form, with precisely controlled parameters. The main purpose of this talk is to give insight into materials synthesis and crystals growth of contemporary superconductors in which high pressure conditions can be used with success. Various examples have been chosen from our own results obtained during the last few years [1-7]. First, I will discuss how the application of high pressure and high temperature affect the phase formation and crystal growth of Fe-based $LnFePnO$ ($Ln1111$, Ln : lanthanide, Pn : pnictogen) oxypnictide superconductors. We could identify the growth conditions which allow obtaining $Ln1111$ crystals with lateral dimensions up to 1 mm [2, 3]. Superconductivity in $LnFeAsO$ single crystals has been induced by partial substitution of O by F or by H, Sm by Th, Fe by Co, As by P or by oxygen deficiency. Underlying correlations and general trends between the composition, structure, magnetism, and superconductivity in these materials will be discussed in details [1-6]. After that I will discuss the growth and physical properties of $MgCNi_3$ single crystals. Based on the low-temperature behavior of the London penetration depth we can clearly state that $MgCNi_3$ is a conventional weak-coupling s -wave superconductor [7]. Then, I will show an important role of extreme conditions in the growth of noncentrosymmetric Mo_3Al_2C superconductor with $T_c=9.3$ K. Firstly available Mo_3Al_2C single crystals allow us determine fine details of the crystal structure and basic physical properties. Finally, the possible multi-gap nature of the superconducting state in high pressure prepared $SrPt_3P$ will be shortly discussed as well.

**This work has been done in collaboration with P. Moll, B. Batlogg, J. Karpinski, S. Katrych, D. Logvinovich, S. Weyeneth, F. Balakirev, L. Balicas, R. Puzniak, R. Khasanov, P. Biswas, L. Fang, U. Welp, K. Kwok, R. Gordon, R. Prozorov*

Key words: superconductors, high pressure, single crystals

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Microstructure - property relations in intercalated iron chalcogenide superconductors

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At the end of 2010 a set of new materials, intercalated iron chalcogenides $A_x\text{Fe}_2\text{Se}_2$ (A: Cs, K, Rb), were found to be superconducting and since then are intensively studied. The mechanism of superconductivity in $A_x\text{Fe}_2\text{Se}_2$, similarly as in iron pnictides or chalcogenides, is still under consideration. Till the discovery of the first „iron superconductor” there was a general belief that even traces of magnetic impurities suppress superconductivity. However, the experimental data evidence the existence of magnetism and superconductivity in iron chalcogenides, though the nature of this coexistence is still unclear. Based on that a hypothesis of the physical separation of magnetic regions from the superconducting domains in crystallites of $A_x\text{Fe}_2\text{Se}_2$ appeared. Studies performed with neutron diffraction, electron microscopy and muon spin relaxation spectroscopy supported the hypothesis of a spatial separation of the magnetic and the superconducting domains. Additionally, up to day the exact composition of superconducting phase is still under discussion and crystals of intercalated superconductors free from the “parasitic magnetic phase” were not yet obtained. A widely utilized high temperature crystal growth from the melt does not allow a precise control of all the intercalation process parameters, therefore new solvothermal low-temperature routes were also applied leading to polycrystalline iron chalcogenides containing molecular spacers inserted between Fe-Se sheets. Those attempts brought already a further improvement of critical temperature ($\sim 44\text{K}$) and an increase of the superconducting volume fraction (above 50%) in the studied system.

key words: intercalated iron chalcogenides, superconductivity, phase separation, magnetic domain

Charge density wave order in 1T-TaS₂ and its relation to superconductivity

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We present combined x-ray diffraction, angle-resolved photoemission and density functional theory study of the charge density wave order 1T-TaS₂. Our x-ray diffraction studies as a function of temperature and pressure prove that the charge density wave, which we characterize in terms of wave vector, amplitude, and the coherence length, indeed exists in the superconducting region of the phase diagram. The data further imply that the ordered charge density wave structure as a whole becomes superconducting at low temperatures, i.e., superconductivity and charge density waves coexist on a macroscopic scale in real space. This result is fundamentally different from a previously proposed separation of superconducting and insulating regions in real space and, instead, provides evidence that the superconducting and the charge density wave gap exist in separate regions of reciprocal space [1]. Furthermore, our density functional theory calculations shed new light onto the origin of the various gaps observed for 1T-TaS₂. Most importantly we find that the previous paradigm of a Mott-gap in this system needs to be reconsidered [2]. Instead we find firm evidence that the corresponding gap is due to the hybridization between the TaS₂-layers directly related to the orbital degrees of freedom. The latter is shown to have a dramatic effect on the band structure close to the Fermi level. We discuss our results in relation to recent time-resolved experiments [3].

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Keywords: charge density wave, multi-band system, orbital order, superconductivity

Investigations of a Bose Insulator Phase in Amorphous Nano-honeycomb Films

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While experimentalists can produce Bose insulator phases in a few different thin film systems, many questions remain about what drives the localization and controls the transport. Our method for creating Bose insulators employs ultrathin films patterned with an approximately triangular array of holes that have attractive features for addressing such questions. We pattern the films by quench depositing metals such as Bi onto the surface of nano-porous Anodized Aluminum Oxide substrates. With increasing thickness these films undergo a bosonic, Cooper Pair Insulator (CPI) to superconductor quantum phase transition (SIT) that is characterized by a vanishing energy scale. The CPI phase is apparent from magneto-resistance oscillations that have a period corresponding to a superconducting flux quantum per unit cell of the hole array. For the superconducting films closest to the thickness tuned SIT, the magneto-resistance oscillations can give rise to multiple magnetic field tuned SIT's. In this talk, I will present insights into what drives the Cooper pair localization, evidence of a new transport regime deep in the CPI phase and the influence of hole array disorder on the thickness and magnetic field tuned SIT's in these films. We are grateful for the support of the National Science Foundation Division of Materials Research.

Keywords: Superconductor-Insulator Transition, Array, Disorder

High critical Temperature Superconductor (HTS) nano-devices and hybrid structures: Quantum tools for probing the nature of HTSs and the detection of Majorana bound states

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Superconductive devices at the nanoscale can have a fundamental role in shedding light into the mechanism leading to High critical Temperature Superconductivity (HTS). Indeed, our recent achievements in nano-patterning of HTS devices such as a single electron transistor (SET) allow us to explore the superconducting state in regimes never accessed before. Indeed, we univocally show via the measurement of the parity effect in a $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ SET that the superconducting order parameter breaks time reversal symmetry in contrast to a pure d-wave symmetry. 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).

At the same time, the advances of nanotechnologies applied to HTS materials can open new perspectives in realizing superconductor-SO-superconductor hybrid structures, where SO represents a material with strong spin orbit coupling such as a topological insulator or a semiconducting nanowire. Such systems are predicted to host Majorana bound states, the main building block of a fault protected topological quantum computer. The several theoretical reports, recently published, refer in particular to the d-wave symmetry of the order parameter in HTS that, together with the large value of the superconducting gap, may allow to design experiments to stabilize and reveal the existence of Majorana bound states still elusive particles in solid state systems. We will present feasibility studies of HTS hybrid structures involving the detection of the proximity effect induced into a normal metal bridging a HTS nano-gap as small as 50 nm.

Keywords: Cuprate high critical temperature superconductor, nano-superconductivity, hybrid devices

Size effects in superconducting thin films coupled to a substrate

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Size effects in superconducting thin films coupled to a substrate

Recent experimental advances in surface science have made it possible to track the evolution of superconductivity in films as the thickness enters the nanoscale region where it is expected that the substrate plays an important role. I will put forward a mean-field, analytically tractable, model that describes size effects in ultra-thin films coupled to the substrate. The study is restricted to one-band and two-band, crystalline, weakly-coupled superconductors with no impurities. This model provides a fair description of experimental results in ultrathin lead films: on average, the superconducting gap decreases with thickness and it is always below the bulk value. We also investigate films of magnesium diboride which is the (two-band) conventional superconductor with the highest critical temperature. Tunneling into the substrate and finite lateral size effects, which are important in experiments, are considered. As a result it is possible to study the interplay between quantum coherence effects, such as shape resonances and shell effects, and the multi-band structure and the coupling to the substrate. No significant enhancement of superconductivity has been observed once the substrate is considered.

Ferromagnetism-induced vortices and a long-range electronic reconstruction at the LaAlO₃/SrTiO₃ interface

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We examine an enduring puzzle of LaAlO₃/SrTiO₃ interfaces: the origin and location of ferromagnetism and its interaction with superconductivity. Resolving this issue experimentally requires us to study heterostructures exhibiting a wide range of carrier densities n_{2D} , leading naturally to a parallel investigation of the sub-interfacial electronic structural evolution.

Regardless of the carrier doping method or total n_{2D} , our LaAlO₃/SrTiO₃ heterostructures develop narrow (≤ 20 nm) superconducting channels below $T_c \sim 300$ mK. We find no evidence for helical superconductivity or non-zero pair momentum; however a giant hysteretic peak emerges in the parallel magnetoresistance below T_c . We argue that hysteresis is principally caused by discrete in-plane ferromagnetic dipoles confined to the interface, whose perpendicular flux components penetrate the underlying superconducting channel as pinned vortices. This heterogeneous magnetic layer generates vortices independently of n_{2D} , suggesting that ferromagnetism in LaAlO₃/SrTiO₃ arises from interfacial defects. Ferromagnetic polarity reversal necessitates vortex depinning within the channel, increasing the coercive field.

For large n_{2D} , carriers occupy states deeper within the SrTiO₃ substrate and Shubnikov-de Haas oscillations appear for in-plane magnetic fields. The angle and n_{2D} -dependence of these oscillations are characteristic of a Fermi surface with predominant $d_{xz,yz}$ orbital character, extending at least 120nm below the interface. Upon increasing n_{2D} to 2×10^{15} cm⁻² by field-effect doping, oscillations emerge in a perpendicular field whose frequency scales with n_{2D} : these are attributed to the almost-degenerate $d_{xy,xz,yz}$ Fermi surface of doped 3D SrTiO₃.

Together, our data reveal a ferromagnetic interface above a superconducting channel, separated from bulk SrTiO₃ by a new $d_{xz,yz}$ -dominated “intermediate” region.

Key words: Vortices, 2D superconductivity, inhomogeneous magnetism, oxide interfaces, quantum oscillations, Fermi surface reconstruction

Magnetic field induced superinsulating state in superconducting NbTiN films

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We present a first experimental observation of the magnetic field induced superconductor-insulator transition in disordered thin NbTiN films. Perpendicular magnetic field drives the critically disordered superconducting film into an insulating state, which transits into a superinsulating one upon decreasing temperature. Appearance of the superinsulator is detected by the upturn from the Arrhenius-type temperature dependence of the resistance evidencing formation of the zero-conducting state at finite temperature. Capacitance measurements support the identification of the charge-ordered nature of the insulating state.

Juxtaposing transport and superconducting properties of NbTiN with those of the earlier investigated TiN films, which demonstrate the superconductor-insulator transition and superinsulating state, we find that partial substitution of titanium by niobium results in a reduction of the carrier density and diffusion constant, increase of superconducting critical temperature and critical magnetic field, and characteristic temperatures of the magnetic-field-induced superconductor-superinsulator transition [1-7].

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key words: superconductor insulator-transition, superinsulator, magnetic field

Chiral and Stripe Charge Order in Cu_xTiSe_2 Probed by STM/STS

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The interplay between superconductivity and ordered electronic phases, especially charge density waves (CDWs), is a persistent puzzle in a range of (low dimensional) superconducting materials. The role of CDWs and charge stripes in the occurrence of high temperature superconductivity remains matter of heated debates and subject to experimental scrutiny. Here we present an STM/STS study of $1\text{T-Cu}_x\text{TiSe}_2$. This layered transition metal dichalcogenide is an attractive model system to address some of these questions. Pristine 1T-TiSe_2 hosts a CDW phase below $T_{\text{CDW}}=220\text{K}$. Upon intercalating Cu, T_{CDW} is reduced and superconductivity appears for $x>0.04$ to reach a maximum T_{C} for $x=0.08$ [Ref 1]. We shall discuss STM/STS micrographs and spectroscopy revealing a distinct chiral CDW in the pristine phase, different from earlier reports,² and the appearance of charge stripe domains with increasing Cu content from $x>0$ to $x<0.08$.

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Key Words: CDW, stripes, chirality, superconductivity, transition metal dichalcogenide, STM

Spin-orbital physics in correlated oxides

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In the last decade, quantum spin-orbital physics in which the orbital frustration and spin-orbit entanglement give rise to novel quantum states has emerged. After some basic introduction to orbital degrees of freedom in transition metal oxides, the talk will give an overview of the recent advances in the field such as interface orbital reconstruction, exotic magnetism in iridium oxides, spin-orbit driven magnetic criticality in Mott insulators, and discuss the challenges and perspectives for materials design via the orbital control.

The role of the interfaces in CaCuO₂ based heterostructure

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A wealth of microscopic mechanisms can be at work at the interfaces between two different constituent oxides and result in a number of novel functional properties [1]. In the case of interfaces between cuprates and other complex oxides, oxygen atoms located at the interface act as a bridge between the two materials driving the electronic charge transfer, atomic relaxation or reconstruction. Theoretical calculations reported in literature predicted that electrostatic instability and atomic reconstruction lead to the oxygen redistribution in a chain-type structure at the interface between non polar SrTiO₃ and the polar infinite-layer copper oxide $ACuO_2$ ($A = Ca, Sr, Ba$), that is the simplest parent compound of cuprate superconductors [2]. Such a chain-type formation may suggest an explanation for the $d3z^2-r^2$ orbital symmetry occurring at the interfaces of several cuprate based heterostructures [3, 4, 5, 6]. To disentangle the role of each constituent block and disclose the mechanism giving rise to the interfacial reconstruction, elemental sensitive spectroscopic techniques can be extremely useful. In particular, we used polarization dependent soft x-ray absorption spectroscopy and bulk sensitive hard x-ray photoelectron spectroscopy. In this talk, I will mainly focus on the results obtained on CaCuO₂/SrTiO₃ (CCO/STO) and CaCuO₂/La_{0.7}Sr_{0.3}MnO₃ (CCO/LSMO) superlattices. In the first system, charge redistribution involving CuO₂ planes gives rise to high-temperature superconductivity, thanks to excess oxygen at the interface. In the second system, apical oxygen contributes to localize extra holes in the optimally doped LSMO block, thus worsening the magnetotransport properties [3]. Our results demonstrate that the interfaces between CCO and complex oxides thin films are not only a breaking symmetry point, but themselves act as a reservoir for localized or doping charges, depending on the presence of apical oxygen atoms and the orbital symmetry of the Cu 3d states.

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Electronic spectrum of twisted bilayer graphene

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We study electronic properties of the twisted graphene bilayer. The material under study consists of two graphene layers rotated with respect to each other by a small (from several degrees down to several tenths of degree) angle θ . The angle θ is assumed to be a rational such that the superstructure exists in the system. Depending on the value of θ the superstructure elementary unit cell contains $\sim 10^2 - 10^4$ carbon atoms. For each angle we construct the tight-binding Hamiltonian of the system and calculate its spectrum numerically. Constructing the Hamiltonian we take into account the effect of environment depending hopping, that is the hopping of electrons between two carbon sites depends not only on the relative positions of these two sites but also on the positions of neighboring carbon atoms [1]. We compare our results with those of other works, both theoretical [2] and experimental [3]. The presence of the band gap due to hybridization between electron states near K and K' Dirac points is demonstrated. The effects of electric potential difference between layers and the electron-electron interactions are discussed.

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Euclidean action of superconductor with “hidden order”

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The superconducting transition in the novel “Euclidian crystal” - quantum ordered state of interacting fermions, that was proposed recently, is considered.

The quantum order parameter (QOP) of electron-hole type plays the role of “hidden order”, that manifests itself in a form of Matsubara time-dependent condensate with zero mean-field expectation value. An exact Euclidian action for QOP is found analytically by a non-perturbative procedure. The part of the Euclidian action that contains superconducting order parameter (SC) and its coupling with QOP is derived consistently from the initial microscopic (bare) model of the correlated Fermi-system to preserve basic symmetries. Depending on the coupling constants ratio in the Cooper and electron-hole channels, two major pictures are considered: with SC gap inside and beyond the Goldstone modes bare gap of QOP. Thermodynamics of the derived Euclidian action for the both cases is considered.

Key words: Euclidian crystal, “hidden order”, non-perturbative Euclidian action, thermodynamics of quantum order

Peculiarities of the orbital effect in the FFLO state in quasi-1D superconductors

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The effect of high magnetic fields on the superconducting state in quasi-low-dimensional structures has been a subject of increasing interest in the last decades because a series of new superconducting compounds with unique properties in magnetic field and pronounced reduced dimensionality has been discovered. Notable examples include the quasi-1D organic Bechgaard salts,¹ polysulfur nitride, the metal-chalcogenide-based compounds,² transition metal carbides,³ the quasi-1D $M_2Mo_6Se_6$ compounds⁴ and lithium purple bronze.⁵ In particular, at low temperature in these compounds the upper critical field exhibits a pronounced upturn with no sign of saturation and its magnitude exceeds the Pauli paramagnetic limit for field oriented in the conducting plane formed by a sheet of highly conducting chains.

The strongly quasi-1D crystallographic structure of these compounds and high values of the Maki parameter convert them into prime candidates for the search of the exotic superconducting phases such as the Fulde-Ferrell-Larkin-Ovchinnikov state. The NMR measurements in some of these compounds revealed a decrease in spin susceptibility consistent with singlet pairing favouring the existence of FFLO state.

In this work we provide the quasi-classical description of the anisotropy of the upper critical field in quasi-1D superconductors. We show that as in the quasi-2D case⁶ the anisotropy of the onset of superconductivity changes in the FFLO state as compared with the conventional superconducting phase and can result in anomalous peaks in the field-direction dependence of the upper critical field. Furthermore, in the FFLO phase appear an additional point $T^{**} = 0.5T_{c0}$ where the orbital effect disappears. Their experimental observation may serve as an evidence for the FFLO phase in quasi-1D superconductors.

M.D.C. acknowledges the support from the BELSPO Return to Belgium Grant.

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Nematic impurity states, transport anisotropy, and neutron resonances in Fe-based superconductors

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The iron-based superconductors exhibit a fascinating interplay between magnetism, structure, and superconductivity. A current controversy is related to the origin and importance of nematic fluctuations and their detection by various experimental probes. In this talk I show how nematic fluctuations get strongly enhanced by disorder near the magnetic phase transition as seen by transport measurements, and how single-site impurity potentials generate completely new emergent extended impurity structures, so-called nematogens. These nematogens are in agreement with recent scanning tunneling measurements on the surface of several different iron pnictide materials which have revealed the presence of electronic dimers. Lastly, I discuss the neutron resonance mode in multi-band systems and its evolution with doping. It is shown, for example, how the resonance may survive even in the absence of a sign-changing gap function.

Enhancing magnetic stripe order in iron pnictides by RKKY interactions

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Recent experimental studies have revealed several unexpected magnetic properties of Mn-doped BaFe₂As₂. These include extension of the stripe-like magnetic $(\pi,0)$ phase to high temperatures above a critical Mn concentration only, the presence of diffuse and largely temperature-independent magnetic (π,π) checkerboard scattering, and an apparent missing structural distortion from tetragonal to orthorhombic. Here, we study the effects of magnetic impurities both below and above the N_el transition temperature within a real-space five-band model appropriate to the iron pnictides. We show how these experimental findings can be explained by a cooperative magnetic impurity behavior of the conduction electrons mediating the Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions between the magnetic impurities.

keywords: magnetic impurity interactions, disorder, iron pnictides.

1111 Iron arsenides viewed by the functional renormalization group: trends and complexity

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We analyze theoretical models for 1111 iron arsenide superconductors by means of the functional renormalization group. In particular we show that tuning the band structures from La-1111 to Sm-1111 reproduces the enhancement of the pairing energy scales as observed experimentally, while the magnetic ordering scale is roughly constant. We also analyze the behavior of the quasiparticle scattering rate in the normal state. Here, in contrast with findings for d-wave pairing in one-band models, the pocket and angle dependence of the scattering rate is found to differ qualitatively from the behavior of the superconducting gap structure.

These works were performed in collaboration with J. Lichtenstein, G. Klingschat, S. Maier, L. Boeri, O.K. Andersen, R. Thomale and C. Platt.

Holography and the strange metals of condensed matter physics

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The holographic duality (or “AdS/CFT” correspondence) of string theory has delivered very recently a series of predictions for novel states of compressible quantum matter. This method addresses physics that is not accessible by conventional field theoretical methods: strongly interacting fermionic matter at finite density, residing behind the “fermion sign problem brick wall”. The fermion signs appear to give rise to long range quantum entanglements of a new kind, translating into the emergence of strongly interacting quantum critical phases with very unusual scaling properties. In turn, these “holographic strange metals” are naturally unstable towards superconducting- and other ordered phases, invoking a generalized form of the Cooper instability. I will review this development, with a special emphasis on the prediction that the transport is governed by a ‘minimal viscosity’ hydrodynamics. This appears to yield a natural explanation for the linear resistivity of the cuprate strange metal, while a number of (falsifiable) predictions follow invoking unconventional experiments.

Decoding Spatial Complexity in Strongly Correlated Electronic Systems

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Inside the metals, semiconductors, and magnets of our everyday experience, electrons are uniformly distributed throughout the material. By contrast, electrons often form clumpy patterns inside of strongly correlated electronic systems (SCES) such as colossal magnetoresistance materials and high temperature superconductors. In copper-oxide based high temperature superconductors, scanning tunneling microscopy (STM) has detected an electron nematic on the surface of the material, in which the electrons form nanoscale structures which break the rotational symmetry of the host crystal. These structures may hold the key to unlocking the mystery of high temperature superconductivity in these materials, but only if the nematic also exists throughout the entire bulk of the material.

Using new methods we have developed for decoding these surface structures [Phillabaum et al., Nat. Commun. 2012], we find that the nematic indeed persists throughout the bulk of the material. We furthermore find that the intricate pattern formation is set by a delicate balance between disorder, interactions, and material anisotropy, leading to a fractal nature of the cluster pattern. The methods we have developed can be extended to many other surface probes and materials, enabling surface probes to determine whether surface structures are confined only to the surface, or whether they extend throughout the material.

Antiferromagnetic states and phase separation in AA-stacked graphene bilayers

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We study electronic properties of AA-stacked graphene bilayers. In the single-particle approximation such a system has one electron band and one hole band crossing the Fermi level. If the bilayer is undoped, the Fermi surfaces of these bands coincide. Such a band structure is unstable with respect to a set of spontaneous symmetry violations. Specifically, strong on-site Coulomb repulsion stabilizes antiferromagnetic order. At small doping and low temperatures, the homogeneous phase is unstable and experiences phase separation into an undoped antiferromagnetic insulator and a metal. The metallic phase can be either antiferromagnetic (commensurate or incommensurate) or paramagnetic depending on the system parameters. The incommensurate AFM phase is mathematically equivalent to the Fulde-Ferrel-Larkin-Ovchinnikov state in superconductors. We derive the phase diagram of the system on the doping-temperature plane and find that, under certain conditions, the transition from the paramagnetic to the antiferromagnetic phase may demonstrate reentrance. When disorder is present, phase separation could manifest itself as a percolative insulator-metal transition driven by doping. The application of the transverse voltage induces the exciton order parameter on the antiferromagnetic background. The value of this second order parameter is proportional to the biased voltage and the value of the nearest-neighbor interplane Coulomb repulsion.

Key words: graphene, phase separation, antiferromagnetic, exciton

Antiferromagnetic spin fluctuations in superconducting LiNH₂-intercalated FeSe

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Despite intensive studies of Fe-based superconductors, the pairing mechanism is still an opened question. Our pressure study of SC FeSe demonstrated that conventional electron phonon pairing plays a secondary role [1,2]. From other hand, appear more experimental facts evidencing that SC can be mediated by AF spin fluctuations acting as a “glue” for superconducting pairing.

In contrast to FeAs-based superconductors, FeSe-based analogues 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 (presumably static) magnetic interactions appear [3]. Application of pressure leads to restoration of superconductivity in Cu-doped FeSe under pressure [4] which could be associated with disappearance of spinglass-type magnetic state.

In the reported study we performed Mössbauer spectroscopic and conductivity measurements under pressure of FeSe intercalated with LiNH₂ showing the superconducting transition temperature of 43 K [5]. Low-temperature Mössbauer studies of pure single-phase superconducting LiNH₂-FeSe have revealed essential magnetic spectral fraction of dynamic nature. Magnetic fluctuations 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. Our high pressure conductivity measurements reveal a cusp-shape anomaly above T_C that could be associated with enhanced magnetic fluctuations prior the superconducting transition. T_C is suppressed with increasing pressure and a cusp-shape anomaly above T_C simultaneously decreases. This observation indicates the interrelation of the superconducting transition and magnetic fluctuations in LiNH₂-FeSe.

Based on mentioned experiments we can draw a conclusion that the superconducting pairing in FeS-based SC is mediated by antiferromagnetic spin fluctuations. This conclusion is in concordance with ⁷⁷Se NMR study pointing toward a positive link between antiferromagnetic spin fluctuations and the superconducting mechanism [6].

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Key words: Iron-based superconductors, Mössbauer effect, Pressure

Anisotropy of Superconducting State Properties in Iron-Based Compounds and Related High-T_c Superconductors

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In Ginzburg-Landau theory the anisotropy is described by the temperature independent effective mass anisotropy. However, a temperature dependent anisotropy was observed in some superconductors, especially in MgB₂, and was explained as a consequence of the presence of two superconducting gaps. Similar temperature dependence was also observed in iron-based superconductors. Furthermore, it was found that the in-plane magnetic penetration depth related to the superconducting carrier density increases with increasing magnetic field. Later on, the study of the cuprate superconductor SmBa₂Cu₃O_{7- δ} has shown that the temperature dependence of the anisotropy is observed also for this class of superconductors. Temperature variation of the anisotropy strongly depends on the doping level and is more pronounced for the samples with lower oxygen content. The weak temperature dependence of the out-of-plane anisotropy parameter for overdoped YBa₂Cu₃O₇ single crystal was found too. It was suggested that such dependence of anisotropy parameter may indicate the presence of two energy scales in the superconducting behavior. This raises the question whether the temperature dependence of the anisotropy is a common property of all layered high-T_c superconductors and how it is linked to the gap structure. Importantly, besides superconductivity, various iron-based compounds exhibit coexisting magnetic order. This order can be influenced by an external magnetic field, making iron-based superconductors a fascinating template for magnetic-field tuned applications.

Keywords: anisotropy, superconducting state properties, iron-based compounds

Evolution of the Fermi Surface Topology in Doped 122 Iron Pnictide

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Based on the minimum two-orbital model and the phase diagram recently proposed by Tai et al [1]. for both electron- and hole-doped 122 iron-based superconducting compounds, we used the Bogoliubov-de Gennes equations to perform a comprehensive investigation of the evolution of the Fermi surface (FS) topology in the presence of the collinear spin-density-wave (SDW) order as well as the superconductivity (SC) order according to the theoretically obtained phase diagram. The SC is assumed to have the s pairing symmetry. In the parent compound like BaFe_2As_2 , the ground state is the SDW order, where the FS is not completely gapped, and two types of Dirac cones, one electron-doped and the other hole-doped emerge in the magnetic Brillouin zone. Our findings are qualitatively consistent with recent angle-resolved photoemission spectroscopy and magneto-resistivity measurements [3]. We also examine the FS evolution of both electron- and hole-doped cases and compare them with measurements as well as with those obtained by other model Hamiltonians. The FS topology could be approached easily by angle resolved photoemission spectroscopic (ARPES) experiments for the parent and very under-doped BaFe_2As_2 compounds in which the gap on the FS is primarily due to the SDW order [3, 4] and for optimal or over doped samples in which the gaps are predominantly or entirely from the SC order [5]. But in the under doped-regime where the gaps of the SDW and SC have the same order of magnitude, it would be difficult for the ARPES experiment to analyze the FS. On the other hand, the FS evolution should have an indirectly impact on the impurity and vortex states as a function of doping according to the phase diagram which could be easily studied by future STM experiments. It needs be point out that our impurity states for optimal electron-doped sample are qualitatively consistent with the calculations based on a five orbital model [6], and our vortex states for hole doped compound like $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ with $x=0.4$ is also consistent with the STM experiments [7]. These results demonstrate that our approach and model should be a valid and reliable one. We are also going to report our theoretical findings on the in-gap states or the local density of states (LDOS) due to a Zn impurity and a magnetic vortex core as the doping level varies. Here the Zn is a nonmagnetic impurity which replaces one of the Fe ions, and its potential has been regarded to be rather strong like that of a unitary impurity. From this study we are able to get a clear understanding of the interplay between the local SDW and SC orders near the Zn impurity site and the vortex core as the doping varies.

Collaborators: Lihua Pan, Jian Li, Yuan-Yen Tai, Matthias J. Graf,3 Jian-Xin Zhu, and Hongyi Chen

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Dirac Fermions in Multilayer Silicene and its stability in air

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Multilayer silicene¹⁻³, the silicon analogue of multilayer graphene, is grown on silver (111) surface with a honeycomb $\sqrt{3}\times\sqrt{3}R(30^\circ)$ reconstruction, as observed by scanning tunnelling microscopy, after the initial formation of the 3×3 reconstructed, silicene monolayer. We mapped the entire Brillouin zone (BZ) of $\sqrt{3}\times\sqrt{3}R(30^\circ)$ reconstructed epitaxial multilayer silicene terraces, by angle-resolved photoemission spectroscopy, showing states with linear dispersion related to π and π^* bands of massless quasiparticles of multilayer silicene.

Thick epitaxial multilayer silicene films are unaffected by oxygen exposure up to 1×10^{10} L ($1\text{L}=1.33\ 10^{-6}$ mbar \times 1 s) in UHV, whereas only weak surface oxidation after 24 hours in air was detected by Auger electron spectroscopy⁴. *Ex-situ* X-ray diffraction as well as Raman spectroscopy performed, without any protective capping, showed the 002 silicene reflection and the G, D and 2D Raman structures, which can be considered the fingerprints of silicene multilayer.

These results are of fundamental importance for exploiting silicene in the existing silicon based device technology.

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Theoretical study of 2D silicon nano-lattices

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Graphene have attracted considerable scientific and technological interest in the last decade. However, the integration of graphene in current Si-based nanotechnologies is still facing important challenges. Recently, the likely existence of silicene, the Si counterpart of graphene, was reported on (111)Ag surface by combining experimental and first-principles simulations. Free standing silicene have been predicted to be gapless semiconductors with linear energy dispersion relations near the K point, like graphene. If one could synthesize free standing silicene layers, their integration into the current nanoelectronic technology would be most likely much favored over their carbon-based counterpart.

A theoretical study of the structural, vibrational and electronic properties of silicene on various substrates, using density functional theory, will be presented. Firstly, the interaction between silicene and Ag(111) surfaces and the comparison of the theoretical results with experimental studies (STM, STS, ARPES and Raman) of the 2D silicon layers grown on Ag will be discussed. The electronic properties of these 2D materials are found to be strongly influenced by their interaction with the underlying substrate. Next, an investigation of silicene on hexagonal layered chalcogenide compounds, namely MoX_2 and GaX ($\text{X}=\text{S}, \text{Se}, \text{Te}$), will be shown. These materials are potentially very interesting as templates for the growth of silicene on non-metallic substrates.

Disorder scattering in cuprate superconductors

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The d-wave superconductivity is very sensitive to imperfections which scatter electrons in random directions. This averaging over momentum directions is incompatible with a strict angular structure of the wave-function in the momentum space. These arguments lead to the conclusion that, unlike s-wave, d-wave superconductors have to be clean. On the other hand, one may extract information about the scattering rate caused by disorder from experimental data. This rate, however, appears to be too large. We may strengthen further this argumentation by the discussion of the Nernst effect in superconducting systems in the normal state. Recently our theory of the Nernst effect, developed for conventional superconducting films in the case of strong disorder (dirty limit), was applied for explanation of experimental data in a cuprate superconductor $\text{La}_{1.8-x}\text{Eu}_{0.2}\text{Sr}_x\text{CuO}_4$. It turns out that our theory describes the data with a very high accuracy. The problem of interest now is how to reconcile all these facts? The conclusion which follows from these observations is that disorder scattering is not weak but has to be rather special: an electron should be scattered mostly backward, but not in the perpendicular directions. Is the physics of stripe responsible for the insensitivity of d-wave superconductivity to random scattering caused by disorder, or are there some chemistry-based factors that make electron scattering predominantly backward?

Metal-to-superconductor transition, mesoscopic disorder and intrinsic charge instability in oxide heterostructures

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Motivated by experiments in oxide interfaces like $\text{LaAlO}_3/\text{SrTiO}_3$ or $\text{LaTiO}_3/\text{SrTiO}_3$ (LXO/STO) heterostructures, we investigate the occurrence of a metal-to-superconductor transition in a two-dimensional electron system with disorder on the mesoscopic scale and possible microscopic mechanisms for electronic phase separation (EPS) based on Rashba spin-orbit coupling (RSOC) [1,2] and/or electrostatic electron confinement at the interface [3]. Disorder induces a distribution of local superconducting critical temperatures accounting well for the transport (resistivity [4] and Hall [5]) and tunnel spectroscopy [6]. With lowering the temperature, global superconductivity establishes as soon as percolation occurs within the superconducting clusters.

Both RSOC and electrostatic confinement could provide an intrinsic mechanism for the observed inhomogeneous phases at the LAO/STO or LTO/STO interfaces and open the way to new interpretations of the observed quantum critical behaviour of LTO/STO [6]. We investigate the effects of temperature 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].

Keywords: oxide heterostructures, electronic phase separation, inhomogeneous superconductivity, quantum criticality

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**Evolution of a complex electronic system to an ordered hidden state: optical quench in
TaS₂ – theory versus experiment**

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Multi-vortex dynamics in charge density waves

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Electronic Crystals is a common form of organization in conducting solids. They take forms of Wigner crystals at hetero-junctions and nano-wires, charge density waves CDWs in chain compounds, spin density waves SDWs in organic conductors, stripes in doped oxides and high-Tc superconductors. In the CDW ground state, the elementary units can be readjusted by absorbing or rejecting pairs of electron. Such a phase-slip process should go via topologically nontrivial configurations: solitons and dislocations – the CDW vortices. An experimental access to those states came from studies of nano-fabricated mesa-junctions, from the STM visualizations and from the X-ray micro-diffraction. We performed a program to model the stationary states and their transient dynamic for the CDW in restricted geometries under the applied field or the passing current. A particular care had to be taken to derive a gauge invariant and current conserving scheme for the interacting condensed and normal charge densities. The model takes into account multiple fields in mutual nonlinear interactions: the amplitude and the phase of the CDW complex order parameter, distributions of the electric field, the density and the current of normal carriers. We have found that vortices are formed stepwise in the junction when the voltage across, or the current through, exceed a threshold. The vortex core concentrates the voltage drop, working as a self-tuned microscopic tunneling junction. The studied reconstruction in junctions of the CDW is a convenient playground for modern efforts of field-effect transformations in strongly correlated material with spontaneous symmetry breakings.

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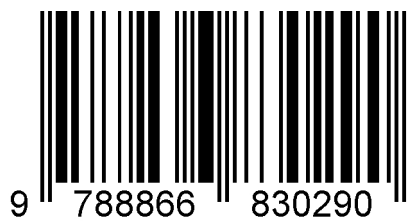
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Superstripes Press Science Series No.5

ISBN 978-88-6683-029-0



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