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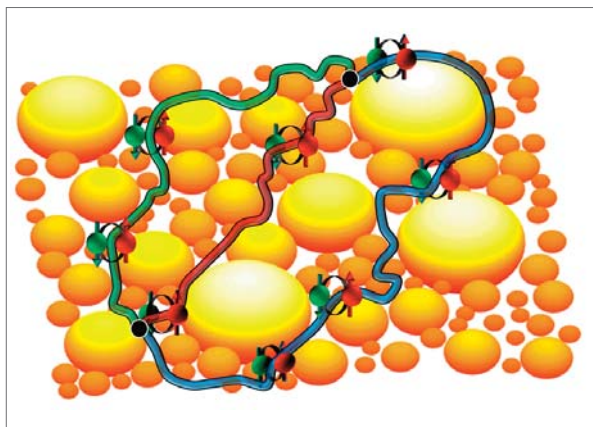
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# SUPERSTRIPES

## 2019

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edited by  
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# SUPERSTRIPES 2019

Quantum Complex Matter

Edited by  
Antonio Bianconi

superstripes press



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\*These authors presented the scientific reports collected in this book at the Superstripes 2019 meeting held in Ischia (It) on June 23-29, 2019

*Superstripes 2019, Ischia June 23-29, 2019*

Papers presented at the international conference

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## Preface

### **Quantum complex matter physics from 1996 to 2019**

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The first stripes conference was held at Rome University in December 1996. The idea was to bring together a small group of scientists who independently were focusing on multi-component electronic complex landscapes after ten years of research in cuprates with emerging role of spin fluctuations, multiple-orbitals, charge density wave, polarons and free carriers [1-6] with the Rome group of Bianconi, Perali, Valletta (BPV) proposing the BPV scenario of multigap Bogoliubov superconductivity in a complex landscape [7,8]. While the standard BCS theory considers only a single BCS isotropic condensate formed by Cooper pairs in a large Fermi surface near zero temperature, and while the resonant valent bond and the bipolaron theories consider a single condensate of preformed pairs, the new proposal for room temperature superconductivity, following Bogoliubov theory, focus on complexity of topology in the real space and k-space with coexisting Cooper pairs, triplet pairs, bipolarons, and intermediate polaron pairs forming multiple coexisting BCS, BEC, and BCS-BEC crossover condensates with both Majorana attractive and Heisenberg repulsive exchange interactions [10-12] not included in the BCS theory. The size of the meeting has grown in the following two stripes conferences in 1998 and 2000 [13] with many top level scientists attracted by the Rome international forum open to confrontations between competing new theories and new experimental results with the participation of Müller, Laughlin, Gorkov, Shirane, Emery between many other top level scientists. The compelling evidence for both a normal broken Fermi surface made of Fermi arcs at room temperature and the presence of nanoscale puddles with short range lattice, spin, charge, orbital stripes at the maximum of

the dome of the critical temperature [13] has stimulated the proposal of the key role of the and the joint role of local strain [14-16] and pressure with doping, to drive a cuprate perovskite to the maximum  $T_c = 160\text{K}$  in the proximity of Lifshitz transitions. The emerging complex scenario of coexisting and intertwined order parameters at nanoscale was called “Superstripes”. [17]. After the Stripes 2000 conference Akimitsu discovered 40K superconductivity in  $\text{MgB}_2$ , which was a practical realization predicted by the BPV model made of a natural heterostructure at atomic limit formed of boron atomic layers where both strain and doping drive the system at the top of the superconducting dome near a Lifshitz transition [18-20]. In 2008 the discovery of superconductivity in iron based superconductivity, a superlattice of atomic Fe layers with two states of different orbital symmetry at the Fermi level provided a second case predicted by the BPV theory for superlattices of atomic quantum wells where a Fano Feshbach and shape resonance occurs driven by exchange interaction between two superconducting gaps near a Lifshitz transition [21,22] confirmed at the 2013 Superstripes conference [23]. However the critical temperature in diborides, iron pnictides and chalcogenides the critical temperature is lower than 100K as expected by the BPV theory which predicts the critical temperature near room temperature for a superlattice of quantum wires [24] or nanotubes [25-26]. The high  $T_c$  multigap superconductivity in  $\text{H}_3\text{S}$  presented at Superstripes 2015 by Eremets [27] and it was assigned to the tuning by pressure of the chemical potential near an electronic topological transition or Lifshitz transition with a Fermi surface spot appearing accompanied by a van Hove singularity [28-30]. At this superstripes 2019 conference the superconductivity at 200K in  $\text{H}_3\text{S}$  has been confirmed by the Tallahassee-Los Alamos group [31] and the discovery of near room temperature superconductivity in pressurized  $\text{LaH}_{10}$  [32,33] confirmed by an independent experiment [34] has confirmed the proposal of room temperature superconductivity in compressed hydrogen [35] and the proposal to tune the chemical potential to a shape resonance driven by exchange interaction in a superlattice of hydrogen quantum nanotubes [25] which is realized in the clathrate structure of  $\text{LaH}_{10}$  [36] which is discussed for superconductivity in a superlattice of hydrogen quantum nanotubes at atomic limit where the maximum of the dome of the critical temperature occurs where the chemical potential has been tuned to a Fano shape resonance [37]. These new results attracted large scientific attention [38-41] and have been object of hot discussions at Superstripes 2019.



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*Superstripes 2019, Ischia June 23-29, 2019*

# Superstripes 2019

## **Orbitals and Nematicity in La-1111 Single Crystals**



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**Keywords:** nematic order, orbitals, Fe-based superconductors

While there is broad consensus that superconductivity in Fe based superconductors is due to an unconventional, most likely electronic pairing, many important aspects of the normal and superconducting state are still unexplored. In particular, the role of orbital degrees of freedom for the normal state electronic properties, nematicity, and pairing is discussed very controversial. In my talk I will present results on a series of large high quality La-1111 single crystals which have been grown for the first time using a method based on anomalous solid state reaction. We have reexamined the phase diagram and studied magnetism and nematic order by means of NMR and strain dependent transport measurements. The possible formation of polaron-like structures will be discussed and evidence for an unusual state with suppressed long range order and soft nematic fluctuations will be presented.

## **Boson—Fermion model for nonconventional superfluids: BCS-BEC crossover**



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**Keywords:** resonant superfluid, Feshbach resonance, BCS-BEC crossover, Superfluid-Insulator transition, Bose-Fermi Hubbard model

The boson—fermion model (BF) with resonant interaction has been proposed to explain high— $T_c$  superconductivity and the BCS-Bose-Einstein condensation (BEC) crossover in ultra-cold fermionic atomic gases with Feshbach resonance [1].

Here, we focus on the evolution of superfluid transition temperature ( $T_c$ ) from the pseudogap state and phase diagrams of a 3D and quasi-2D boson—fermion resonant model on a lattice, which are obtained in the self-consistent many-body T-matrix approach.

The main features of BCS-BEC crossovers for  $T_c$  and other quantities vs. the position of the bosonic level ( $\Delta_B$ ) and converting interaction ( $I$ ), for various total fillings ( $n$ ), in the BF model are reviewed.

At fixed  $I$ , a reentrant BCS-BEC crossover vs.  $\Delta_B$ , involving pairing of fermionic holes, is observed near the quantum superfluid-band insulator transition, which occurs for integer filling  $n=2$ . The density driven crossover across this QCP is examined.

The coupled mixture of hard-core (charged) bosons and fermions is also discussed, especially for  $n=2$ , which allows the superfluid-boson Mott insulator transition and a possibility of charged Kondo state.

Finally, we examine the effect of boson on-site repulsion on the superfluidity in the Bose-Fermi Hubbard model with Feshbach converting interaction, by using the coherent state path integral method [2].

**References**

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## **Emergent electronic phenomena in mixed valence rare-earth fullerides**



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Molecular solids whose cooperative electronic properties are based purely on  $\pi$ -electrons from carbon atoms offer a fertile ground in the search for exotic states of matter, including unconventional superconductivity and quantum magnetism. Of particular interest are the families of molecule-based strongly correlated f-electron fullerides with stoichiometry  $\text{RE}_{2.75}\text{C}_{60}$  (RE = Sm, Yb, Eu) in which the presence of the electronically-active  $\text{C}_{60}$  anions is combined with mixed valence rare earth ions potentially leading to properties unattainable in other systems currently available. Strong correlations dominate the electronic properties of both the rare-earth cation and the  $\text{C}_{60}$  anion sublattices and unambiguous signatures of electronically-driven valence transitions with changes in external stimuli (temperature, pressure) are found in the variation of the elastic and electronic properties of these mixed valence solids.

## Mechanism of s-wave superconductivity in heavy fermion $\text{CeCu}_2\text{Si}_2$ and Fe-based superconductors

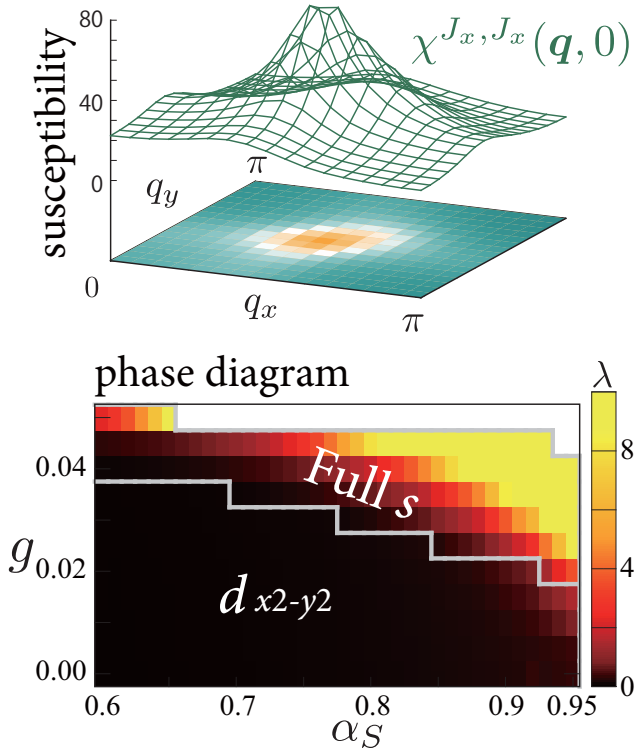


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**Keywords:** heavy fermion systems, Fe-based superconductors, superconductivity, electronic nematic state

We study the mechanism of s-wave superconductivity in  $\text{CeCu}_2\text{Si}_2$  and Fe-based superconductors, by focusing on the orbital and multipole degrees of freedom. In  $\text{CeCu}_2\text{Si}_2$ , it is widely believed that the d-wave state with sign-reversal appears due to the strong electron correlation. However, recently discovered fully-gapped s-wave state in  $\text{CeCu}_2\text{Si}_2$  has clarified that strong attractive pairing interaction can appear even in heavy-fermion systems. To understand the origin of attractive force, we develop the multipole fluctuation theory by focusing on the inter-multipole many-body interaction called the vertex corrections. By analyzing the periodic Anderson model for  $\text{CeCu}_2\text{Si}_2$ , we find that hexadecapole fluctuations mediate strong attractive pairing interaction. Therefore, fully-gapped s-wave superconductivity is driven by pure on-site Coulomb repulsion, without introducing electron-phonon interactions. The present theory will be useful to understand rich variety of the superconducting states in heavy fermion systems as well as Fe-based superconductors.



(a) Antiferro magnetic dipole susceptibility. (b) Obtained phase diagram. Fully-gapped s-wave state appears when the magnetic fluctuations are strong.

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## Theoretical possibilities for flat-band superconductivity



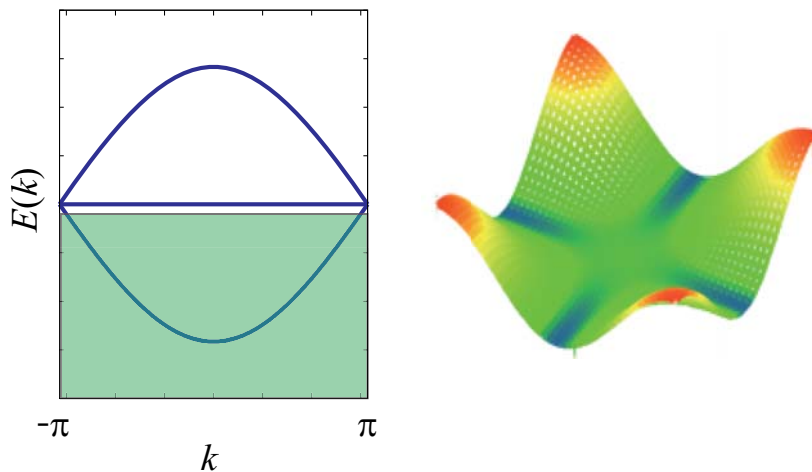
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**Keywords:** flat band, topological systems

One novel arena for designing superconductors with high  $T_c$  is the flat-band systems. A basic idea is that flat bands give unique opportunities for enhancing  $T_c$  with (i) many pair-scattering channels between the dispersive and flat bands, and (ii) an even more interesting situation when the flat band, arising from quantum mechanical interference, is topological. Here we view the route in two ways: we start with multi-band systems where a flat band coexists with dispersive one(s). We can show that this can indeed induce superconductivity when the flat band is “incipient” (close to, but away from, the Fermi energy) [1]. We then move on to propose that a simplest possible one-band case in which a portion of the band is flat does harbour the flat-band superconductivity too, with many pair-scattering channels between the flat and dispersive portions [2]. This occurs when the flat portion is incipient, where the flatness exerts an effect on the superconductivity sensitively dominated by the Fermi energy with curious pairing symmetries emerging. We also detect non-Fermi-liquid behavior. I shall discuss various implication of these.



Left: An example of multi-band model comprising flat and dispersive bands.

Right: An example of one-band model where the band comprises flat and dispersive portions.

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## Electron jamming and charge configurational state dynamics in correlated 2D chalcogenides, new devices, CDW, unconventional electronic transitions, jamming

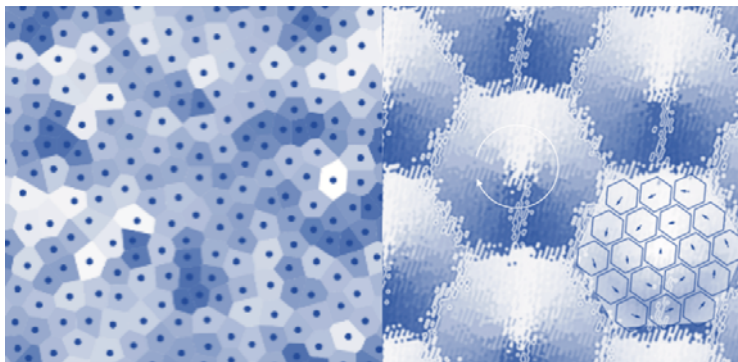


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**Keywords:** Quantum materials, quenched disorder, quasi-2D materials, Correlated disordered systems

Many body quantum systems whose constituents self-organize under highly non-equilibrium conditions can lead to entirely unexpected emergent states [1-6]. Apart from symmetry-breaking phase transitions, entirely novel mechanisms may come into play. We present laser-excited experiments in combination with scanning tunneling microscopy that reveal metastable hyper-uniform amorphous electronic matter (Fig. 1) and chiral mesoscopic configurational states (Fig. 2) created through a topological transition and quantum jamming respectively. The relaxation of such configurational states shows temperature-independent processes which can be attributed to quantum tunneling between configurational states at low temperatures. Multi-tip nanoscale conductivity measurements and tunneling spectroscopy reveal an electronically gapless state in which localized charges resonantly coexist with conduction electrons [3]. Such unusual metastable states not only reveal new non-equilibrium physics, but open the way to new all-electronic memory devices [4-6].



**Fig. 1**

**Fig. 2**

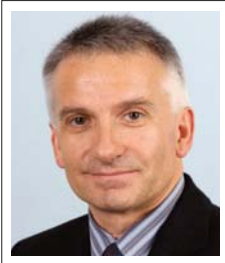
Fig. 1. Electron distribution in a jammed 2D electronic crystal

Fig. 2. Chiral structure in a 2D electronic crystal. Both were created under non-equilibrium conditions and show STM data.

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## Unprecedented Optical Anisotropy in Optimally Doped Iron-Based Superconductor



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**Keywords:** optical properties, iron-pnictide superconductors

The temperature-doping phase diagram of almost all iron-based superconductors is characterized by an antiferromagnetic dome centred at the parent compound. The onset of the magnetically ordered state is coincident with or follows a tetragonal-to-orthorhombic structural phase transition, that is driven by electronic nematic order. The latter breaks the tetragonal symmetry of the underlying lattice, without altering the translational symmetry. Superconductivity emerges in proximity of such a broken symmetry state, at the bottom of the magnetic dome in both electron- and hole-doped systems. It is currently debated to what extent nematic fluctuations contribute to the pairing-mechanism. In my talk, I offer a comprehensive optical investigation of the optimally hole-K-doped 122 material over a broad spectral range, as a function of temperature and of tunable applied stress, which acts as an external symmetry breaking field. It can be shown that the stress-induced optical anisotropy in the infrared spectral range, which is reversible upon sweeping the applied stress, occurs only below the superconducting transition temperature. These findings demonstrate that there is a large nematic susceptibility at optimal doping which extends right under the superconducting dome.

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## Dynamics of propagating and localized electronic excitations analyzed by femtosecond photoelectron spectroscopy



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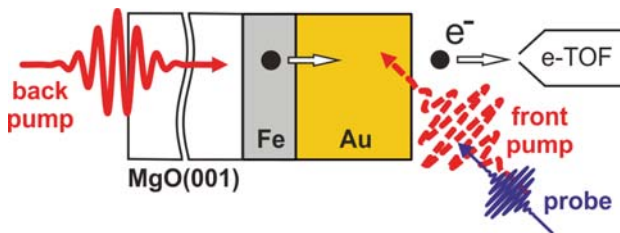
**Keywords:** Ultrafast dynamics

An excited electron in condensed matter propagates with its momentum  $k$  at an energy  $E(k)$  and experiences elastic and inelastic scattering processes, which lead to relaxation. Experiments employing femtosecond time-resolved photoelectron spectroscopy exploited so far very successfully the surface sensitivity of photo-electron spectroscopy and probed such scattering processes locally at the surface or the surface near region in the time domain [1]. Here, we report on first experimental results which analyze the non-local dynamics of excited electrons in two-photon photoemission (2PPE). In these experiments one photon excites in a Au/Fe/MgO(001) heterostructure electrons in Fe. Electron propagation through the layer stack to the Au surface is detected in 2PPE in back-pump front-probe experiments, similar to pioneering femtosecond pump-probe experiments in condensed matter, which revealed time-dependent changes in the linear optical reflectivity of free standing Au films [2]. Electrons which propagate through the layer stack in the intermediate state are detected, similar to a time-of-flight analysis. We observe pronounced differences between front- and back-pumping the hetero-structure which are attributed to electron transport contributions through the layer stack. Given the investigated Au film thickness  $5 \text{ nm} \leq d_{\text{Au}} \leq 30 \text{ nm}$ , the Fermi velocity of Au of  $v_{\text{F}}=1.4 \text{ nm/fs}$ , and the 2PPE cross correlation width on the Au surface of 70 fs we are setup to distinguish ballistic and superdiffusive transport contributions. We identify elastically and inelastically scattered electrons which propagate in a su-

perdiffusive regime [3]. Furthermore, absence of ballistic contributions at electron energies of 1-2 eV above the Fermi level for the thicker Au films are attributed to enhanced scattering at the Fe-Au interface.

Furthermore, we investigate the relaxation of delocalized Bloch electron in the charge density wave / Mott system 1T-TaS<sub>2</sub> with femtosecond photoelectron spectroscopy. In addition to previous work on the ultrafast doublon dynamics [4] we observe scattering of Bloch electrons with doublon excitations, which limit the relaxation timescales at quasiparticle energies up to 1.5 eV to 50 fs. This is in clear contrast to metals in which electron-electron scattering timescales of few femtosecond are found. Calculations by a quantum Boltzmann equation [5] support the experimental observation and allow to estimate the interaction energies.

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Scheme of time-resolved photoelectron spectroscopy to analyze non-local electron dynamics in a back-pump, time-of-flight like configuration.

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## Recent developments on iron-based superconductors – magnetic and nematic orders and their fluctuations



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**Keywords:** Iron-based superconductivity

Multiple building blocks and competing interactions characterize many strongly correlated electron systems. In iron-based superconductors, they manifest through electronic orders and their fluctuations. Here, I will first address quantum criticality and the involved degrees of freedom, including our early prediction of a quantum critical point based on a field theory [1] and the subsequent experimental evidence [2], as well as our recent study in multi-orbital Hubbard models that treats both the Hubbard and Hund's couplings [3]. Our result connects the quantum criticality with the underlying electronic degrees of freedom.

The second issue concerns the variety of nematic orders. I will introduce a new formulation via a broken mirror symmetry and show how this approach connects to the spatial patterns of magnetic fluctuations [4]. I will discuss the types of magnetic fluctuations that stabilize a B(2g) nematic order and how the mechanism provides a natural understanding of surprising recent experiments in the heavily hole doped iron pnictides.

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## Field-dependent specific heat in cuprates - pseudogap, quantum criticality and phase separation



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**Keywords:** thermodynamics, pseudogap, QCP, superfluid density, phase separation

The electronic specific heat to 300 K captures the full spectrum of low-lying spin and charge excitations up to about 100 meV [1]. In the case of the cuprates measurements of the electronic specific heat have provided deep insights [2,3] into the various correlated states that compete with superconductivity, especially the still-enigmatic pseudogap [4]. We present measurements of the field-dependent electronic specific heat with a view to addressing current controversies in the field of cuprate physics. In particular these measurements allow, amongst other things, the superfluid density to be extracted. We show (i) that the temperature scale of the pseudogap is very high – far above the reported  $T^*$  features commonly reported [5]; (ii) the reported phase transitions [5] at  $T^*$  are extremely weak and are unrelated to the pseudogap; (iii) the reported coincidence of the pseudogap with a Lifshitz transition [4,6] is not supported, and neither is the associated re-entrant superconductivity [6]; and (iv) in the overdoped state a progressive phase separation takes place causing the superfluid density to increasingly weaken, with the ultimate total suppression of superconductivity. It seems that in many of the cuprates there is only one location in the phase diagram where the electronic ground state is homogenous and coherent, namely at the critical doping of  $p=0.19$  holes/Cu.

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## **Coexistence of spin density wave and metallic phases under pressure**



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**Keywords:** electronic phase separation, imperfect nesting, pressure effects  
Using a simple and rather general model of the system with imperfect nesting of the Fermi surface, we show that the spin density wave (SDW) and normal metal (or, at low temperature, a superconductor) can coexist within a certain pressure range due to the electronic phase separation. The model predicts the SDW state at low pressure, then, nucleation of the paramagnetic (PM) droplets or islands within the SDW host at higher pressure. When the pressure continues to increase, the droplets transform to rods (or pillars) and, finally, to slabs. With the further growth of pressure, a uniform metallic phase arises. The theory agrees well with the experiment and, even in its simplest version, can capture an essential physics of the systems under study.

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## Anomalous Phonons and Dynamic Charge Stripes



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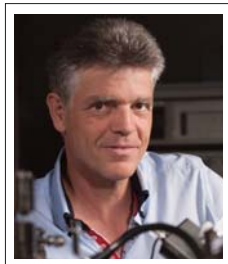
**Keywords:** Dynamic charge stripes, nickelates

The insulator-to-metal transition continues to be a challenging subject, especially when electronic correlations are strong. In layered compounds, such as  $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$  and  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ , the doped charge carriers can segregate into periodically spaced charge stripes separating narrow domains of antiferromagnetic order. Earlier we found direct spectroscopic evidence of charge-stripe fluctuations, which demonstrated that these dynamic (fluctuation) charge stripes are strongest in  $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$  close to the charge-stripe melting temperature and appear as inelastic scattering near the stripe-ordering wavevector. [1] In my talk I will discuss recent results of an inelastic neutron scattering investigation of the Ni-O bond-stretching phonons. Appearance of dynamic charge stripes is associated with a pronounced softening and broadening of these phonons near the stripe-ordering wavevector. This effect is similar to the giant phonon anomalies in cuprates that I will illustrate primarily on the example of our new work on  $\text{HgBa}_2\text{CuO}_{4+x}$ .

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## Staggered charge order and possible orbital order in the unit-cell slabs of $1T\text{-Cu}_x\text{TiSe}_2$



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**Keywords:** CDW, Orbital order, Transition metal dichalcogenides, STM, STS

Charge density wave (CDW) phases permeate the phase diagram of many correlated electron systems, and despite decades of research, they are still lacking a detailed understanding in many compounds. There is renewed interest in CDWs motivated by the possible competition of this quantum phase with superconductivity, in particular in high temperature superconductors. Combining high-resolution STM imaging [1], advanced analysis techniques [2] and DFT modelling [3], we achieve unprecedented insight into the atomic and electronic structure of the CDW ground state in  $1T\text{-Cu}_x\text{TiSe}_2$ . We find that charge ordering resides primarily on the top and bottom Se sites, staggered along the c-direction, perpendicular to the ab-plane. STM further reveals possible orbital ordering on the Ti sites. Energy dependent STM imaging reveals a striking energy dependent CDW patchwork and clear contrast inversion – something only rarely reported for any CDW system. Both features hint at an unusual CDW gap opening below the Fermi level, large and shifting to higher binding energies upon Cu intercalation. We conclude on possible consequences of these observations on the interplay between the CDW and superconducting ground states in  $1T\text{-Cu}_x\text{TiSe}_2$ .

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## Superconductivity in non-centro symmetric $\text{Re}_6\text{Zr}$ probed by Point contact Andreev reflection spectroscopy



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$\text{Re}_6\text{Zr}$ , is a non-centrosymmetric superconductor with a superconducting transition temperature ( $T_c$ ) of 6.78 K and has a simple  $\alpha$ -Mn cubic crystal structure. Recent muon spectroscopic measurements on this system has suggested that its superconducting state breaks time reversal symmetry implying a mixture of spin singlet-spin triplet states leading to a complex order parameter in this system. We report point contact Andreev Reflection (PCAR) measurements on a single crystal of  $\text{Re}_6\text{Zr}$  where at the lowest temperature of  $T = 1.6$  K, we observe multiple gap features in the PCAR spectra appearing at voltages  $1.0 \pm 0.1$  mV,  $0.75 \pm 0.05$  mV and  $0.45 \pm 0.1$  mV. Out of these, the bulk gap ( $2\Delta = 1.95 K_B T_c = 1.1$  meV) is less frequent, mostly visible with ferromagnetic tips. Besides, it also appears with low weightage in spectra where all the gap features are visible. Spectral features associated with all three gaps disappear at the bulk  $T_c$ . The two smaller gaps seem to be fully gapped. Our results suggest an unconventional superconducting order in this compound: Multiband singlet states dominated by inter-band pairing or singlet mixed with triplet states, both of which can break the time reversal symmetry.

## The Fate of the Topological Mott Insulator and Novel Quantum Criticality of Interacting Dirac Fermions on the Honeycomb Lattice



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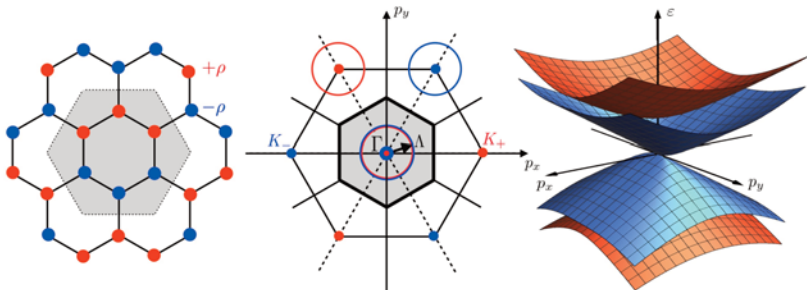
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**Keywords:** Quantum Criticality; Dirac Fermions; Charge-Density Waves

We consider the extended half-filled Hubbard model on the honeycomb lattice for second nearest neighbour interactions. Using a functional integral approach, we find that collective fluctuations suppress topological states and instead favor charge ordering, in agreement with previous numerical studies. However, we show that the critical point is not of the putative semimetal-Mott insulator variety. Due to the frustrated nature of the interactions, the charge ordered ground state remains metallic with semi-Dirac excitations. We show that translational and rotational symmetry breaking is connected to emergent gauge fields in the low-energy effective field theory. Using a renormalisation group analysis we demonstrate that the quantum-phase transition is not in the Gross-Neveu universality class.





## Dirac and Rashba bands in non-symmorphic BaNiS<sub>2</sub>



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**Keywords:** Dirac points, Rashba coupling, topological materials

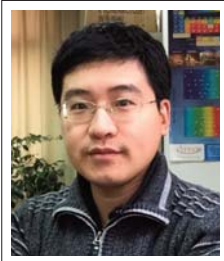
By means of a systematic ARPES study combined with ab initio first-principles calculations, we report on the peculiar co-existence of Dirac and Rashba bands in the quasi-2D system, BaNiS<sub>2</sub> [1-3], characterized by a peculiar non-symmorphic crystal structure formed by a square network of puckered NiS<sub>5</sub> pyramids. We first show that this symmetry property leads to the appearance of four Dirac points in low symmetry points along the gamma-M symmetry line [3,4], which opens the possibility of engineering the position of the Dirac bands as a function of electronic doping or strain. Second, we discuss the link between the symmetry properties of the above bands and of previously reported Rashba bands [5] and the non-symmorphic symmetry. Specifically, we highlight the possibility of manipulation of the topological properties of both bands in view of future spintronics applications. These results support the evidence that strain has been shown to be a key physical variable controlling the superconducting critical temperatures in the diborides [6], cuprates [7], and pnictides [8].

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## Manipulating electronic structure of novel correlated materials by tailoring superlattices



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Recently, a number of novel phenomena at complex quantum materials' interfaces have been discovered. Charge confinement/deconfinement in multiple valence heterostructures, coupling of structural instabilities, and continuity of the electric displacement field at interfaces have been applied as the guiding principles to manipulating electronic structure of novel correlated materials through building superlattices.

Following these principles, we successfully fabricated a series of  $[(\text{SrIrO}_3)_m/(\text{SrTiO}_3)]_n/\text{SrTiO}_3(100)$  superlattices using the layer-by-layer oxide molecular beam epitaxy. In this series of superlattices, the metal-insulator transition (MIT) is introduced by tuning the thickness of  $\text{SrIrO}_3$  interlayer. Besides, the emergent interfacial magnetism by such an artificial dimensionality control of iridates is realized. The mechanism of this MIT has been then investigated by in-situ angle-resolved photoemission spectroscopy (ARPES). Our results could provide a comprehensive understanding of the phase transition in this spin-orbit Mott insulator.

Moreover, using ARPES, we studied the electronic structure evolution of  $(\text{PbSe})_{1.16}(\text{TiSe}_2)_m$  superlattices ( $m=1, 2$ ), which are naturally occurring van der Waals heterostructures (VDWHs), and discovered several striking charge transfer effects. When the thickness of the  $\text{TiSe}_2$  layers is halved from  $m=2$  to  $m=1$ , the amount of charge transferred increases unexpectedly by more than 250%. This is accompanied by a dramatic drop in the electron-phonon interaction strength far beyond the prediction by first-principles calculations and, consequently, superconductivity only exists in the

m=2 compound with strong electron-phonon interaction. These findings of anomalous charge effects lay a foundation for further understanding and tuning VDWHs based on the manipulation of superlattices.

## Many-body effects in twisted bilayer graphene



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We theoretically study the effects of electron-electron interaction in twisted bilayer graphene [1]. When the twist angle is not very small, the electronic spectrum of the bilayer consists of four Dirac cones inherited from each graphene layer. An applied bias voltage leads to the appearance of two hole-like and two electron-like Fermi surface sheets with perfect nesting among electron and hole components. Such a band structure is unstable with respect to exciton band-gap opening due to the screened Coulomb interaction. The exciton order parameter is accompanied by spin-density-wave order. The gap depends on the twist angle, and can be varied by a bias voltage. Our results [2] correlate well with recent transport measurements [3].

We also study many-body properties of twisted bilayer graphene at the so-called 'first magic angle', where both superconductivity [4] and Mott-type many-body insulating states [5] were detected. At small twist angles, no Dirac cones exist near the Fermi level, and the bilayer's single-electron spectrum consists of weakly-dispersing partially degenerate bands. This weak dispersion makes electrons susceptible to the effects of the interactions. We consider two excitonic order parameters with spin-density-wave-like structure, and demonstrate that they lift the band degeneracy: one order parameter separates the eight bands into two quartets with the gap between the quartets. The other order parameter pulls the bands in the quartets apart, generating four doublets. The spectrum structure depends non-trivially on the doping level, which allows us to reproduce qualitatively [6] the behavior of the conductivity observed recently in experiments [5].

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## **Effects of molecular adsorption on carrier scattering in graphene**



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**Keywords:** graphene, molecular adsorption

Since graphene has a large specific area, its electronic property is easily modified by molecular adsorption. Previously, we clarified the mechanism of charge transfer between graphene and molecules [1]. The doping efficiency of electron acceptor (EA) molecules is determined by the difference between the Fermi energy of graphene and the HOMO level of the molecules. In this study, we consider how the molecules affect the carrier scattering in graphene. EA molecules were deposited on graphene in vacuum, and transport property was measured in situ. As a result, both the hole density and the scattering rate increased with an increase in the molecular density. This means that a molecule donates a hole to work as a Coulomb scatterer. The scattering rate increases in proportion to the carrier density, where the proportionality coefficient is constant for almost all molecules. However, one EA molecule did not affect the mobility in spite of hole accumulation. The possible origin is discussed in connection with the interaction between molecules.

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## Electron-phonon coupling and superconductivity in SrTiO<sub>3</sub>



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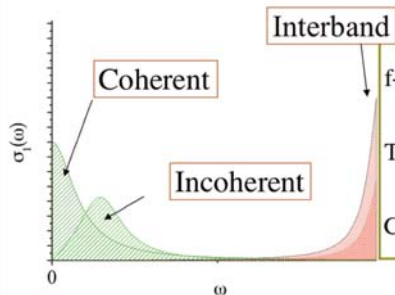
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**Keywords:** superconductivity, electron-phonon interaction, ferro-electricity, quantum criticality, isotope effect, polaron, SrTiO<sub>3</sub>

Doped STO is a superconductor with a maximal  $T_C$  rising from zero at zero doping to 400 mK around 0.005 electrons per Ti atom, and dropping to zero above 0.02 electrons per Ti atom. Substituting the heavier O-18 isotope for the natural O-16 in the samples results in a strong increase of  $T_C$  with an isotope coefficient some 20 times larger and of opposite sign as predicted by the Bardeen-Cooper-Schrieffer (BCS) model. Such a very strong isotope effect with opposite sign was theoretically anticipated based on a model where the superconducting pairing in STO is mediated by the optical phonons which are associated to the para- to ferro-electric phase transition in the undoped insulating compound, the so-called TO1 mode. Here we demonstrate from experimental data that the spectral weight of the TO1 mode is anomalously large, providing a strong indication for the so-called “charged phonon” effect discussed for the first time by MJ Rice et al in the context of organic conducting materials. Here the experimentally observed value of the charged phonon is used to determine the nature and strength of the electron-phonon coupling to the transverse polarized TO1 mode, and the quantitative implication for the corresponding channel of superconducting pairing is presented.



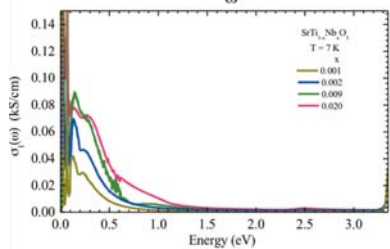
## Electrons coupled to phonons



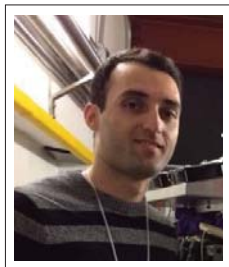
f-sumrule: 
$$\int_0^{\infty} \sigma_1(\omega) d\omega = \frac{\pi e^2}{2} \frac{n}{m_e}$$

Total free charge spectral weight: 
$$\frac{\pi e^2}{2} \frac{n_f}{m_b}$$

Coherent free charge spectral weight: 
$$\frac{\pi e^2}{2} \frac{n_f}{m^*}$$



## Exploring Two-Dimensional Layered Materials Beyond Graphene



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**Keywords:** 2D materials, Magnetic Semiconductor, topological superconductivity, Weyl-Semimetal

Transition metal dichalcogenides (TMDs), a family of 2D layered materials like graphene, have been subject to tremendous experimental and theoretical studies not only due to their exciting physical properties but also as systems that may solve critical technological problems. I will describe a few TMD

systems with novel electronic properties, where the application of hydrostatic pressure and uniaxial strain lead to large and unexpected effects [1-3]. These include the Weyl semimetal Td-MoTe<sub>2</sub> (where a strong pressure effect on superfluid density, its linear scaling with T<sub>c</sub>, as well as a possible sign changing s+- gap were observed), metallic NbSe<sub>2</sub> (where a large negative uniaxial strain effect on T<sub>c</sub> with a plateau region around zero strain is observed) and semiconducting 2H-MoTe<sub>2</sub> (where we provide the first evidence for involvement of magnetic ordering in the physics of TMDs). I will discuss these results from an experimental perspective using a combination of muon-spin rotation, X-ray/Neutron powder diffraction, and atomic-resolution scanning tunneling microscopy techniques.

These results support evidence of the key role of strain controlling functionality in dichalcogenides as it was shown in cuprates [4-5] diborides [6-8] pnictides [9].

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## Nonlinear electric and optical responses in van der Waals nanostructures



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**Keywords:** Nonreciprocal transport, superconductivity, bulk photovoltaic effect, transition metal dichalcogenide, nanotube

The effect of inversion symmetry breaking on electric and optical properties is one of the central issues in condensed matter physics. Such inversion symmetry breaking can be easily realized in van der Waals nanostructures by using the ionic liquid gating technique or crystal engineering. In this presentation, I will talk about the recent progress on the study of nonlinear electric and optical responses in van der Waals nanostructures without inversion symmetry.

Nonreciprocal electric transport, which is the second order nonlinear electric response and indicate that the forward and backward current becomes inequivalent because of inversion symmetry breaking, have been observed in various van der Waals nanocrystals [1-3]. I will also report the bulk photovoltaic effect in van der Waals nanostructures, which is the second order nonlinear optoelectronic response. Photo-induced spontaneous current appears in noncentrosymmetric van der Waals nanostructures [4].

Characteristic behavior and potential mechanism of both phenomena will be discussed.

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## Microfocus laser-ARPES on encapsulated mono-, bi- and few-layer 1T'-WTe<sub>2</sub>



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**Keywords:** 2D van der Waals materials, quantum spin Hall effect, WTe<sub>2</sub>, micro-ARPES

Two-dimensional crystals of semimetallic van der Waals materials hold much potential for the realization of novel phases. A prominent example is 1T'-WTe<sub>2</sub>, where recent magneto-transport experiments discovered a quantum spin Hall insulating phase in the monolayer [1,2] and a metallic state with macroscopic electrical polarization in bi- and tri-layers [3]. Understanding these phases is particularly challenging because little is known from experiment about the momentum space electronic structure of ultrathin crystals. In this talk, I will discuss direct electronic structure measurements of exfoliated mono- bi- and few-layer 1T'-WTe<sub>2</sub> by laser-based micro-focus angle resolved photoemission [4]. This is achieved by encapsulating a flake of WTe<sub>2</sub> comprising regions of different thickness with monolayer graphene. Our data support the recent identification of a quantum spin Hall state in monolayer 1T'-WTe<sub>2</sub> and reveal strong signatures of the broken inversion symmetry in the bilayer. We finally discuss the sensitivity of encapsulated samples to contaminants following exposure to ambient atmosphere.

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## BiS<sub>2</sub>-based layered superconductor with thick superconducting layers



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**Keywords:** new superconductor; BiS<sub>2</sub>-based layered superconductor; La<sub>2</sub>O<sub>2</sub>Bi<sub>2</sub>M<sub>2</sub>S<sub>6</sub>

In 2012, we have discovered new layered superconductors with BiS<sub>2</sub>-type conducting layers, such as Bi<sub>4</sub>O<sub>4</sub>S<sub>3</sub> [1] and REO<sub>1-x</sub>F<sub>x</sub>BiS<sub>2</sub> [2]. Since the layered crystal structure resembles to those of cuprates and Fe-based superconductors, many researchers have explored new BiS<sub>2</sub>-based superconductors and the possibility of higher transition temperature ( $T_c$ ) and unconventional nature of the superconductivity mechanisms in the system. Recently, we synthesized several La<sub>2</sub>O<sub>2</sub>Bi<sub>2</sub>M<sub>2</sub>S<sub>6</sub>, where M is metal (Pb, Ag, Cd, In, Bi, Sn, etc.). For example, the phase with M = AgBi (La<sub>2</sub>O<sub>2</sub>Bi<sub>3</sub>AgS<sub>6</sub>) is composed of alternate stacks of the La<sub>2</sub>O<sub>2</sub>Bi<sub>2</sub>S<sub>4</sub>-type layer and the rock-salt-type (Bi,Ag)S<sub>2</sub> layer [3]. La<sub>2</sub>O<sub>2</sub>Bi<sub>3</sub>AgS<sub>6</sub> shows superconductivity at  $T_c \sim 0.5$  K [4]. We will show the substitution effects and an increase in  $T_c$  in the La<sub>2</sub>O<sub>2</sub>Bi<sub>2</sub>M<sub>2</sub>S<sub>6</sub> system.

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## Cuprate quantum phase transition probed by nanoscale density wave inhomogeneity



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**Keywords:** cuprate, charge order, superconductivity

The cuprate phase diagram exhibits a number of ordered phases in addition to high temperature superconductivity. Determining the relationships among broken symmetries, Fermi surface structure, and superconductivity remain key challenges to understanding the complex phenomenology. Here, we use the d-form factor density wave (DW), imaged via scanning tunneling microscopy, to probe the ground state evolution of  $(\text{Pb,Bi})_2(\text{Sr,L a})_2\text{CuO}_{6+\delta}$  (Bi-2201). We employ local inhomogeneity to simultaneously image the DW and Fermi surface structure with continuous access to doping across the quantum phase transition where mysteriously open arcs become a conventional large Fermi surface. We discover a commensurate to incommensurate DW transition directly linking the DW instability to the k-space phenomenology.

## From weak to strong-coupling magnetism in Fe-based compounds



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**Keywords:** Magnetism, strong correlations, orbital physics, superconductivity

Iron pnictides and chalcogenides have the same structural elements. Yet, the magnetism in FeSe, for instance, displays properties of localized moments while the pnictides develop spin density waves. Thus the question as to strong *versus* weak coupling magnetism arises. Raman scattering experiments are sensitive to the type of ordering and we show how the response from a weakly coupled itinerant systems can be distinguished from that of a Heisenberg-type localized magnet. Our numerical simulations using exact diagonalization of a  $4\times 4$  cluster reproduce the experiments semi-quantitatively in the limit of a nearly frustrated spin-1 Heisenberg model (localized spins). The results indicate that the electrons in some of the orbitals are more localized in FeSe than in the pnictides and re-open the discussion on the type of nematic fluctuations observed recently.

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## Scaling between the Fano effect of the Fe-As stretching mode and $T_c$ in K-doped Ba-122



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**Keywords:** high  $T_c$  superconductivity, Fano-effect, pnictides, infrared spectroscopy

I will present a detailed infrared spectroscopy study of the Fano-effect of the Fe-As stretching mode in  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$  (BKFA) single crystals. In particular, I will show that the Fano-parameter  $1/q^2$  (and thus of the electron phonon coupling) scales with the superconducting critical temperature  $T_c$ . The origin of the underlying interband transitions and their relationship with the antiferromagnetic spin fluctuations will be discussed.

## Density of States in few layers of FeSe



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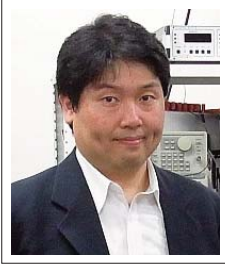
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We present X-ray absorption near edge spectroscopy (XANES) in  $\text{FeSe}_x\text{Te}_{1-x}$ . The spectra can be modelled assuming an inhomogeneous electronic structure. This inhomogeneity reflects nanoscale phase separation of coexisting magnetic ordered region of FeTe and nonmagnetic FeSe. Resonant Inelastic X-ray Scattering (RIXS) yields information about the electronic structure as it probes both unoccupied states above the Fermi level, and occupied states below. We present calculations of RIXS spectra in  $\text{FeSe}_x\text{Te}_{1-x}$  for  $x=1, 0.75, 0.50, 0$ . For these calculations we use a Density Functional Theory approach, based on a one-electron approximation that expresses the cross section as a result of the convolution of the x-ray absorption spectra and x-ray emission spectra. We use the same structural model used to model XANES spectra. [1] These calculations show the same trends observed in experimental RIXS spectra. [2] We thus conclude that the electronic structure resulting from nanoscale phase separation is reflected both for excited states above the Fermi level and occupied valence band states.

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## Time-reversal symmetry breaking in the superconducting state of FeSe



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The iron-based superconductor FeSe has attracted special attention because it uniquely has a pure nematic phase without a magnetic ordering. It is considered as a key material for investigating the influence of nematicity on superconductivity. The superconducting state inside the nematic phase also has unique properties, and it has been recently proposed that the superconducting order parameter breaks the time-reversal symmetry near the nematic twin boundaries. The lifting of superconducting gap nodes due to twin boundaries has been observed in scanning tunneling spectroscopy [1] and angle-resolved photoemission spectroscopy [2], which is consistent with the induced imaginary component. However, these measurements of the gap structure provide only indirect evidence for time-reversal symmetry breaking (TRSB), and thus the observation of spontaneous internal magnetic field generated by TRSB is indispensable. Here we report on the zero-field muon spin rotation ( $\mu$ SR) measurement, which is one of the most sensitive magnetic probes, in high-quality single crystals of FeSe. We find that the relaxation rate starts to grow just below  $T_C$  ( $=9$  K). This indicates that weak but finite internal magnetic field is induced in the superconducting state, providing strong evidence for TRSB state in FeSe.

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## Spin fluctuation in $\text{LaFePO}_{1-x}\text{H}_x$ superconductor



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**Keywords:**  $\text{LaFePO}_{1-x}\text{H}_x$ , inelastic neutron scattering

Spin fluctuations are widely believed to play an important role in the superconducting mechanisms of unconventional high temperature superconductors. Spin fluctuations have been observed in iron-based superconductors as well. However, in some iron-based superconductors such as  $\text{LaFePO}_{0.9}$ , they have not been observed by inelastic neutron scattering (INS).  $\text{LaFePO}_{0.9}$  is an iron-based superconductor with a low superconducting transition temperature ( $T_c = 5$  K), where line nodes are observed in the superconducting gap function. The line-node symmetry typically originates from sign reversal of the order parameter in spin-fluctuation-mediated superconductivity. This contradiction has been a longstanding mystery of this superconductor. Herein, spin fluctuations were found at high energies such as 30–50 meV with comparable intensities to an optimally doped  $\text{LaFeAs}(\text{O},\text{F})$  [1]. Based on this finding, the line-node symmetry can be explained naturally as spin-fluctuation-mediated superconductivity.

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## Imaging the local electronic and magnetic properties of intrinsically phase separated $\text{Rb}_x\text{Fe}_{2-y}\text{Se}_2$ superconductor using scanning microscopy techniques



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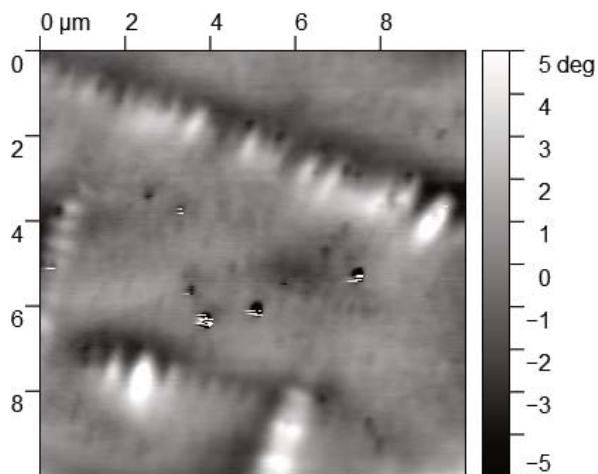
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Alkali-metal-intercalated iron selenide ( $\text{A}_x\text{Fe}_{2-y}\text{Se}_2$ , A = alkali metal) superconductors are of particular interest owing to their relatively high transition temperatures of 30 K and the co-existence of the superconducting state with antiferromagnetic ordering. Intrinsic phase separation on the mesoscopic scale is known to occur in single crystals of these compounds, adding to the complexity of interpretation of bulk property measurements. In this study, we investigate the local electronic structure and chemistry of  $\text{Rb}_x\text{Fe}_{2-y}\text{Se}_2$  crystals using scanning microscopy techniques. Nano-focused angle-resolved photoemission spectroscopy (NanoARPES) has enabled the band structure of the minority superconducting phase and the non-superconducting matrix to be measured independently and linked to the surface chemistry from the same regions using core-level spectroscopy. Valence band mapping reveals the characteristic microstructure of these crystals, but does not have sufficient spatial resolution to enable the precise morphology of the superconducting phase to be elucidated. Cryogenic magnetic force microscopy (MFM) has shown that the superconducting phase has a fine-scale stripey morphology that was not resolved in the SPEM experiment. The correlation of these findings with previous microstructural studies, bulk measurements and first-principles DFT calculations paves the way for understanding the intriguing electronic and magnetic properties of these compounds.



Magnetic Force Microscopy image of  $\text{RbxFe}_{2-y}\text{Se}_2$  at 4 K in an applied field of 100 nT, The minority superconducting phase appears bright in this image.

## Role of Fe-vacancy in FeSe and Related Superconductors



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The exact superconducting phase of FeSe and  $K_{2-x}Fe_{4+y}Se_5$  has been controversial since its discovery due to its intrinsic multiphase in early material. In an attempt to resolve this mystery, we have carried out systematic structural studies on a set of well controlled samples with exact chemical stoichiometry  $Fe_{4+x}Se_5$  and  $K_{2-x}Fe_{4+x}Se_5$  ( $x=0-0.3$ ) that are heat-treated at different temperatures. The stoichiometric  $Fe_4Se_5$  and  $K_2Fe_4Se_5$  compounds, which are Mott insulators, exhibit well-ordered Fe-vacancy with no Fe occupancy at 4d sites. Using high resolution synchrotron radiation X-ray diffraction, our investigations have determined the superconducting transition by focusing on the detailed temperature evolution of the crystalline phases. Our results show that superconductivity appears only in those samples that have been treated at high enough temperature and then quenched to room temperature. The superconducting transition strongly depends on the annealing temperature used. The most striking result is the observation of a clear contrast in crystalline phase between the non-superconducting parent compounds  $Fe_4Se_5$  (or  $K_2Fe_4Se_5$ ) and the superconducting  $Fe_{4+x}Se_5$  (or  $K_{2-x}Fe_{4+y}Se_5$ ) samples. The results strongly suggest that superconductivity in  $Fe_{4+x}Se_5$  and  $K_{2-x}Fe_{4+y}Se_5$  critically depends on the occupation of Fe atoms on the originally empty 4d site.

## **Host-guest interactions in iron-based chalcogenides intercalated with adducts of alkali metals and Lewis bases**



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**Keywords:** layered chalcogenides, intercalation, structure

Iron-based monochalcogenides intercalated with adducts of alkali metals and Lewis bases are recently intensively studied due to their intriguing magnetic and superconducting properties. The ability of iron-chalcogenides for hosting of various organic species between the inorganic layers opens the possibility for fine tuning of physical properties by controlling the type/shape, amount and orientation of the organic co-intercalant. Here, the main aspects governing chemical intercalation of layered iron chalcogenides and their consequences to the magnetic and electric properties of the hybrid intercalates will be discussed.



## A novel nematic state in heavily hole-doped iron-pnictides



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**Keywords:** iron-based superconductor; orbital-selective Mott phase; electronic nematic state

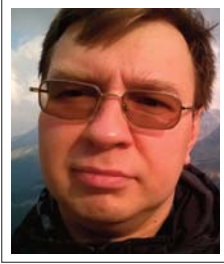
In iron pnictides and iron chalcogenides the superconductivity often emerges in the vicinity of the  $B_{1g}$  (Fe-Fe direction) nematic states [1,2] with doping or applying pressure on their parent compound with  $3d^6$  configuration of Fe atom. On the other hand, it has recently been pointed out that electron correlations are strongly enhanced with hole doping in  $BaFe_2As_2$  system, leading to a proximity to a possible half-filled Mott insulating state with  $3d^5$  configuration [3]. This fact implies that the other exotic electronic states may emerge in the heavily hole-doped regime of iron pnictides similar to underdoped cuprates [4,5]. In our elastoresistance and specific heat measurements on heavily hole-doped  $Ba_{1-x}Rb_xFe_2As_2$ , it is found that  $B_{2g}$  (Fe-As direction) nematic fluctuations develop and the specific heat exhibits two-fold oscillations in the superconducting states. These results provide evidence for the nematicity with  $B_{2g}$  symmetry in iron-pnictide superconductors with  $3d^{5.5}$  configuration.

In collaboration with K. Ishida, M. Tsujii, O. Tanaka, T. Shibauchi (Department of Advanced Materials Science, University of Tokyo), S. Ishida, A. Iyo, H. Eisaki (National Institute of Advanced Industrial Science and Technology, Japan) K. Grube, T. Wolf, Hilbert. v. Löhneysen (Karlsruhe Institute of Technology, Germany), and R. M. Fernandes (University of Minnesota, Unites States of America).

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## Spin resonance peak in the superconducting state of iron-based materials



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**Keywords:** Fe-based superconductors, pnictides, chalcogenides, spin fluctuation theory of pairing, multiband models, unconventional superconductivity, magnetic susceptibility, inelastic neutron scattering

Multiband systems, which possess a wide parameter space, allow to explore a variety of competing ground states. Bright examples are the iron-based pnictides and chalcogenides, which demonstrate metallic, superconducting, and various magnetic phases. The superconducting state is unconventional and thus the system demonstrates unusual spin response with the spin resonance feature that can be observed in the inelastic neutron scattering experiments. Here, the spin resonance in the superconducting state of Fe-based materials within the multiorbital model with unequal anisotropic gaps on different Fermi surface sheets is discussed. On the basis of the model gap function and the one calculated within the spin fluctuation theory of pairing, we show that the resonance peak shifts to higher frequencies with increasing the zero-amplitude gap magnitude. On the contrary, with increasing the gap anisotropy, it shifts to lower frequencies and loses some intensity. Obtained results lead to the adjustment of the condition that allows us to make a comparison of experimental data on the peak frequency and gaps to answer the question on whether the observed peak is the true spin resonance originating from the  $s_{\pm}$  state.

This work was supported in part by Presidium of RAS Program for the Fundamental Studies No. 12, Gosbudget Program No. 0356-2017-0030, and Foundation for the advancement of theoretical physics and mathematics “BASIS”.

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## Low temperature scanning tunneling microscopy and spectroscopy study of $\text{FeSe}_x\text{Te}_{1-x}$ at the nematic quantum critical point



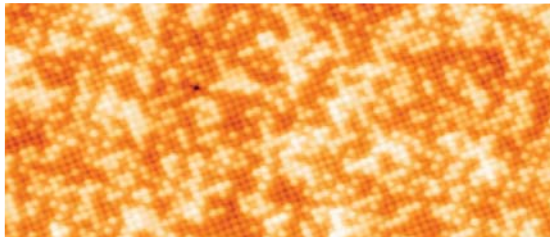
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**Keywords:** Iron-based superconductor, scanning tunneling microscopy and spectroscopy, electronic nematicity

FeSe has the simplest crystal structure among Fe-based superconductors and is considered to be an ideal play ground to understand the pairing mechanism of Fe-based superconductors because of the simplicity. By replacing 60% of Se with Te,  $\text{FeSe}_{1-x}\text{Te}_x$  ( $x=0.6$ ),  $T_c$  increases from 9 K to 14 K and the superconducting gap shape changes from nodeful to fullgap together with the disappearance of the nematic phase transition.

However, a well-known phase separation region ( $0 < x < 0.5$ ) so far prevent a full understanding of the system. We successfully grew single crystals in this region and performed electronic transport and low temperature scanning tunneling microscopy and spectroscopy measurements. The details will be discussed in the presentation.



The topographic image of  $\text{FeSe}_{0.6}\text{Te}_{0.4}$  taken with a low-temperature STM.

## Two-dimensional correlations and strong spin-orbit coupling in a single atomic plane



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**Keywords:** Mott physics, electronic correlations, charge-density-wave

Two-dimensional (2D) surface systems consisting in  $1/3$  monolayer of a tetravalent metal atom (Pb,Sn) adsorbed on a tetravalent semiconducting surface (Si, Ge, SiC) constitute simple model systems to investigate the physics of correlated electrons in 2D [1]. A particularly interesting case is the one of  $1/3$  monolayer of Pb/Si(111). While simple DFT calculations predict a half-filled 2D metal, DMFT calculations predicted the ground state to be at the border between a Mott state, a metallic state and a charge-order state [2]. Using scanning tunneling spectroscopy (STS) at  $T=0.3$  K and fully relativistic DFT+U first-principles calculations, we could study this system and furnish a consistent picture of its electronic and structural properties [3]. We found that spin-orbit coupling play an important role, in addition to strong on-site Coulomb repulsion and electron-lattice interaction, making this system a 2D correlated metal.

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## Polaron transitions in a realistic model of strongly correlated electron systems



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**Keywords:** high-Tc cuprates, polarons, strong electron correlations, electron-phonon interaction, phonon spectral function

There is major interest in description of the properties of polarons in systems with competing strong electron-electron and strong electron-phonon interactions. Sharp transitions and non-trivial topological effects found in models with electron-phonon vertex, which depends not only the phonon momentum  $q$ , but also on the quasiparticle momentum  $k$ , draw particular attention to this problem [1,2]. Here we consider realistic two-dimensional multiband pd-model with electron-phonon coupling comes from the modulation of both the on-site energy of electrons and their hopping parameter. We discuss transitions in the properties of the polarons and show that competition of diagonal and non-diagonal electron-phonon interactions results in the formation of new excitations in the phonon spectral function.

The reported study was funded by the Russian Foundation for Basic Research, Government of Krasnoyarsk Territory and Krasnoyarsk Regional Fund of Science according to the research project: "Features of electron-phonon coupling in high-temperature superconductors with strong electronic correlations" No. 18-42-240017.

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## Termination dependent electronic structure of YBCO studied by micro-ARPES



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**Keywords:** cuprates, Micro-ARPES

Utilizing angle-resolve photoemission spectroscopy with several tens of microns spot size (micro-ARPES), we disentangled surface electronic inhomogeneity of the high-T<sub>c</sub> cuprate superconductor YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> [1]. Two surface terminations consisting of either a CuO or BaO layer are identified through a chemical-states-specified core-level intensity distribution. This enables us to perform termination-selective ARPES measurements that uncover the different charge fillings and electronic configurations depending on the surface termination. By combining the real-space and electronic information, we propose a simple model to explain the termination-dependent surface electronic reconstruction. Further, we will also present new observations of peculiar superconducting states as well as zero-energy surface states on the heavily overdoped BaO surface.

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## Is magnetism relevant to cuprate superconductivity? lanthanides versus charge-compensated cuprates



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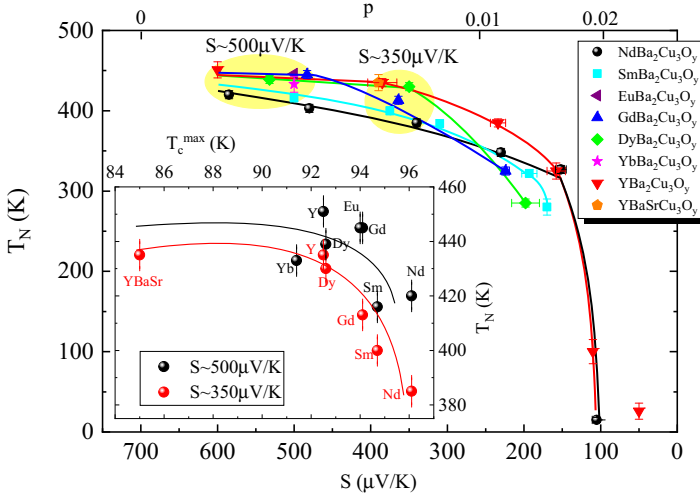
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**Keywords:** Critical Temperatures, magnetism, superconductivity, mechanism, muon spin rotation,

We address what seemed to be a contradiction between the lanthanide series  $REBa_2Cu_3O_y$  (RE123) and the charge-compensated series  $(Ca_xLa_{1-x})(Ba_{1.75-x}La_{0.25+x})Cu_3O_y$  (CLBLCO) regarding the super-exchange ( $J$ ) dependence of the maximum superconductivity (SC) critical temperature  $T_c^{\max}(J)$ ; RE and  $x$  are implicit variables. This is done by measuring the Néel temperature and the temperature dependence of the magnetic order parameter for RE=Nd, Sm, Eu, Gd, Dy, Yb, Y, and for Y(BaSr)Cu<sub>3</sub>O<sub>y</sub>, at various very light dopings. The doping is determined by thermopower, and the magnetic properties by muon spin rotation. We find that the normalized-temperature dependence of the order parameter is identical for all RE123 in the undoped limit (with the exception of Gd123) implying identical out-of-plane magnetic coupling. The extrapolation of  $T_N$  to zero doping suggests that, despite the variations in ionic radii,  $J$  varies too weakly in this system to test the relation between SC and magnetism. This stands in contrast to CLBLCO where both  $T_c^{\max}$  and  $T_N^{\max}$  vary considerably in the undoped limit, and a positive correlation between the two quantities was observed.



**Néel temperature summary.** versus the thermoelectric power Seebeck coefficient  $S$  as measured at room temperature for the different samples. The larger the  $S$  the smaller the doping. A rough estimate of the doping  $p$  is obtained from the relation  $S=700\exp(-100p)$  (see text). As the doping decreases the variation in becomes smaller. Two groups of samples are highlighted, each with similar value of  $S$ . The inset show  $T_C^{\max}$  of each family .For  $S\sim 350\sim\mu$  V/K anti-correlation between  $T_C^{\max}$  and  $T_N$  is observed for all samples excluding YBaSr. However, for  $S\sim 500\sim\mu$  V/K the variation in is not systematic.

## **Fluctuations and quantum critical points in cuprates**



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**Keywords:** cuprate, superconducting fluctuations, Quantum critical points

The phase diagram of underdoped superconducting cuprates is known to be extremely rich and complex. In addition to a transition from an antiferromagnetic insulator at half-doping to a strange metal at optimal doping, and the opening of a pseudo gap in the density of states, the normal state is also the location for a charge ordering and a Fermi surface reconstruction. By analyzing  $\text{La}_{1-x}\text{Sr}_x\text{CuO}_4$  thin films resistivity under high pulsed magnetic field for various doping, we carefully inspect the behavior of superconducting thermal and quantum fluctuations. We propose a tentative (H,T) phase diagram and we discuss the interplay between charge ordering and superconductivity.

## Four-legged starfish-shaped Cooper pairs with ultrashort antinodal length scales in cuprate superconductors



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We apply brand new ARPES-based methods [1,2] that allow us to reconstruct the shape and size of the pairs in  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ . The pairs are seen to form a characteristic “starfish” shape that is very long ( $>50\text{\AA}$ ) in the near-nodal direction but extremely short ( $\sim 4.5\text{\AA}$ ) in the antinodal (Cu-O) direction. We find that this ultrashort antinodal length scale, which is of order a lattice constant, is approximately constant over a wide range of doping levels even as many other parameters including the pairing strength change. This suggests that this new length scale, along with the pair shape, is one of the most fundamental characteristics of the pairs. Further, the shape and ultrashort length scale should make the pairs create or intertwine with variations in charge and pair density, center on various types of lattice positions, and potentially explain aspects of the nematic order in these materials.

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## Development of ferromagnetic fluctuations in heavily overdoped Bi-2201 high-Tc superconductors



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**Keywords:** High-Tc cuprate, Bi-2201, ferromagnetic fluctuation, muon spin relaxation, electrical resistivity, magnetization, specific heat

It has been theoretically proposed [1] and experimentally suggested in La-214 cuprates [2] that a ferromagnetic (FM) phase exists and is related to the suppression of superconductivity in the heavily overdoped (HOD) regime of the hole-doped high-Tc cuprates. In order to clarify the details of FM fluctuations, we have investigated transport and magnetic properties using HOD single crystals of Bi-2201 cuprates [3]. It has been found that the magnetization curve shows the tendency to be saturated in high magnetic fields at low temperatures, suggesting the precursor phenomenon toward a FM transition at a lower temperature. The development of spin fluctuations has been observed at low temperatures from muon spin relaxation. The resistivity and specific heat have shown the temperature depen-

dence characteristic of a metal with two-dimensional (2D) FM fluctuations. It has been concluded that the 2D FM fluctuations exist in the HOD regime of Bi-2201, suggesting the universality of FM fluctuations in HOD cuprates.

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## Phase diagram of cuprates under extreme conditions



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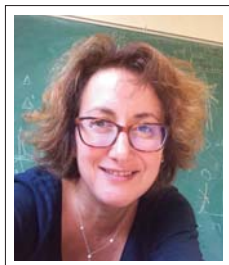
**Keywords:** Cuprates, Superconductivity, Hydrostatic pressure, High magnetic fields

The CDW observed in the cuprates superconductors is associated with a Fermi surface reconstruction that takes place in the underdoped side of the phase diagram and leads to the sign change of the Hall coefficient (RH). This sign change of RH provides a useful bulk probe to track the evolution of the CDW as the material is tuned across the phase diagram. Here we have used hydrostatic pressure to change  $T_c$  in YBCO and magnetic fields up to 38T to suppress superconductivity, so that the normal state behaviour of RH can be studied [1]. Results will be presented showing how the CDW evolves with pressure and doping in YBCO samples. I will also show the evolution of the Hall coefficient up to room temperature way above the CDW.

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## **Pseudo spin Higgs mechanism in cuprate superconductors**



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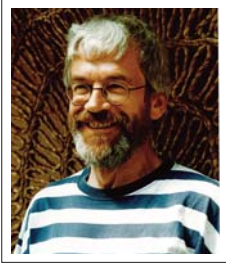
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**Keywords:** cuprate superconductors, pseudo gap, Higgs mechanism

We present a mechanism for the pseudo-gap phase of cuprate superconductors where a special Higgs mechanism in the pseudo spin space is unveiled. At  $T^*$ , the system hesitates between forming Excitonic pair and Cooper pairs. The frustration is resolved by freezing the global phase between the two fields, hence opening a spectral gap which goes as the mean square of the Excitonic and Cooper pair gaps. The plausibility case for the under doped Cuprates is addressed.



## Superconductivity in the two-dimensional Hubbard model for weak repulsion



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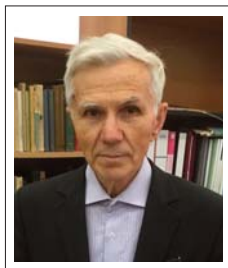
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The two-dimensional Hubbard model has been extensively studied during the last three decades, both analytically and numerically. Many questions have been answered, but several issues are not yet settled. Numerical simulations are typically limited to relatively small lattices (hundreds of sites) and therefore not capable of revealing the dominant ordering tendencies for small values of the on-site repulsion  $U$ . In order to be able to treat larger lattices (millions of sites) I have used a sophisticated variational ansatz, which performs extremely well for small values of  $U$  [1]. Expanding the energy in powers of  $U$ , one obtains explicit expressions which are readily evaluated numerically. So far I have concentrated myself on superconductivity with d-wave pairing. A finite order parameter is found away from half filling, but its  $U$ -dependence is at odds with conventional wisdom, namely I obtain a power law instead of the BCS-like exponential predicted by the exchange of spin fluctuations.

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## Asymmetry of superconducting gap dispersion in e- and h- doped cuprates



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**Keywords:** e-and h-doped cuprates, superconducting gap dispersion, high order harmonic

The dependence of the superconducting gap on the wave vector contains important information on the nature of the Cooper-pairing mechanism. The measurements with increasing accuracy provide grounds for the inclusion of higher harmonics with the d wave symmetry in the gap dispersion for both hole- and electron-doped cuprates. It was found that the behavior of the gap along the Fermi contour can be described by the phenomenological expression  $\Delta\phi = \Delta_0(B\cos(2\phi) + (1 - B)\cos(6\phi))$ , where the angle is measured from the antinodal direction in the Brillouin zone [1–5]. In hole-doped cuprates the amplitude  $(1 - B) > 0$ , whereas in electron-doped case  $(1 - B) < 0$ . Another points are the critical temperatures of h- and e-doped cuprates are different by factor 2-3 and there are contrast behavior between spin excitation and plasmon spectra. In my talk I will discuss the origin of this asymmetry.

Recently the solutions of the Bardeen–Cooper–Schrieffer equation for the superconducting gap including superexchange, spin–fluctuation, long-range Coulomb (plasmon), and phonon pairing mechanisms were obtained for  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  and  $\text{Pr}_{0.89}\text{LaCe}_{0.11}\text{CuO}_4$  [6.7]. The calculations reproduced correctly the values of quantities  $\Delta_0$  and  $(1 - B)$  for both compounds. It is found that in  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  the dependence proportional to  $\cos(6\phi)$  is due to the spin–fluctuation and phonon mediated interactions. In case  $\text{Pr}_{0.89}\text{LaCe}_{0.11}\text{CuO}_4$  the high order harmonic of gap is originated

from combined spin–fluctuation and plasmon mediated pairing. The difference between critical temperatures is mainly attributed to the presence of the tree-site correlation term, which suppresses the supexchange pairing in e-doped case.

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## **An accurate first-principles treatment of doping-dependent electronic structure of high-temperature cuprate superconductors**

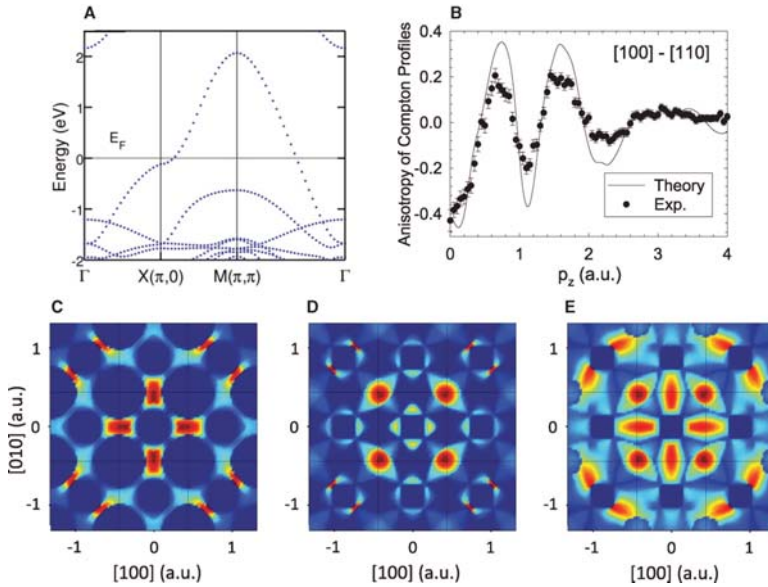


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**Keywords:** Cuprates, DTF, magnetic moments

A first-principles density-functional description of the electronic structures of the high- $T_c$  cuprates has remained a long-standing problem since their discovery in 1986, with calculations failing to capture either the insulating (magnetic) state of the pristine compound or the transition from the insulating to metallic state with doping. Here, by taking lanthanum cuprate as an exemplar high- $T_c$  cuprate, we show that the recently developed non-empirical, strongly constrained and appropriately normed density functional accurately describes both the antiferromagnetic insulating ground state of the pristine compound and the metallic state of the doped system. Our study yields new insight into the low-energy spectra of cuprates and opens up a pathway toward wide-ranging first-principles investigations of electronic structures of cuprates and other correlated materials.

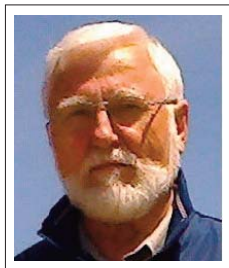


Theoretical electronic structure of LSCO from Ref. [1]: (A) Band structure; (B) anisotropy of Compton profiles; (C) 2D-EMD contribution between  $-0.4$  eV and  $+0.1$  eV; (D) 2D-EMD contribution between  $-0.8$  eV and  $-0.4$  eV; and (E) 2D-EMD contribution between  $-0.8$  eV and  $+1.3$  eV. Error bars in (B) indicate SEM. a.u., atomic units.

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## The electron-hole dimers and unconventional properties of normal and superconducting state in cuprates



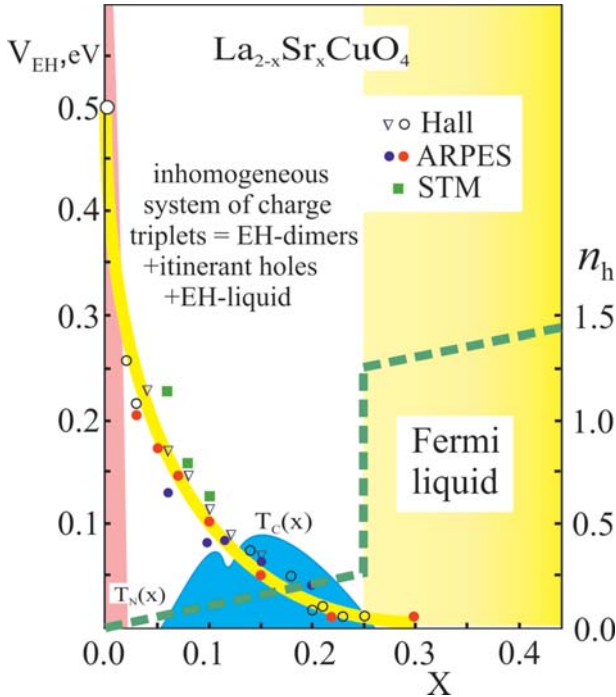
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**Keywords:** cuprates, electron-hole dimers, HTSC

Theoretical and experimental efforts have not yet led to a decisive breakthrough in explaining the unconventional properties of the normal and superconducting states of cuprates. Here we would like to draw attention to two important universal properties of parent cuprates which could explain their unusual behavior under nonisovalent doping. First, these systems are close to a so-called polarization catastrophe [1]. In practice this can implicate an insulator-to-metal transition, charge ordering, or other form of the high-polarization state. Second, energy gap over which the bounded electron-hole (EH) pairs, or highly polarizable EH dimers are thermally activated in parent cuprates, are unusually small:  $U_{th} = 0.4$  eV [2]. It means the three charge states of the  $\text{CuO}_4$  cluster,  $[\text{CuO}]^{5-}$ ,  $[\text{CuO}]^{6-}$ ,  $[\text{CuO}]^{7-}$  (nominally  $\text{Cu}^{3+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Cu}^{1+}$ ), or a charge triplet, could be considered on equal footing within the framework of an “unparticle”  $S=1$  pseudospin description [2]. The EH-dimer looks like a peculiar “quantum” of the diagonal site and/or bond charge order and off-diagonal (superfluid) order generated by a two-particle (“composite boson”) transfer. Nonisovalent substitution in cuprates stimulates the formation of the complex fluctuating inhomogeneous system of the charge triplets which is composed of traces of the parent phase, itinerant holes/electrons, stable EH dimers [3], and Bose-like EH liquid [2], whose spectral weight depends on the doping level. It is the EH Bose liquid that is responsible for the formation of the low-density superconducting Bose condensate at  $T = T_C$ , whereas the EH binding energy  $V_{EH}$

defines the pseudogap [3]. The EH dimers survive down to small  $V_{EH}$  values [3], then we arrive at EH recombination with a global transition to the Fermi liquid (Fig. 1).



Model “phase diagram” for LSCO cuprate. The doping dependence of the binding energy  $V_{EH}$  is shown according to the data of [3] and [2] ( $V_{EH}$  at  $x = 0$ ). The dotted line shows the doping dependence of carrier concentration with a jump at the EH recombination point. The regions of the long-range antiferromagnetic order and superconductivity are distinguished.

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## **Topological Superconductivity in HgTe-based Devices**



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Suitably structured HgTe has been shown to be a topological insulator in both 2- (a quantum well wider than some 6.3 nm) and 3 (an epilayer grown under tensile strain) dimensions with favorable properties for quantum transport studies, i.e. a good mobility and a complete absence of bulk carriers.

In this talk I will summarize the results of our efforts (in collaboration with colleagues all over the globe) to induce superconductivity in the topological surface states of these materials. Special emphasis will be given to recent results on the ac Josephson effect. We will present data on Shapiro step behavior that is a very strong indication for the presence of a gapless Andreev mode in our Josephson junctions.



## **Metallic glass for spintronics**

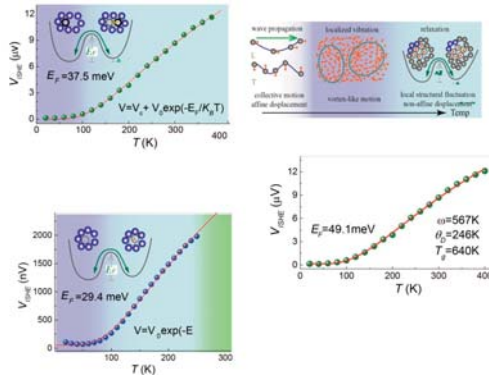
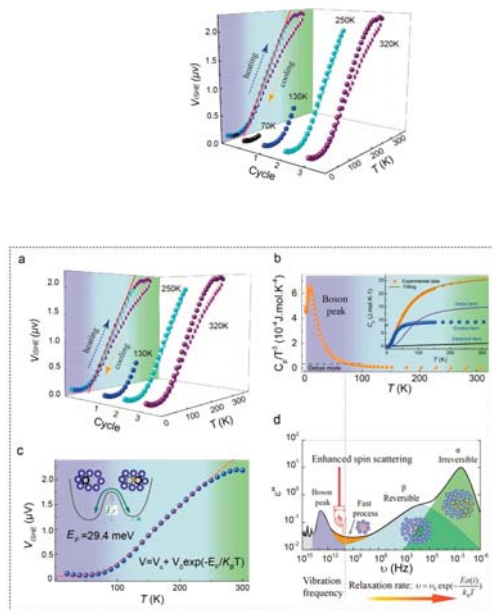


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**Keywords:** spintronics, metallic glass, Rashba effect

The idea of spintronics is to do both computation and data storage with spins, thus minimizing energy loss due to Joule heating. But to communicate with outside world spin current has to be converted to charge current, using the inverse spin Hall effect (ISHE), whereas at present the ISHE is too weak to make spintronics viable. The ISHE is based upon the Rashba effect which requires strong spin-orbit coupling and the local electric field (absence of inversion symmetry). A glass of heavy elements satisfy both requirements, and indeed we found recently Au and Pd based metallic glasses show strong ISHE [1]. I discuss the effect of local non-phonon topological excitations coupling to the crystal-field resulting in local spin fluctuations. How local spin fluctuations contribute to the ISHE was recently theorized [2]. This represents a new strategy in finding better materials for spintronics.



ISHE due to topological excitation

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## **Singlet-triplet mixing and superconducting spin currents**



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Equal-spin pairs can be generated at interfaces between conventional superconductors and spin-polarised materials, and allow for superconducting spin currents, long-range supercurrents across ferromagnets, and novel Josephson effects controlled by geometric phases. We propose a mechanism for the generation of pure superconducting spin-current carried by equal-spin triplet Cooper pairs in a superconductor sandwiched between a ferromagnet and a normal metal with intrinsic spin-orbit coupling and enhanced spin susceptibility. Our results demonstrate the crucial role of Landau Fermi-liquid interaction in combination with spin-orbit coupling for the creation of spin supercurrent in superconducting spintronics and give a possible explanation of a recent experiment utilizing spin-pumping via ferromagnetic resonance.

## **Anomalous planar hall-effect in topological semimetals**



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**Keywords:** Weyl semimetals, axial anomaly

Weyl semimetals are characterized by nodes in their linear electronic dispersion acting as Berry curvature monopoles. The simultaneous application of electric and magnetic fields is predicted to favor a particular Weyl fermion chirality. The suppression of carriers characterized by a given chirality leads to an axial current, predicted to lead to a very large planar Hall-effect which is small effect observed in anisotropic magnetic materials. Here we show that this effect is observable in the Weyl type I semi-metal TaAs. However, superimposed onto this signal we also observe a signal that is odd both in angle and in field, as a conventional Hall-effect although the field is applied in the same plane of the electrical current. This effect was reported for  $ZrTe_5$ , but here we show that it is observable also in TaAs, in GdBiPt and in the  $Fe_3GrTe_2$  which is claimed to be a topological nodal line semimetal.

## Doping and momentum dependence of coupling strength in cuprate superconductors



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**Keywords:** coupling strength, normal self-energy, pairing self-energy, spin excitation, cuprate superconductor

Superconductivity is caused by the interaction between electrons by the exchange of collective bosonic excitations, however, this bosonic glue forming electron pairs is manifested itself by the coupling strength of the electrons to collective bosonic excitations [1,2]. Here [3] the doping and momentum dependence of the coupling strength of the electrons to spin excitations in cuprate superconductors is studied within the framework of the kinetic-energy-driven superconducting mechanism [4,5]. The normal self-energy in the particle-hole channel and pairing self-energy in the particle-particle channel generated by the interaction between electrons by the exchange of spin excitation are employed to calculate the coupling strengths of the electrons to spin excitations in the particle-hole and particle-particle channels, respectively. It is shown that below the superconducting transition temperature, both the coupling strengths in the particle-hole and particle-particle channels around the antinodes consist of two peaks [3], with a sharp low-energy peak located at around 5 meV in the optimally doped regime, and a broad high-energy peak appeared at around 40 meV. In particular, this two-peak structure in the coupling strength in the particle-hole channel is directly responsible for the striking peak-dip-hump structure observed in the quasiparticle excitation spectrum of cuprate superconductors [6,7], and can persist into the normal-state. However, these coupling strengths are doping dependence, and the positions of the peaks in the coupling strengths

in the underdoped regime around the antinodes are shift towards to higher energies with the increase of doping [3]. Moreover, the coupling strengths show a striking momentum dependence, with the positions of the peaks in the coupling strengths that move to lower energies from the antinode to node. In particular, the coupling strength in the particle-particle channel vanishes at the nodes due to the d-wave type symmetry of the superconducting gap. The theory also predicts that both the coupling strengths in the particle-hole and particle-particle channels fade away around the hot spots on the electron Fermi surface.

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## Phase diagram and mechanism of superconductivity in correlated electron systems



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**Keywords:** strong correlation; mechanism of superconductivity; spin fluctuation; charge fluctuation; Hubbard model; d-p model

The mechanism of high-temperature superconductivity has been studied intensively since the discovery of cuprate high-temperature superconductors. It is certain that the electron correlation plays an important role in cuprate superconductors since parent materials without doped carriers are insulators. It is important to clarify the phase diagram of electronic states in the  $\text{CuO}_2$  plane. We investigate the ground state of the strongly correlated electronic models based on an optimization variational Monte Carlo method to clarify the mechanism of high-temperature superconductivity [1,2]. We consider the two-dimensional Hubbard model and also the three-band d-p model. The wave function is optimized by introducing variational parameters in an exponential-type wave function beyond the Gutzwiller function. The many-body effect plays an important role as an origin of superconductivity in a correlated electron system. There is a crossover between weakly correlated region and strongly correlated region, where two regions are characterized by the strength of the on-site Coulomb interaction. Our argument is that high-temperature superconductivity occurs in the strongly correlated region.

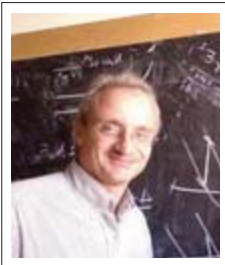
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## Dynamical Charge Density Waves pervading the phase diagram of high-T<sub>c</sub> superconducting cuprates



Marco Grilli

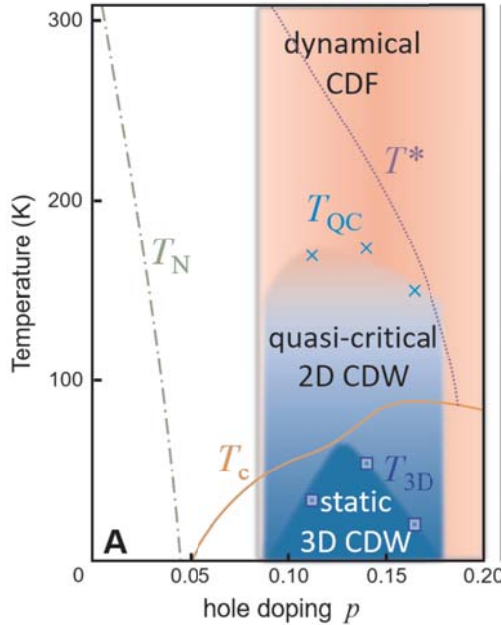
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**Keywords:** cuprates, Charge-Density-Waves, Marginal Fermi Liquid

Here is increasing consensus that charge modulations are a common occurrence in all families of high temperature superconducting cuprates. According to an old proposal [1] recently revised and extended [2], charge density waves (CDW) arise from a quantum critical point around optimal doping, but, due to the near two-dimensionality of the  $\text{CuO}_2$  planes and competition with superconductivity, the quantum charge fluctuations usually stay dynamical without forming a long-ranged CDW. Resonant Inelastic X-ray Scattering (RIXS) provides a clear evidence that strong, very short-ranged dynamical charge fluctuations are present up to very large T above the pseudogap region and in the overdoped region [3] of Nd-123 samples. This finding will stimulate a revision of the current understanding of the CDW phenomenon in cuprates also because these dynamical fluctuations could in fact provide a possible mechanism for the Marginal Fermi Liquid behavior of these systems [4].

The unexpected occurrence of quite long-ranged CDW fluctuations even in the overdoped region of Bi2201 cuprates [5] further confirms that CDW in cuprates are a pervasive effect in these systems

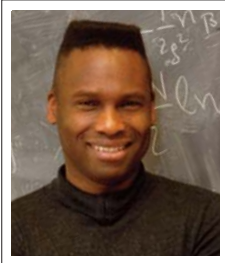


(From [4]) Summary NBCO phase diagram from RIXS experiments. Increasing blueish hue corresponds to more well-defined CDW correlations.

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## Moire is different: Wigner solidification at magic angles in doped twisted bi-layer graphene



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**Keywords:** Quantum Criticality

In a recent paper, the MIT group led Pablo Jarillo-Herrero has found that doping twisted bi-layer graphene can generate strongly correlated insulating states and superconductivity at particular twist angles called magic angles. This problem has excited the condensed matter community because it establishes that graphene, normally viewed as a weakly interacting system, is a new platform for strongly correlated physics. The experimentalists as well as a host of theorists have attributed the insulating states to Mottness. However, this interpretation has been called into question because the simplest experimental set-up in which one charge resides in each unit cell exhibits metallic transport not Mott insulation. I will review the experiments and 1) explain why the one-electron/unit cell case is a metal, 2) show that the insulating behavior is consistent with a series of Wigner crystalline states that are enhanced by hydrostatic pressure as observed in the newest experiments of Dean and Young, and 3) discuss how superconductivity arises from doping such crystalline states.

## The new NMR shift and relaxation scenario of the cuprates



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**Keywords:** Cuprates; NMR

Based on earlier experiments, as well as a comprehensive literature analysis of cuprate NMR shift and relaxation data we present the new scenario for the cuprates [1-3]. It has almost ubiquitous fermionic excitations that govern the nuclear relaxation above  $T_c$  and begin to disappear below  $T_c$ . For cuprates with the highest doping, this nuclear relaxation is in agreement with the Korringa relation for a simple Fermi liquid. Contrary to hitherto believes, it is argued that cuprates can have suppressed shifts, even when overdoped, which is the reason for the failure of the Korringa law. This means, no enhanced nuclear relaxation due to spin fluctuations has to be invoked, even not for doping levels that are significantly below optimal doping. The suppression of the shifts above  $T_c$  must be related to the pseudogap physics that does not show up in nuclear relaxation. It is argued that two antiferromagnetically coupled spin components that have different orbital origin can explain all the data, even the NMR orbital shift conundrum. More details will be discussed.

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<https://doi.org/10.3390/condmat2020016>

## Superconductivity in oxides generated by percolating electron- or hole-bipolarons



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**Keywords:** cuprates, tungstates, bipolarons

It is remarkable that in over three decades since the discovery of high temperature superconductivity (HTS) in cuprates no other class of materials has been found which exhibits this property above the liquid nitrogen boiling point at ambient pressure. Here we describe the conformation of hole- and electron-bipolarons in doped cuprates and tungstates. Important similarities and differences between them are discussed. Both hole- and electron-bipolarons can percolate forming filaments or clusters in the bulk or on the surfaces as well. Upon cooling these electronic objects can show superconducting properties. It is proposed that oxygen reduced tungsten oxide  $WO_{3-x}$  in bulk or thin film form is a promising material to explore the HTS [1]. Such material would be another example of bipolaronic superconductivity similar to cuprates. However, there is also an important difference: in the cuprates holes predominantly enter the oxygen orbitals and hole bipolarons are composed of three-spin polarons, whereas in the tungstates doped electrons are located on tungsten ions and  $W^{5+} - O^{2-} - W^{5+}$  electron bipolarons form from  $5d^1 W^{5+}$  polarons.

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## Overdoped cuprates: beyond BCS?



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**Keywords:** overdoped cuprates, XAFS, dynamics

Results from a large number of experiments on O- and photo-doped  $\text{UO}_2(+x)$ , a 5f Mott insulator, are best and perhaps only interpreted as demonstrating that the polarons aggregate and self organize into a Bose-Einstein condensate. The basis for this is Fröhlich's prediction of a non-equilibrium condensate composed of specific phonons that become coherent because of dipole interactions that are enhanced by anharmonicity. The charge-transfer that we have observed in  $\text{UO}_2$  would be an extreme case of that. An evaluation of the electronic density-of-states also shows that the polaronic quantum phase meets the conditions for stabilization by a Fano-Feshbach resonance [1-3]. Evidence will be presented for typical condensate properties as well as several that have not been predicted.

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## Hints of orbital-selectivity and charge-order in $\text{AFe}_2\text{As}_2$ (A = Cs, Rb) iron-based superconductors by means of $^{75}\text{As}$ nuclear quadrupole resonance



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**Keywords:** Charge order, nematic order, quadrupole resonance

We discuss the results of  $^{75}\text{As}$  nuclear quadrupole resonance in  $\text{AFe}_2\text{As}_2$  (A = Cs, Rb) single crystals. We demonstrate a crossover in the nuclear spin-lattice relaxation rate associated with the onset of an inhomogeneous local charge distribution causing the broadening or even the splitting of the spectra. We argue that this crossover, occurring at temperatures well above the phase transition to the nematic long-range order, is associated with a charge disproportionation at the Fe sites induced by competing Hund's and Coulomb couplings. These different trends are discussed in light of an orbital-selective behavior expected for the electronic correlations. Moreover, in  $\text{RbFe}_2\text{As}_2$  we observe a peak in the spin-lattice relaxation rate which is possibly associated with the critical slowing down of electronic nematic fluctuations on approaching the transition to the nematic long-range order.

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## Annealing effect on electronic state in electron-doped cuprate



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**Keywords:** electron-doped, XANES

Ce-substitution and reduction annealing effects on the electronic states at copper sites were systematically studied by Cu K-edge x-ray absorption near-edge structure measurements in  $\text{Pr}_{2-x}\text{Ce}_x\text{CuO}_4$  alpha-delta (PCCO). Absorption near-edge spectra were modified by both Ce-substitution and reduction annealing in a similar manner with increasing  $x$  and  $\delta$ . Considering the increase of electron number by Ce-substitution, this similarity indicates an electron-doping at the copper sites due to oxygen reduction annealing ( $n_{\text{AN}}$ ). Thus, the total number of electrons is determined by the amount of Ce and oxygen ions. Furthermore, quantitative analyses of the spectra clarified that the number of  $\text{Cu}^+$  sites, corresponding to the induced electron number by Ce-substitution  $n_{\text{Ce}}$  increases linearly with  $x$  in the as-sintered PCCO ( $\delta = 0$ ), whereas  $n_{\text{AN}}$  is not exactly equal to twice of  $\delta$ , which is expected from charge neutrality. For each  $x$ -fixed sample,  $n_{\text{AN}}$  tends to exceed  $2\delta$  with increasing  $\delta$ , suggesting the emergence of two types of carrier due to annealing. These results will be discussed in connection with spin correlations investigated by neutron scattering measurements.

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## Disappearance of the second magnetization peak in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ single crystals in the presence of static stripe order



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**Keywords:** LSCO single crystals, second magnetization peak, static stripe order

The investigation of the second magnetization peak (SMP) in “self-nanostructured” (striped)  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  single crystals can offer useful information about its nature. Optimally doped and overdoped specimens ( $x > 0.15$ ) exhibit an SMP in a large temperature  $T$  interval. By decreasing  $x$ , with the external magnetic field  $H$  oriented along the crystallographic  $c$  axis, the SMP completely disappears in the doping domain of well developed static charge and spin stripes ( $x \sim 1/8$ ), and reappears for  $x > 0.10$ . This behavior follows the instability of the quasi-ordered vortex solid (the Bragg vortex glass) in the presence of static stripe order (as revealed using small-angle neutron scattering experiments), which is confirmed by the determined temperature variation of the normalized vortex-creep activation energy. If  $H$  is parallel to the  $(a,b)$  planes, the SMP occurs even for specimens with static stripes, accompanied by an elastic vortex creep–plastic creep crossover. The results support the scenario in which the SMP is generated by the pinning induced disordering of the Bragg vortex glass in the dynamic conditions of dc magnetic measurements [2].

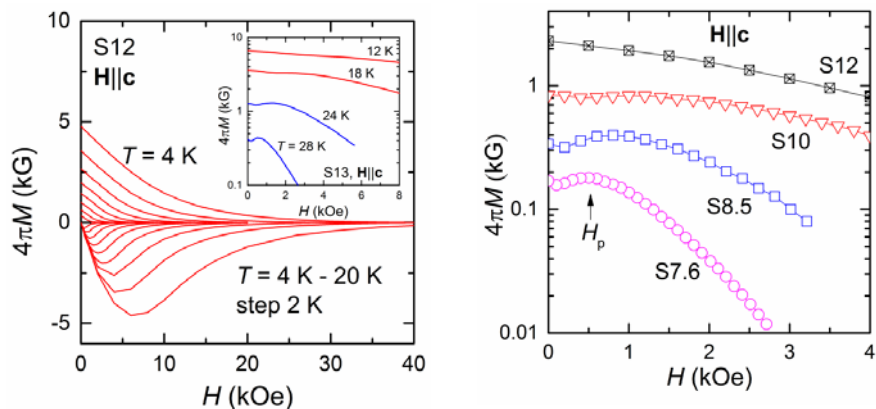


Fig. 1. (Left) Main panel: dc  $M(H)$  curves registered for S12 (in the doping range of the 1/8 anomaly) for  $H$  oriented along the  $c$  axis. No SMP was observed up to  $T_c \sim 27.5$  K. The inset shows that for S13 the SMP can be seen above  $\sim 18$  K, but it disappears at lower temperatures. (Right) While the SMP is absent in S12, strongly underdoped LSCO single crystals (S10, S8.5, S7.6) exhibit an SMP, with the peak field  $H_p$  detected on the descending  $M(H)$  branch ( $H$  parallel to the  $c$  axis,  $T \sim 0.4T_c$ ). Sample notation  $S_x$  indicate Sr with  $x$  in %.

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## Large negative thermal Hall response in the pseudogap phase of cuprates



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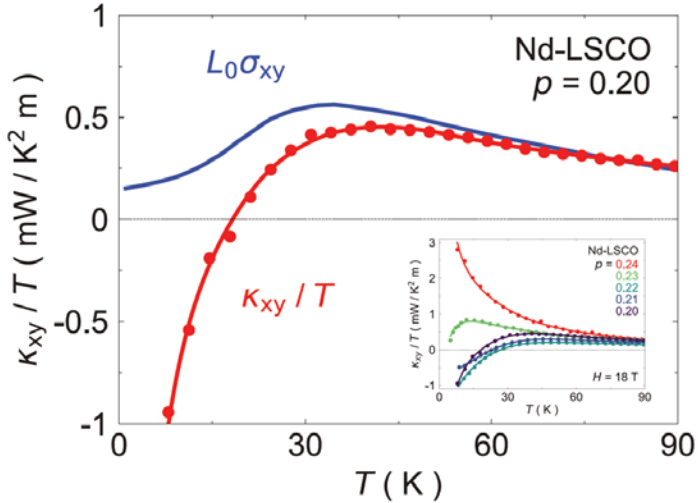
**Keywords:** cuprates, pseudogap, thermal Hall, spin chirality

The nature of the pseudogap phase of cuprate superconductors remains a mystery. In that phase, the Fermi surface is transformed even though translational symmetry is not broken [1]. A possible explanation is a spin-liquid-like state with topological order [2].

The thermal Hall conductivity  $\kappa_{xy}$  has recently emerged as a powerful probe of insulators with unusual forms of magnetism, such as quantum spin liquids [3] and quantum spin ice [4].

We report extensive measurements of the thermal Hall conductivity  $\kappa_{xy}$  in several families of cuprates across a wide range of dopings. We observe a large and negative thermal Hall response at temperatures below the pseudogap temperature  $T^*$ , which appears immediately below the pseudogap critical doping  $p^*$ . The negative  $\kappa_{xy}$  contrasts with the positive electrical Hall conductivity  $\sigma_{xy}$  and, moreover, the magnitude of  $\kappa_{xy}$  increases as doping is reduced towards  $p = 0$ , whereas  $\sigma_{xy}$  vanishes as the material becomes an insulator.

The negative  $\kappa_{xy}$  is therefore due to neutral heat carriers and it points to spin chirality [5], or perhaps topological excitations.



Thermal Hall conductivity function of temperature at  $H = 18\text{T}$  in the cuprate Nd-LSCO at hole doping  $p = 0.20$   $p^*(= 0.23)$ : one observes that the transverse heat channel of conduction  $\kappa_{xy} / T$  (red) departs from the charge channel  $L_0\sigma_{xy}$  (blue) at temperatures close to  $T^* \approx 70\text{ K}$ . Inset:  $\kappa_{xy} / T$  vs  $T$  for Nd-LSCO at four different dopings  $p = 0.20, 0.21, 0.22, 0.23, 0.24$  on each side of the pseudogap critical doping  $p^* = 0.23$

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## **Evidence of a Coulomb-Interaction-Induced Lifshitz Transition and Robust Hybrid Weyl Semimetal in Td-MoTe<sub>2</sub>**



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Using angle-resolved photoemission spectroscopy (ARPES) we probed the electronic structure of Td-MoTe<sub>2</sub>. We found that on-site Coulomb interaction leads to a Lifshitz transition, which is essential for a precise description of the electronic structure. A hybrid Weyl semimetal state with a pair of energy bands touching at both type-I and type-II Weyl nodes is indicated by comparing the experimental data with theoretical calculations. Unveiling the importance of Coulomb interaction opens up a new route to comprehend the unique properties of MoTe<sub>2</sub>, and is significant for understanding the interplay between correlation effects, strong spin-orbit coupling and superconductivity in this van der Waals material.

## Experimental signatures and control of entanglement transitions in quantum spin clusters



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**Keywords:** Quantum magnetism, entanglement

We address a simple model of a single-molecule nano-magnet with  $N$  interacting spins in a transverse applied magnetic field, and consider the experimental implications of the entanglement transition [1]. We consider the general spin-1/2 anisotropic antiferromagnetic Heisenberg model, and from numerical diagonalization for  $N=4,6,8,10,12$  we calculate the magnetisation, low-energy gap and neutron-scattering cross-section. We find that there are  $N/2$  level crossings between the ground state and first excited state as the field is increased, with zeros in the energy gap and magnetisation jumps at the crossings. The last crossing corresponds to the entanglement transition in which, for all  $N$ , the ground state is fully factorised into a product wave function, with a dramatic rearrangement of spectral weight in the spin-spin correlation function on going through the entanglement transition. We find there is a large shift in spectral weight from antiferromagnetic ferromagnetic positions as the nature of the entangled state changes through the factorisation field. The changes are robust to non-zero temperature. Neutron scattering experiments should therefore be able to detect the entanglement transition.

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## Impact of magnetic ions state on local structure of pyrochlores $\text{Ln}_2\text{Ti}_2\text{O}_7$ (Ln=Gd, Tb, Dy)



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**Keywords:** geometrically frustrated magnetic materials, complex rare-earth oxides, XAFS (EXAFS and XANES)

We report temperature dependent XAS study of geometrically frustrated magnetic pyrochlores  $\text{Ln}_2\text{Ti}_2\text{O}_7$  (Ln=Gd, Tb, Dy). These compounds have the same crystal structure, but their magnetic structure is quite different, that is, long-range ordered, spin-liquid, and spin-ice state for  $\text{Gd}_2\text{Ti}_2\text{O}_7$ ,  $\text{Tb}_2\text{Ti}_2\text{O}_7$ , and  $\text{Dy}_2\text{Ti}_2\text{O}_7$ , respectively [1]. The XAS spectra were taken at Ti K- and Ln L<sub>3</sub>- absorption edges in transmission mode in the temperature range of 10–300 K. The temperature dependences of the interatomic bond lengths Ln – O and Ti – O were obtained from EXAFS data analysis. We also calculated the Debye-Waller factor and the Einstein temperature to evaluate the stiffness of bonds and the degree of their local static and dynamic disorder. Basing on XAS and XRD data, we discuss the impact of magnetic state of a rare-earth ion on the local structure features in  $\text{Ln}_2\text{Ti}_2\text{O}_7$  and demonstrate that the stabilization energy of a magnetic ion in a crystal field plays an important role.

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## Exceptional points in energy spectrum of magnetic materials



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Non-conservative physical systems admit a specific type of spectral degeneracy known as exceptional point (EP), at which eigenvalues and eigenvectors of the corresponding non-Hermitian Hamiltonian coalesce. Slow encircling of individual EPs in a parameter space can lead to non-adiabatic evolution of the system, resulting in non-reciprocal dynamics. Building on the recent progress in understanding parity-time-symmetric magnetic systems, we utilize the topological properties of EPs for chiral non-reciprocal transmission of spin. The range of optimal protocol parameters for high-efficiency operation of an asymmetric spin filter based on this effect is obtained. This result offers a platform for non-reciprocal spin devices crucial for applications in spintronics and magnonics.

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## Pressure-induced dimerization and Kitaev spin liquid regime of $\alpha$ -RuCl<sub>3</sub>



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**Keywords:** Kitaev-Heisenberg magnet, quantum spin liquid, dimerisation

The Kitaev model on a honeycomb lattice has become a particularly hot topic in the field of frustrated magnetism, due to its exact solubility and its quantum spin-liquid ground state. Recently, the honeycomb material  $\alpha$ -RuCl<sub>3</sub> has been identified as a possible realization of the Kitaev model, rendering this material an ideal platform for exploring Kitaev magnetism experimentally. However, the onset of long-range magnetic order at  $T_N = 7$  K and ambient pressure, i.e. the absence of a spin liquid ground state, implies that  $\alpha$ -RuCl<sub>3</sub> deviates from the ideal Kitaev model under these conditions. We therefore set out to elucidate whether  $\alpha$ -RuCl<sub>3</sub> can be driven into the true Kitaev regime by means of hydrostatic pressure. Our high-resolution x-ray diffraction studies reveal a rich structural phase diagram, including pressure induced Ru-Ru dimerization as well as a high-symmetry rhombohedral phase. The latter is indeed found to be very close to the ideal Kitaev model.

## ESR spectroscopy of two-dimensional van der Waals magnets



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Layered van der Waals magnetic compounds attract currently large attention as they may display an intrinsically low-dimensional magnetic behavior and as such offer an extensive materials base for exploring fundamental magnetic properties of strongly correlated two-dimensional (2D) electron systems. In the talk the results of a detailed electron spin resonance (ESR) spectroscopic study of two representatives of this family will be discussed:

1)  $\text{Cr}_2\text{Ge}_2\text{Te}_6$  is a quasi-2D magnet showing intriguing intrinsic ferromagnetism down to atomically thin films [1]. Here we could obtain new detailed insights into the magneto-crystalline anisotropy which should be responsible for the stabilization of magnetic order in the 2D limit and find evidence for an intrinsically 2D character of the dynamics of Cr spins even in bulk single crystals [2].

2)  $\text{MnBi}_2\text{Te}_4$  is the first antiferromagnetic topological insulator featuring Dirac cones in the electronic structure due to the topological surface states [3,4]. In this material we observe a surprisingly anisotropic spin dynamics of bulk conduction electrons and Mn localized states which, as we argue, could be responsible for the persistence of the bandgap in the topological surface state even above the magnetic ordering temperature.

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## Spin excitation spectroscopy reveals single atom magnetism



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**Keywords:** Spin excitations, Single atoms, Kondo effect, Scanning tunneling probes

Recently, correlation-driven transport asymmetries, reminiscent of spin-polarized transport in a magnetic field, have been observed in the tunneling spectra between two magnetic impurities, one at the tip of a scanning tunneling microscope, the other one on the sample surface [1]. Here we apply this technique in zero magnetic field and at a temperature of 0.5 K, to reveal the spin of an individual Ce adatom on the surface of a CuN ultrathin film. The presence of the Ce 4f spin manifests itself in the differential conductance spectra recorded in a tunneling junction between a PtIr tip, functionalized with a Ce-cluster at its apex, and a single Ce adatom on the sample surface. By identifying this cluster as a Ce-trimer at the tip apex via its Kondo and spin excitation spectrum, a fundamental understanding of the manifestations of the 4f spin in Ce adatoms is obtained. The three Ce adatoms forming the trimer are shown to couple ferromagnetically to a total spin of  $3/2$  with a degenerate Kondo ground state of spin  $1/2$  [2]. The degeneracy of the ground state of the Ce-trimer at the tip is gradually lifted by decreasing the tunneling resistance (decreasing the tip surface distance) and thereby increasing the interaction with the 4f spin of a single Ce adatom at the sample surface. The induced splitting of the Ce trimer Kondo resonance of about 2 meV corresponds to an effective magnetic field of 5 Tesla [3]. Thus, employing the vertical atom manipulation capabilities of the STM, the functionalized tip is used as a spin detector for single magnetic Ce adatoms in the absence of an external magnetic field. This achievement

validates an alternative route to the study of magnetic nanostructures [4], circumventing the application of spin-polarized STM tips. When individual Ce adatoms assemble to create a superlattice on Ag(111) with an interatomic lattice spacing of 3.2 nm [5], a Kondo lattice is formed. The differential conductance spectra obtained on single Ce-adatoms within the superlattice reveal a considerably broadened Kondo resonance of about 70 meV as compared to the one of 1 meV found for isolated Ce-trimers, indicating the presence of antiferromagnetic indirect exchange interactions (RKKY) in the superlattice[6]. In the light of these results, the present study opens new insights into the interplay between Kondo physics, localized spin-flip excitations, and the magnetic exchange interaction.

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## Spin waves in the ferrimagnetic spin spiral of FeP

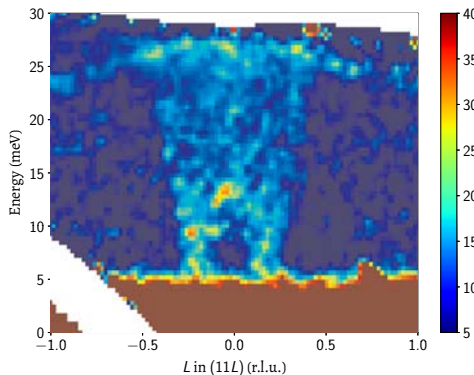


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**Keywords:** spin spirals, incommensurate antiferromagnet, iron phosphide

Iron phosphide (FeP) represents an itinerant non-collinear magnet, in which a spin-spiral ground state is realized. In contrast to conventional helimagnets, though, two nonequivalent magnetic moments lead to a highly unusual twisted ferrimagnetic type of spin arrangement. Using inelastic neutron scattering, we investigated the spin-wave dispersions in this material. We find two types of incommensurate spin-wave modes emanating in the vicinity of the structurally allowed and forbidden zone-center reflections. The corresponding spin-wave velocities are very anisotropic, as seen in the



much steeper dispersion along the  $b$  direction of the crystal, which is in agreement with expectations based on band structure theory. The spin-wave dispersion in the direction of the spiral propagation is reminiscent of the “hourglass” dispersion that was famously observed in some incommensurate antiferromagnets, including doped copper oxides.

“Hourglass”-shaped spin-wave dispersion emanating from the incommensurate magnetic satellites of the structurally forbidden (110) Bragg reflection in FeP.

## Pseudo Jahn-Teller effect in spin-orbit entangled Mott insulators



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**Keywords:** spin-orbit coupling, Jahn-Teller effect

The consequences of Jahn-Teller (JT) orbital-lattice coupling for magnetism of pseudospin  $J_{\text{eff}}=1/2$  and  $J_{\text{eff}}=0$  compounds are addressed [1]. In the former case, represented by iridium oxide  $\text{Sr}_2\text{IrO}_4$ , this coupling generates, through the so-called pseudo-JT effect, the orthorhombic deformations of a crystal concomitant with magnetic ordering. The orthorhombicity axis is tied to the magnetization and rotates with it under magnetic field. Theory resolves a number of hitherto unexplained puzzles in  $\text{Sr}_2\text{IrO}_4$  such as metamagnetic behavior, field dependence of the magnon gaps, etc. In case of pseudospin  $J_{\text{eff}}=0$  systems, the pseudo-JT effect leads to a spin-nematic transition well above the magnetic ordering, which may explain the origin of “orbital order” in  $\text{Ca}_2\text{RuO}_4$ .

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## Mott transition and collective charge pinning in electron doped $\text{Sr}_2\text{IrO}_4$



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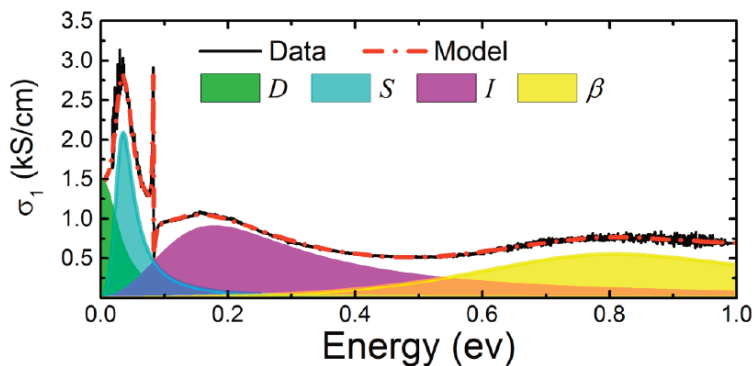
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Many body systems involving strongly interacting electrons exhibit various rich and interesting physical phenomena, among them the well known Mott insulator. Undoped cuprates and iridates belong to this class, and have in common that the Mott-insulating state is formed by half-occupying a single non-degenerate band. In the case of the cuprates doping holes or electrons in the Mott-insulating phase results in high  $T_c$  superconductivity, the exact mechanism of which is still not fully established. Based on strong similarities in crystal structure and the common feature of the Mott-insulating parent state, the effect of doping  $\text{Sr}_2\text{IrO}_4$  is expected to result in a superconducting state. While superconductivity has not yet been established in this family of materials, a peculiar gap in the density of states is observed both in iridates and in cuprates. In the cuprates the pseudo-gap feature shows up in various different types of charge and spin spectra, in particular in the infrared optical spectra. An important unanswered question concerns the relation and/or interplay between the pseudo-gap state and the superconducting state: are they competing phases or is the former a precursor of the latter? Here we present optical data on an iridate compound, and investigate the doping and temperature dependence of the pseudo-gap at low en-

ergies. We argue that the pseudo-gap is a signature of the presence of residual correlations unrelated to pair-formation, which are inherited from the correlated insulating state.



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## Topological superconductivity in the 5d Mott insulator $\text{Sr}_2\text{IrO}_4$



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We study superconducting pairing instabilities of the hole-doped 5d Mott insulator in the presence of antisymmetric Dzyaloshinskii-Moriya exchange, applicable to  $\text{Sr}_2\text{IrO}_4$ . Within the random phase approximation, we compute the spin-fluctuation-mediated pairing interactions as a function of filling and  $\text{IrO}_6$  octahedron canting angle. We find that paramagnon exchange near a spin-density-wave instability gives rise to a strong singlet d-wave pairing interaction. Besides, a Rashba type spin-orbit coupling splits the spin degeneracies of the bands and enhance the ferromagnetic contribution, which leads to mixing of even and odd parities in the superconducting order parameter. We find that mixed singlet-triplet superconductivity,  $d+p$ , is generated as a result of the antisymmetric exchange originating from a quasi-spin-orbit coupling. As a possible candidate of topological superconductivity, we study a possible trace of the nodal structure of the superconducting gap, as the edge states. These edge modes are spin polarized and emerge as zero-energy flat bands, supporting a symmetry-protected Majorana state, verified by evaluation of the winding number and  $Z_2$  topological invariant. Together with this prediction, we discuss a possible method for experimentally observing the zero-energy nontrivial edge states via the STM-based QPI approach [1].

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## Phase separation at the dimer-superconductor transition and absence of dimer fluctuations in iridium ditelluride based superconductors



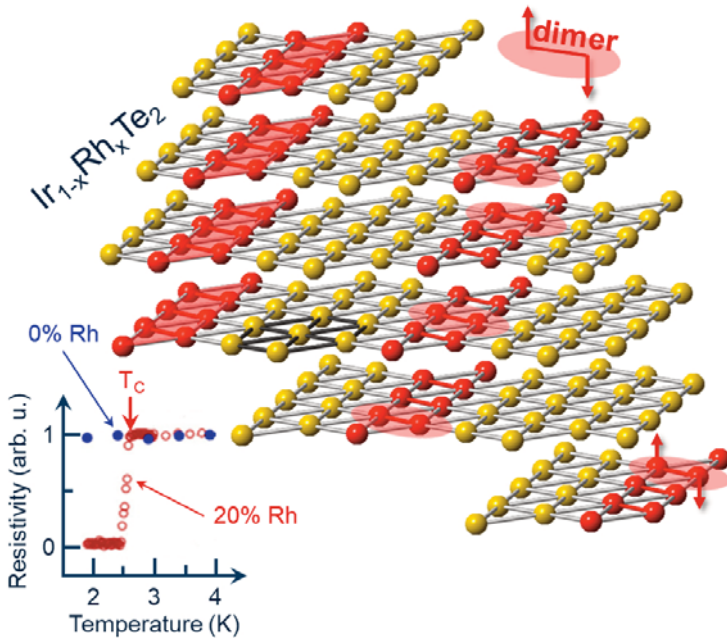
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**Keywords:** local atomic structure, phase separation, dimerization

The compound  $\text{IrTe}_2$  is known to exhibit a transition to a modulated state featuring Ir-Ir dimers, with large associated atomic displacements. Partial substitution of Rh or Pt for Ir destabilizes the modulated structure and induces superconductivity. It has been proposed that quantum critical dimer fluctuations might be associated with the superconductivity. Here we test for such local dimer correlations and demonstrate their absence [1,2]. The detailed evolution of the local atomic structure across the  $(x,T)$  phase diagrams of  $\text{Ir}_{1-x}(\text{Rh,Pt})_x\text{Te}_2$  superconductors is obtained from high-quality x-ray total scattering data using the atomic pair distribution function method. The observed hysteretic thermal structural phase transition from a trigonal to a triclinic dimer phase for low Rh and Pt content emphasizes the intimate connection between the lattice and the electronic properties. In the superconducting compositional regime, and away from the dimer/superconductor boundary the structural transition is absent. The local structure of  $\text{Ir}_{0.95}\text{Pt}_{0.05}\text{Te}_2$  and  $\text{Ir}_{0.8}\text{Rh}_{0.2}\text{Te}_2$  with compositions just past the dimer/superconductor boundary is explained well by a dimer-free model down to 10 K. In the narrow range of compositions close to the boundary structural phase separation is observed, suggestive of weak first-order character of the doping induced dimer-superconductor quantum phase transition. Samples from this narrow range show weak anomalies in electronic trans-

port and magnetization, hallmarks of the dimer phase, as well as superconductivity albeit with incomplete diamagnetic screening. This implies competition of the dimer and superconducting orders. The observations rule out the possibility of there being nanoscale dimer fluctuations in this regime. This is inconsistent with the proposed quantum-critical-point-like interplay of the dimer state and superconductivity and precludes scenarios for dimer fluctuations mediated superconducting pairing.

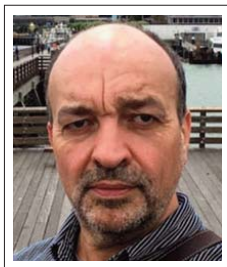


Atomic structure (iridium sublattice) of the low temperature phase of IrTe<sub>2</sub> featuring Ir<sup>4+</sup> dimers (red) ordered on a triangular Ir network. Inset: low temperature electrical resistivity of pure and Rh-substituted IrTe<sub>2</sub>.

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## Jeff=1/2 exciton Fano resonances in pyrochlore iridates with all-in/all-out magnetic order



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**Keywords:** spin-orbit coupling, Mott insulator, exciton, Fano resonance

Pyrochlore iridates are predicted to realize exotic quantum states over a certain range of relative correlation  $U/W$  and spin-orbit coupling  $\lambda/W$  strengths. We used spectroscopic ellipsometry to determine the dielectric function of  $A_2\text{Ir}_2\text{O}_7$  ( $A = \text{In}, \text{Lu}, \text{Y}$ ) polycrystalline samples in the spectral range from 10 meV to 6.5 eV at temperatures from 7 K to 300 K. Comparing the spectra with the results of relativistic LSDA+U band structure calculations for the noncollinear all-in/all-out magnetic state, we quantitatively classify pyrochlore  $A_2\text{Ir}_2\text{O}_7$  as spin-orbital Jeff=1/2 Mott insulators with the on-site Coulomb interaction  $U \approx 1.5$  eV and the electronic bandwidth  $W = 0.3 \div 0.5$  eV. Exciton doublets with pronounced Fano line shapes were identified in  $\text{Y}_2\text{Ir}_2\text{O}_7$  upon cooling below the magnetic ordering temperatures  $T_N = 150$  K. The formation of exciton complexes observed at the absorption edge is accompanied by distinct phonon anomalies in the infrared spectra. Our results indicate considerable effects of long-range Coulomb interaction and spin-orbit-lattice coupling in the 5d-pyrochlore compounds and the need for a detailed analysis of their influence on the Jeff=1/2 states. Newly synthesized  $\text{In}_2\text{Ir}_2\text{O}_7$  does not exhibit the absorption edge and phonon anomalies below  $T_N = 45$  K and thus serves as a reference.

## **Superconductivity and structural inhomogeneity in perovskite-based materials**



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I will present the finding of a universal superconducting precursor regime in several perovskite-based superconductors, including the cuprates and strontium titanate [1,2]. The unconventional precursor was studied using nonlinear magnetic response, that unambiguously separates the superconducting from the normal-state response. The measurements reveal an unusual exponential temperature dependence, which is shown to be related to intrinsic structural inhomogeneity. We find a characteristic stress scale for this inhomogeneity, and demonstrate that the precursor (and the superconducting transition temperatures) can be manipulated by compressive plastic deformation at ambient conditions. The experiments establish unexpected similarities between very different unconventional superconductors, and show the important role played by self-organized local structure inhomogeneity.

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## Instantons related structure of the Density Wave systems in high-Tc superconductors



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**Keywords:** negative energy antiferromagnetic instantons, ‘hidden order’ in HTSC, instantonic guage fields structure

An emergence of the magnetic boson of instantonic nature, that provides a Cooper-pairing glue, is considered in the repulsive ‘nested’ Hubbard model of superconducting cuprates. It is demonstrated, that antiferromagnetic instantons [1] of a spin density wave type may have negative energy due to coupling with Cooper pair condensate. A set of Eliashberg-like equations is derived and solved self-consistently, proving the above suggestion. An instantonic propagator plays the role of pairing boson Green’s function. Simultaneously, the instantons defy condensation of the mean-field SDW order. We had previously demonstrated in analytical form [2-4] that periodic ‘chain’ of 0+1D instantons along the axis of the Matsubara’s time, a ‘quantum crystal’, has zero scattering cross section for weakly perturbing external probes, thus representing a ‘hidden order’. We show, that instantons in 2+1D Euclidean space may cause different DW structures in high-Tc superconductors. A comparison of the theoretically deduced and experimentally observed DW patterns and excitations brunches as fingerprints of the instantonic structure is made.

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## Exact phase diagram of the infinite-dimensional extended Falicov-Kimball model



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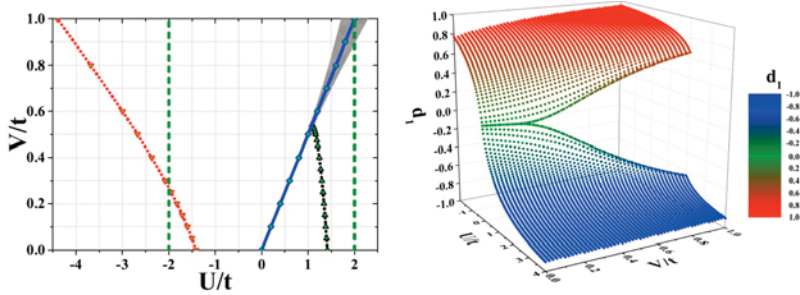
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**Keywords:** extended Falicov-Kimball model, phase diagram, charge-order, exact results, intersite interactions, dynamical mean field theory

The Falicov-Kimball model [1,2] is a simplified version of the Hubbard model, where only electrons with, e.g., spin down, can hop. The half-filled extended Falicov-Kimball model, which includes also the intersite density-density interactions, is studied within the DMFT formalism [3-6] on the Bethe lattice in infinite dimensions, which is a rigorous approach in this limit. We determined the exact phase diagrams of the model both in the ground state [5] and at finite temperatures [6]. Using analytical formulas we showed that in the ground state the system is an insulator and we detected the discontinuous transition between two different charge-ordered phases [5]. The finite temperature diagrams contain several types of ordered phases, both conductive and insulating [6]. The transitions between them are either continuous or discontinuous. What is more, it turns out that in a certain range of interaction parameters the order-disorder phase transition may be discontinuous.

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Left: Ground state diagram as a function of on-site  $U$  and intersite  $V$  interactions. Solid line at  $U=2V$  denotes a discontinuous transition. Right: The overall behavior of the difference of number of itinerant electrons in both sublattices as a function of  $U$  and  $V$  in the stable phases [after: Phys. Rev B 96, 205102 (2017)].

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## Spin-Peierls dimerization and orbital ordering in quasi one dimensional Ti compounds $\text{TiPO}_4$ and $\text{NaTiSi}_2\text{O}_6$



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**Keywords:** Mott insulator, Spin-Peierls dimerization, Jahn-Teller effect, Quantum magnetism

Quasi one dimensional Ti compounds  $\text{TiPO}_4$  and  $\text{NaTiSi}_2\text{O}_6$  are investigated by NMR technique using  $^{23}\text{Na}$ ,  $^{29}\text{Si}$ ,  $^{31}\text{P}$ , and  $^{47,49}\text{Ti}$  resonances in several magnetic fields: 4.7, 8.5 and 14.1 Tesla. Both compounds undergo at low temperatures  $T < T_c$  Ti spin dimerization to singlet state from paramagnetic state. In  $\text{TiPO}_4$  dimerization takes place through incommensurate phase  $T_{c1} = 73\text{K} < T < T_{c2} = 112\text{K}$ . On the other hand in  $\text{NaTiSi}_2\text{O}_6$  at  $T < T_c = 210\text{K}$  starts Ti orbital ordering and spin dimerization simultaneously. In spite of both compounds have direct Ti spin-spin strong exchange interaction of the same order  $J = 900\text{--}1000\text{K}$ , the detailed behavior is very different. These differences are experimentally established and analyzed taking account of different structures of crystal lattices and orbital degeneracy of Ti d-orbitals.

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## Chiral anomaly and dynamics of charge density waves



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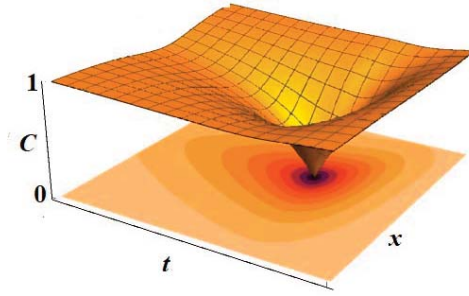
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**Keywords:** chiral anomaly, electronic vortices, dynamical topological defects, phase slips, space-time vorticity

Many experiments addressed the charge density waves in nano-junctions, under electric field, together with real space visualizations by STM and micro X-ray diffraction. This activity returns the interest to stationary or transient states with static and dynamic topologically nontrivial configurations: electronic vortices, instantons, and microscopic solitons. Describing and modeling these states and processes calls for a theory which takes into account the degenerate order parameter, various kinds of normal carriers and the electric field. The commonly employed time-depend Ginzburg-Landau approach suffers with violation of the charge conservation law resulting in unphysical generation of particles which is particularly strong for nucleating or moving electronic vortices. We present a consistent theory which exploits the chiral transformations taking into account the principle contribution of the fermionic chiral anomaly to the effective action. On this basis we perform the numerical modeling of a spontaneously generated coherent sequence of phase slips - the space-time vortices - serving for the conversion among the injected normal current and the collective one.



Single electronic vortex

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## Charge susceptibility and diffusion in bad metals



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**Keywords:** bad metal, strange metal, charge susceptibility, diffusion, doped Mott insulator

The study of transport within the fermionic Hubbard model by its realization in the cold-atom setup will be presented. Applying long wave-length external potential and inducing particle density modulation, which decayed with time after the turn-off of the external potential the diffusion constant was measured. Additionally, the charge susceptibility or compressibility was estimated by measuring the variation of the particle density with position in the harmonic trapping potential. This allowed the estimate of the resistivity via the Nernst-Einstein relation and its temperature dependence by measuring the temperature dependence of both diffusion constant and charge susceptibility. In a wide high temperature regime, the resistivity shows linear-in-temperature dependence and violates the upper boundary extracted from the Mott-Ioffe-Regel limit. This is a typical behavior of a bad metal. The measured behavior will be compared to the numerical simulations by Finite Temperature Lanczos Method (FTLM), Dynamical Mean Field Theory (DMFT) and Determinantal Quantum Monte Carlo (DQMC). The satisfactory agreement between all these approaches coherently states that in a wide high temperature regime ( $T > 0.3t$  for  $U=7.5t$  and  $n=0.83$ ), the resistivity of a Hubbard model can be understood only when temperature dependence of both diffusion constant and charge susceptibility (or respectively scattering rates and

static effects) are considered. I will further discuss in more detail the observed difference between the resistivities obtained by DMFT and by FTLM and demonstrate that the main origin of the difference are the vertex corrections.

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## **Exotic electronic states of the multi-layered cuprates revealed by laser-ARPES**



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I will introduce our recent ARPES studies of several multi-layered cuprates, which exhibit exotic electronic states coming from the charge nonuniformity over the multiple  $\text{CuO}_2$  layers. The possible coexistence of antiferromagnetism (AFM) and superconductivity (SC) is one of such intriguing properties, which has been suggested by NMR study. Whereas the single and double layered systems exhibit the famous phase-diagram with separated AFM and SC phases, the mixed region of these has been found to emerge in the underdoped regime with further increasing the number of  $\text{CuO}_2$  plane per unit cell. Most importantly, the deep inner plane of  $\text{CuO}_2$  in these systems is protected from the dopant layers, which induce the inhomogeneous in-plane electronic state. Therefore, the clean, thus ideal  $\text{CuO}_2$  plane is realized in the inner  $\text{CuO}_2$  plane, which would provide yet unveiled phase diagram, which is inherent but has been hidden so far in cuprates.



## Nanoscale devices to explore the phase diagram of high temperature superconductors



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The phase diagram of the cuprates superconductors is dominated by various nanoscale symmetry breaking orders, such as Charge Density Waves (CDWs) that are strongly intertwined with superconductivity.

In this contribution we present our recent experiments where we use newly engineered nanowires of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-y}$ , as a function of doping, to disclose the effects of local orders on the normal and superconducting properties of nanodevices.

We have found that untwinned and underdoped  $\text{YBa}_2\text{Cu}_3\text{O}_{7-y}$  nanowires, with thicknesses below 10 nm, show a strong normal state anisotropy already at room temperature and the disappearance of the pseudogap feature, in the  $R(T)$  transition, in the  $b$ -axis direction. In these samples Resonant Inelastic X-ray Scattering, RIXS experiments have revealed the absence of the CDW peak along the  $a$ -axis direction which points towards a strong correlation between the  $R(T)$  behavior and the charge density wave order. Analogously the nanowire superconducting properties are also affected. The switching voltage, in the current voltage characteristic, connected to the quasiparticle diffusion time, is anisotropic and strongly dependent on the doping, reaching the maximum value close to optimal doping. These findings clearly show that transport properties of nanodevices, at extreme length scale, encode the properties of local orders which might shed new insights into the microscopic mechanism for high critical temperature superconductivity.

## Current-induced atomic diffusion limits the dissipative state of high temperature superconducting bridges



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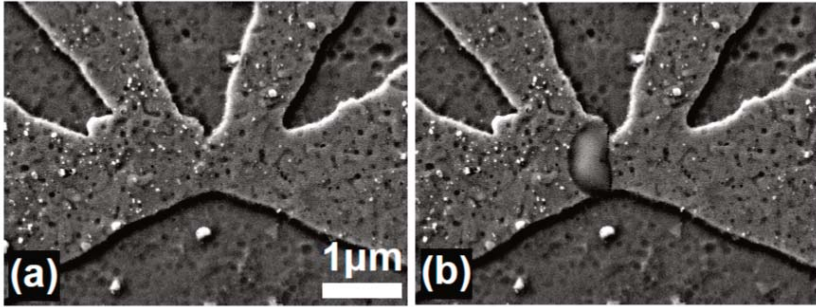
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**Keywords:** electromigration, resistive switching, electric field oxygen doping, superconductor-insulator transition

The current stimulated atomic diffusion in  $\text{YBa}_2\text{Cu}_3\text{O}_7$  superconducting bridges is investigated. A superconductor to insulator transition can be induced by direct current controlled electromigration process whereas partial recovery of the superconducting state can be achieved by inverting the polarity of the bias. Interestingly, the temperature dependence of the current density  $J_m(T)$ , above which atomic migration takes place intersects the critical current density  $J_c(T)$  at certain temperature  $T^*$ . Therefore, for  $T > T^*$  the superconducting dissipative state cannot be accessed without leading to irreversible modifications of the material properties. This phenomenon may also become an important mechanism of local sample deterioration in high critical temperature superconducting lms abruptly penetrated by thermomagnetic instabilities.



Scanning electron microscopy images of (a) a virgin sample (before electromigration) and (b) after electromigration failure.

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## Study of dissipation in hybrid ferromagnetic Josephson junctions



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**Keywords:** Hybrid Josephson junctions, phase dynamics, macroscopic quantum phenomena

The interfacial coupling of two materials with different ordered phases, such as a superconductor (S) and a ferromagnet (F), is driving new fundamental physics and innovative applications. Examples are: the possibility to switch the ground state of a Josephson junction (JJ) from a 0 to a  $\pi$  phase state, the existence of JJs having a doubly degenerate ground state with an average Josephson phase  $\psi = \pm\varphi$ , the possibility to carry spin-triplet supercurrent in the presence of certain types of magnetic inhomogeneity. Therefore, Josephson coupling between superconductors and ferromagnetic layers is providing new solutions for superconducting electronics and quantum circuits [1].

We will report on a comprehensive study of dissipation in ferromagnetic Josephson junctions composed by pure metallic ferromagnetic layers (SFS) [2], by an insulating barrier and a ferromagnetic metallic layer (SIFS) [3], and by a ferromagnetic-insulator barrier (SIFS) [4,5]. Through measure-

ments of switching current distributions, different dissipation sources can be highlighted, reflecting different properties of the barriers and of the composition of the junctions. This study provides the electrodynamic characterization [2,6] necessary for the possible use of these systems in more complex circuits, as cryogenic memories or spintronic devices, and suggests new solutions of hybrid JJs in superconducting qubits.

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## **Superconducting proximity effect in half-metallic ferromagnetic lateral Josephson junctions**



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It is established that spin-triplet superconducting correlations can emerge at s-wave superconductor/ferromagnet interfaces [1,2]. With the exception of a few experiments using half-metallic ferromagnets [3-5], the majority of experiments have focused on triplet pairing in transition metal ferromagnets which have a spin-polarization of less than 50% at the Fermi energy. Here we report lateral Josephson junctions with the half-metallic ferromagnetic manganite  $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$  (LCMO) with and without spin-mixer interfaces of  $\text{SrRuO}_3$  (SRO113) and Nb superconducting electrodes.

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## Signatures of fluctuating nematic order in YBCO nanostructures



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**Keywords:** YBCO, nanowire, noise, nematicity

The microscopic origin of superconductivity and the related phase diagram of High Critical Temperature Superconductors (HTS) is far from being fully understood. During the last few years Charge Density Wave (CDW) order has been ubiquitously observed in these materials unifying the behavior of the various HTS compound families [1]. Recently, transport measurements have been instrumental to detect signatures of CDW [2,3]. In this respect resistance noise measurements can be a powerful tool to understand the properties of these materials in the phase under study and to detect symmetry breaking orders [4,5]. Here we present resistance noise measurements performed on  $\text{YBa}_2\text{Cu}_3\text{O}_{7-y}$  (YBCO) nano-structures, as a function of temperature and hole doping? Our measurements reveal a clear indication that oxygen dynamics is the dominant mechanism responsible for the  $1/f$  flicker noise [6]. The noise also shows unexpected strong two level fluctuators (TLFs) with distinct characteristic activation energies. These TLFs can be studied by performing cross-correlation noise measurements on YBCO X-bars Fig.1(a). The measurements show anti-correlation in the spectral phase, this points to a symmetry breaking characteristic of fluctuations in a nematic ordered phase (e.g. CDW).

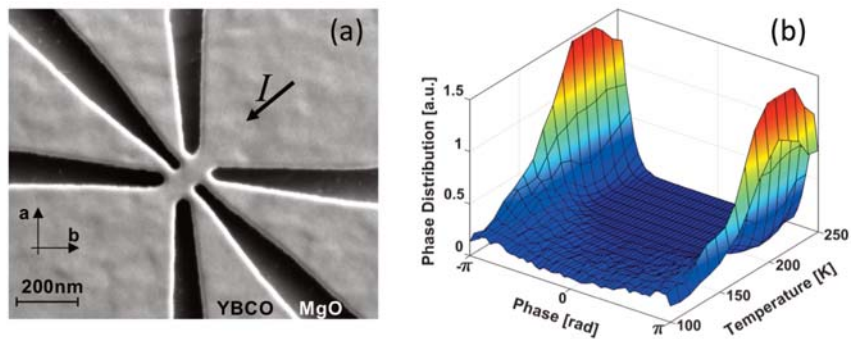


Fig. 1: (a) SEM picture of a measured device. The current bias flows along I, the voltage is measured simultaneously along  $V_{a+-}$  and  $V_{b+-}$ . (b) Phase distribution of the cross-correlated spectra as function of temperature. The phase collects around  $\pi$  for the temperature where the TLF are pronounced as expected for anti-correlated noise, giving indication of nematic order.

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## Particle-hole crossover in the vortex cores of the multi-band superconductor FeTeSe



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**Keywords:** Vortex core, pnictides, STM, disorder

The Abrikosov vortices in fully gapped type-II superconductors host bound electronic states, which can be probed with the scanning tunneling microscope. In most materials, these states form a quasi-continuum and cannot be individually resolved. In the quantum regime, however, the size of the vortices is comparable with the Fermi wavelength and the theory predicts experimentally resolvable discrete levels. Recent experiments [1,2] have reported vortex spectra with discrete levels for the iron-chalcogenide  $\text{FeTe}_{0.55}\text{Se}_{0.45}$ . This low-density multi-band system with nearly compensated electron and hole carriers realizes the quantum regime. It is furthermore microscopically disordered, which is expected to affect the vortices due to their small sizes. We present a microscopic multi-band tight-binding model to describe  $\text{FeTe}_{0.55}\text{Se}_{0.45}$  and investigate the discrete vortex-core states. We determine their angular momenta and observe a crossover from hole-like to electron-like behavior with increasing energy, a feature that is peculiar to multiband systems. We also find that the vortex properties are only weakly affected by the chemical disorder and we study how the observed disorder in vortex positions influences the vortex-core spectroscopy.

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## **Non-equilibrium vortex states in the high-temperature superconductors caused by current and magnetic impulses**



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**Keywords:** High-temperature superconductors, numerical simulation, Monte-Carlo method, current impulse, vortex states

Numerical modeling of the vortex system in a layered high-temperature superconductor under the influence of short-time impulses of the transport current as well as magnetic field are carried out. The calculations were performed by the Monte Carlo method in the framework of a two-dimensional model of a layered high-temperature superconductor. It is assumed that the vortices enter the superconductor under the influence of the intrinsic field of the transport current at the sample boundary. The algorithm is realized taking into account the processes of creation, annihilation, motion of vortices and annihilation of a pair of vortices of the opposite sign in the center of the sample. The electric field strength in the superconductor was calculated from the energy released during annihilation at the center of the vortices of the opposite sign, the value of which is proportional to the number of pairs annihilated during the calculation. For the critical current is accepted, at which the field strength is 1 mV/cm. The results of calculations show that in a pulsed regime, a superconductor can withstand a current several times higher than the critical current, determined from the current-voltage characteristic. The dependences of the threshold pulse duration on its amplitude are calculated, as well as the maximum values of the current flowing through the superconductor without the release of energy. The influence of various parameters of artificial pinning centers on the threshold duration and pulse amplitude is analyzed. The cases of a regular (rectangular

and triangular lattice with different periods) and a chaotic arrangement of defects are considered. It is shown that a regular lattice of defects can lead to a decrease in the threshold amplitude and pulse duration. Vortex configurations that arise when a current pulse is applied to a superconductor are obtained.

The research was done under support of Russian Foundation for Basic Research (grant 17-29-10024).

## Superconducting vortex clusters in S/F hybrids



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**Keywords:** Vortex/antivortex, S/F topological defects, MFM

We used low temperature scanning probe microscopy techniques to investigate superconducting vortex confinement in planar Superconductor/Ferromagnet (S/F) heterostructures realized by Nb/Py thin films. In these systems, new physical phenomena can be observed due to the interaction between superconducting vortices in Nb layer and the periodic, stripe-like, Py magnetic domains.

In general, the arrangement of superconducting vortices in bulk superconductors is only set by their reciprocal repulsion, which leads to a hexagonal vortex lattice formation, also called “Abrikosov lattice”. Nevertheless, when a confinement potential is imposed to the superconductor, the vortex distribution may result strongly affected. In particular, in presence of a ferromagnetic template underneath the superconductor, the nucleation of vortex chains and vortex clusters have been reported.

In this framework, we studied vortex clusters pinned at the bifurcations of stripe-like magnetic domains by using magnetic force microscopy (MFM) and scanning tunneling microscopy and spectroscopy (STM/STS). Mag-

netic imaging of such dislocations, above and below the  $T_c$  critical temperature, is crucial to get insight into both their magnetic topology and their confinement power for superconducting vortices. Indeed, low temperature MFM experiments allow the imaging of superconducting vortices being sensitive to the magnetic field decay from the normal vortex core, on the scale of the London penetration depth  $\lambda$ . On the other hand, once the magnetic structure is known, low temperature STM/STS, sensitive to the amplitude of the superconducting order parameter rather than the magnetic profile, allows detailed measurements of the electronic density of states outside and inside the vortex core, with a sub-nanometric spatial resolution. We find that intrinsic bifurcations of the stripe-like magnetic pattern can act as confinement sites for superconducting vortices. Such dislocations, can be particularly effective for vortex pinning because of the local enhancement of the magnetic out-of-plane stray field as well as because of their peculiar magnetic topology.

## Two-dimensional topological superconductivity in Pb/Co/Si(111)



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The examination of supposedly well-known condensed matter systems through the prism of topology has led to the discovery of new quantum phenomena that were previously overlooked. Just like insulators can present topological phases characterized by Dirac edge states, superconductors can exhibit topological phases characterized by Majorana edge states. Two-dimensional (2D) superconductors are expected to exhibit propagating Majorana edge states characterized by a Dirac-like dispersion. We have recently observed some hint of dispersive Majorana edge states in a single atomic layer Pb superconductor coupled to a buried Co-Si nano-magnet [1]. In addition to their dispersive edge states, 2D topological superconductors are also supposed to support Majorana bound states localized on topological defects, our recent measurements seem to support this theoretical prediction [2].

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## **In-gap excitations due to defects in topological superconductor with spin-orbit coupling**



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**Keywords:** spin-orbit coupling, magnetic texture, monoatomic layer, topological defect, vortex, Majorana pair

Recent microscopy experiments on superconducting monolayer of lead (Pb) grown over clusters of cobalt atoms have raised urgent questions about in-gap electronic states in presence of strong spin-orbit coupling and magnetism. Using analytics and numerics we find that a topological defect in Rashba spin-orbit coupling (in contrast to a vortex in superconducting pairing) fully explains puzzling features of this experiment: 1) Two different zero-modes, one point-like at center of island and the other ring-shaped around it; 2) The zero mode pair is protected by a large energy gap; 3) The localization lengthscale inside the island is far smaller than superconducting coherence length, but comparable to it outside. The theory predicts that this is a Majorana pair, with remarkable isolation in energy thanks to the defect in strong spin-orbit coupling.

We discuss the role of magnetic textures in our theoretical scenario.

## **Formation of the Majorana bound states on defects**



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**Keywords:** Majorana bound states, impurities, defects

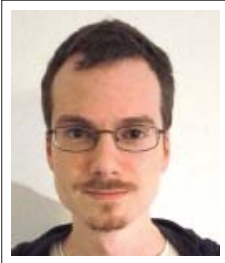
Zero-energy Majorana bound states can emerge at the edge of a low dimensional systems [1]. Due to the Non-Abelian statistics of such states, Majoranas are a good candidate for the realization of qubit for topological quantum computer. However, If they are to be used in creation of quantum computer, it is crucial to obtain an intentional creation and manipulation of this type of bound states. We show such a possibility in a setup of several systems (e.g. optical trap [2] or quantum dot-nanoring [3] hybrid system) in which we artificially create a ‘defect’ (inhomogeneity) region via electrostatic means. In such scenario, apart from non-trivial Majorana bound states, some trivial states like Andreev bound states can also be detected. We study the differences between those bound states and the possibility of their manipulation.

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## Experimental results on the predicted Weyl semimetal PrAlGe



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**Keywords:** Topology, Hall Effect, Magnetization, Neutron Scattering

Topological materials have many interesting properties and are the focus of intense theoretical and experimental research. The material PrAlGe has recently been predicted to be a Weyl semimetal with broken time reversal and inversion symmetries [1]. We present experimental results on various properties of PrAlGe single crystals such as magnetization, neutron diffraction, and electrical transport with a focus on the origin of the anomalous Hall effect. This data is compared to theoretical calculations involving the Berry curvature of the Weyl nodes in the system and interpreted in light of other recent measurements of topological materials [2, 3].

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## Topologically protected Majorana zero modes around the edge of a magnetic skyrmion



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**Keywords:** Majorana fermions; Topological superconductors; skyrmions

Magnetic skyrmions are topological spin textures currently at the forefront of research in spintronics because of their fundamental properties as well as their possible applications for memory devices. From another perspective, the question of the interplay of magnetic textures and superconductivity has naturally arisen as attempts to engineer topological superconductivity intensify. In that context, previous work has shown that magnetic skyrmions can host a Majorana zero mode (MZM) in their core when proximitized by a conventional s-wave superconductor. In contrast, we find a highly degenerate flat band of Majorana zero modes on the edge of the skyrmion that is robust to local perturbations be they electronic or geometric. We show that these states can be interpreted as the topologically protected end states of Rashba wires. In addition, the number of MZMs in the flat band surprisingly grows linearly with the perimeter of the edge of the texture, irrespective of its precise shape. In turn, this implies that the MZM are localized on the nanometer scale which potentially allows for their individual addressing. We finally argue that the system considered here implements a Majorana island suitable for the experimental realization of the topological Kondo effect and of electron “teleportation” and suggest possible physical realizations.

## Topology-controlled thermopower oscillations in multiterminal Andreev interferometers



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**Keywords:** Quantum coherence, thermoelectric effect, Josephson effect, Aharonov-Bohm effect, non-equilibrium superconductivity

We theoretically investigate coherent oscillations of the thermopower  $S$  as a function of the magnetic flux  $\Phi$  in six-terminal Andreev interferometers. We demonstrate that the thermopower behavior is determined by a number of contributions originating from the Josephson-like and Aharonov-Bohm-like effects as well as from electron-hole asymmetry. The relative weight of these contributions depends on the relation between temperature, voltage bias and an effective Thouless energy of our setup. We particularly emphasize the role of the system topology that may have a dramatic impact on the behavior of  $S(\Phi)$ .

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## Three dimensional Dirac electrons in antiperovskites



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The  $A_3BO$  type antiperovskites ( $A=Ca, Sr, Ba$ ;  $B=Sn,Pb$ ) are a relatively new class of topological material which host bulk three-dimensional (3D) Dirac electron as well as symmetry-protected surface states. Because of the variety in a possible composition, designing the property of Dirac electron could be envisaged simply by a composition control, or ultimately by using an artificial heterostructure. To this end, we have developed the epitaxial technique for the growth of antiperovskites  $Sr_3PbO$  and  $Sr_3SnO$ .

In this presentation, we first introduce the growth strategy and chemistry of MBE grown antiperovskites. In particular, we utilize X-ray photoelectron spectroscopy (XPS) to uncover an unusual valence state of Pb and Sn. Next, we focus on the low temperature magnetotransport which exhibits quantum interference effects. The results point to the role of real spin texture originating from a unique orbital texture in Dirac electrons. The importance of valley degree of freedom is emphasized to disentangle pseudospin and real spin physics.

## Charge trapping and super-Poissonian noise centers in a cuprate superconductor



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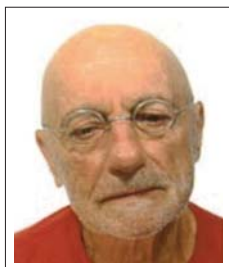
**Keywords:** high-temperature superconductors, noise spectroscopy, STM

I will present evidence for highly polarizable insulator properties in a cuprate high-temperature superconductor through novel, atomic-scale noise spectroscopy. Our results indicate that charge can be trapped on macroscopic timescales in the cuprates and provide new insight into the mystery of their highly anisotropic transport characteristics. Above the superconducting transition these materials are perfectly metallic along the crystal planes (ab-plane), but are insulating in the c-axis, with ratios exceeding 104. We employ our newly developed scanning noise spectroscopy technique [1] and discover surprising deviations from the expected Poissonian noise of uncorrelated electrons. Such behavior can only happen in highly polarizable insulators and represents strong evidence for trapping of charge in the charge reservoir layers of the cuprates [2]. I will discuss how this connects to the physics of the cuprates including the c-axis transport characteristics.

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## **Intrinsic structure of composites in superconducting systems**



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Collective excitations in superconducting systems can be described in terms of fermionic composites. Such objects, including the composite representing the Goldstone mode, are not point-like. I present a general method to determine their intrinsic structure.

## Near room temperature superconductivity in hydrides at high pressures



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**Keywords:** high temperature superconductivity, high pressure

We will present our recent results on the high temperature superconductivity [1-3] in different hydrides. The superconductivity has been proved by observation of zero resistance, Meissner effect, isotope effect, and X-ray diffraction studies [4]. Recent results on infrared and Raman studies will be presented. Pure hydrogen also will be discussed. The observed apparently conventional superconductivity will be discussed in view of numerous theoretical works. Recent proposals of new superconducting materials and prospects for achieving higher critical temperatures of superconducting transition will be discussed too.

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## Near room-temperature superconductivity in superhydrides at megabar pressures



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Recent predictions and experimental observations of high  $T_c$  superconductivity in hydrogen-rich materials at very high pressures are driving the search for superconductivity in the vicinity of room temperature [1,2]. We confirmed the existence of a new class of such materials – superhydrides ( $MH_x$ , with  $x > 6$ ) – and developed preparation techniques for their syntheses and characterization, including measurements of structural and transport properties, at megabar pressures. Four-probe electrical transport measurements of lanthanum superhydride samples display signatures of superconductivity at temperatures ranging from 150K to above 260K near 200GPa. The experiments are supported by pseudo-four probe conductivity, critical current determinations, and low-temperature x-ray diffraction measurements. These measurements of near-room temperature superconductivity are in good agreement with density functional and BCS theory-based calculations.

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## **High field probe of superconducting order in high-*t*c hydrides**

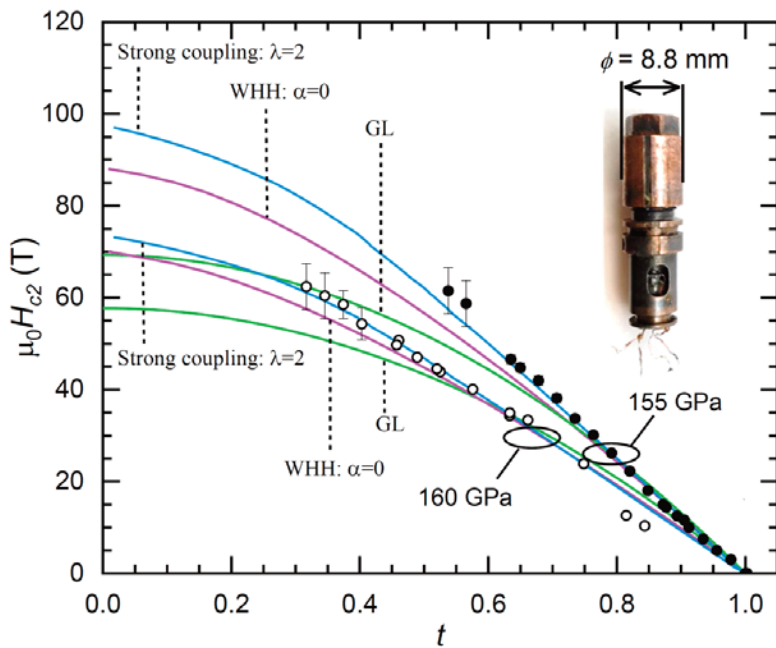


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**Keywords:** Hydrides, superconductivity

A combination of diamond anvil cells and pulse magnets allows us to controllably tune and probe candidate systems at the extremes of pressure-field-temperature parameter envelope. Here we directly investigate the robustness of the superconducting order in sulphur hydride in magnetic fields as high as 65T. Sulphur hydride forms a metallic phase and becomes superconducting at temperatures as high as 203 K at 155 GPa [1,2]. Magnetotransport measurements of the superconducting phase-diagram under high magnetic fields could provide detailed information about underlying superconducting coupling. We find experimentally determined characteristic critical field to be in close agreement with the Werthamer, Helfand, and Hohenberg (WHH) formalism in the vicinity of the superconducting transition, while noticeable deviations from WHH appear at experimental limit of 65 T [3]. The projected zero-temperature upper critical field surpasses 100T.

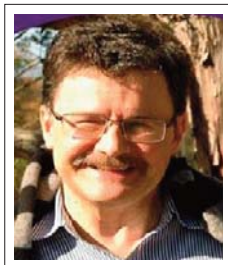


Upper critical fields as a function of reduced temperature for the superconducting sulfur hydride samples under 155 GPa and 160 GPa pressure. Solid lines are fits to different theoretical models: Ginzburg-Landau (GL), Werthamer, Helfand and Hohenberg (WHH), and strong-coupling model. Inset: high pressure diamond anvil cell with sulfur hydride sample used in this study.

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## Structure and composition of novel polyhydrides at high pressures



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**Keywords:** polyhydrides, structure, high pressure, superconductivity

Synchrotron X-ray diffraction, IR spectroscopy, and Raman spectroscopy have been used to study chemical reactions of molecular hydrogen with various elements at high pressures [1-3].

We synthesized selenium trihydride at 5 GPa and found that it is stable up to 40 GPa at 100-200 K, similar to Cccm H<sub>3</sub>S.

The results for tellurium polyhydride will be reported at the meeting. Inspired by theory predictions, we have synthesized a number of novel uranium polyhydrides in addition to a well-known alpha-UH<sub>3</sub> and beta-UH<sub>3</sub>. These include fcc UH<sub>5</sub> and UH<sub>8+y</sub> and hcp UH<sub>5</sub> and UH<sub>7</sub>.

The results for other polyhydrides including those of rare-earth elements will be discussed at the meeting concerning to recently discovered high-temperature superconductivity [3].

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## Puddles in superconductors: a phenomenon which reaches from low- $T_c$ to high $T_c$ superconductors



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**Keywords:** polarons, multi-component superconductivity, perovskites

High- $T_c$  superconductors HTS [1] cuprates [2,3] diborides, [4-6] pnictides [7] and pressurized hydrides [8] are made of multiple electronic components [9,10]. While it is rather well established that HTS show spatial inhomogeneity made of puddles emerging from CDW order with filamentary superconductivity in a hyperbolic space [11,12], this concept has not been used for low  $T_c$  BCS type systems.

Here we show, that the extremely low carrier density multigap superconductor, doped  $\text{SrTiO}_3$  [13], is not a homogeneous system, but is highly inhomogeneous consisting of charge rich metallic filaments embedded in a polar matrix. Only, as long as this coexistence remains, superconductivity survives. This is confirmed experimentally by probing two identically doped crystals for superconductivity where one part is polished and thus has only few filaments, whereas the other is roughened with increased filament density. In addition, the embedding matrix surrounding the filaments is shown to be polar and insulating with a crossover regime in the contact region. This is proven by local piezoelectric measurements which confirm the polar character of the matrix. Further support is derived from theory which predicts that local lattice modes soften reminiscent of ferroelectricity. A schematic sketch of this scenario is shown in Figure 1.

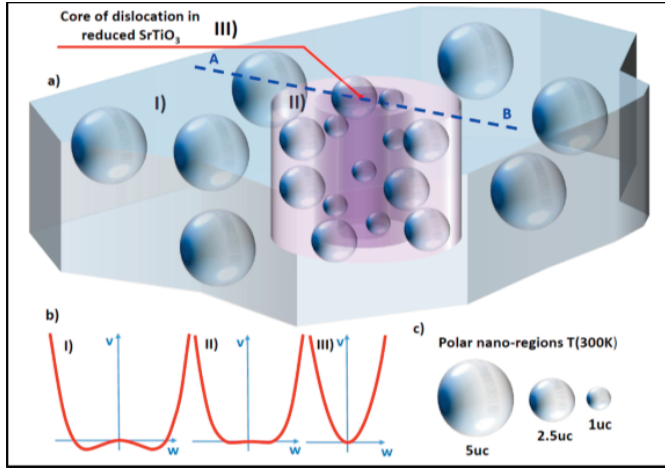


Figure 1. Sketch of the distribution of polar nano clusters in reduced STO (insets a, and the corresponding local potential b-I), close to the conductive core of the dislocation (insets a, with the potential b-II) and inside the core (insets a, and potential b-III).

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## **Normal and superconducting states of cuprates: an emergent Bose liquid?**



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Besides the puzzling high-temperature superconductivity, cuprates also features numerous unusual normal-state properties. This talk will present a simple picture of an emergent Bose liquid (EBL) and demonstrate several non-Fermi liquid characteristics of EBL that seems to capture the essence of the normal and superconducting states of cuprates. These include: 1) bad metal behavior (linear resistivity beyond the Mott limit), 2) mid-infrared features in optical conductivity, 3) non-Fermi liquid scattering rate, 4) zero-temperature phase diagram, 5) diminishing superfluid stiffness at high doping, and 6) weak doping dependence of superconducting gap. The similarities in these highly unusual characteristics [1-4] suggest strongly that cuprates are a prototype of EBL, and EBL might often take place in strongly correlated materials that complements the standard textbook Fermi liquid in condensed matter systems.

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## Hourglass magnetic dispersion and nature of the spin liquid phase in cuprates



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**Keywords:** Hourglass dispersion, spin liquid

We resolve the problem of the magnetic ground state and magnetic excitations in underdoped cuprates. Modelling cuprates by the extended t-J model we show that there is a dimensionless parameter  $\lambda$  which drives magnetic criticality. Hence we derive the zero temperature  $\lambda$ - $x$  phase diagram ( $x$  is doping).

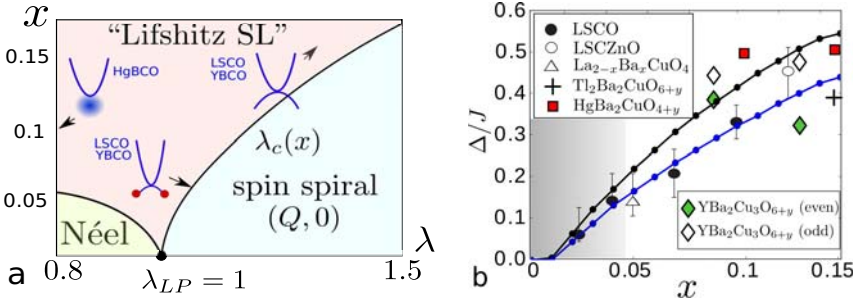
We argue that all underdoped cuprates are close to the quantum tricritical point  $x=0$ ,  $\lambda=1$ .

The three phases “meet” at the tricritical point:

- (i) Neel antiferromagnet,
- (ii) Spin spiral,
- (iii) Algebraic spin liquid similar to the Ioffe-Larkin spin liquid in frustrated magnets.

Underdoped cuprates belong either to the spin liquid phase or they are on the borderline between the spin liquid and the spin spiral.

We explain the hourglass magnetic dispersion and compare calculated dispersions with experimental data at different doping levels. We propose new experiments that can directly prove the developed theory.



A: Zero temperature  $\lambda$ - $x$  phase diagram consists of three phases, Neel, Ioffe-Larkin-type Spin Liquid, Spin Spiral. The tricritical Lifshitz point is  $\lambda=1$ ,  $x=0$ .

Blue lines indicate different types of hour-glass dispersion.

B: The spin liquid gap versus doping. Solid lines represent theory, two lines indicate an uncertainty. Points show experimental data.

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## **Evolution of the spin excitations in doped cuprates**



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**Keywords:** cuprates, Hubbard, spin excitations, spectroscopies

Understanding the interplay between spin and charge degrees of freedom lies at the heart of the “cuprate problem”. In this talk we summarize our recent works on the problem of the evolution of the collective spin excitations in the doped cuprates. We start by showing that the Hubbard model [1, 2] is enough to explain this phenomenon. Next, we present how a finite next nearest neighbor hopping as well as the lattice dimensionality influences the Hubbard model result [3]. Finally, we show that one can easily understand the evolution of the spin excitations in the 1D models [4] and discuss whether one can use this result to understand the 2D cuprate case.

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## Fingerprints of Mn12: the forefather of molecular nanomagnets



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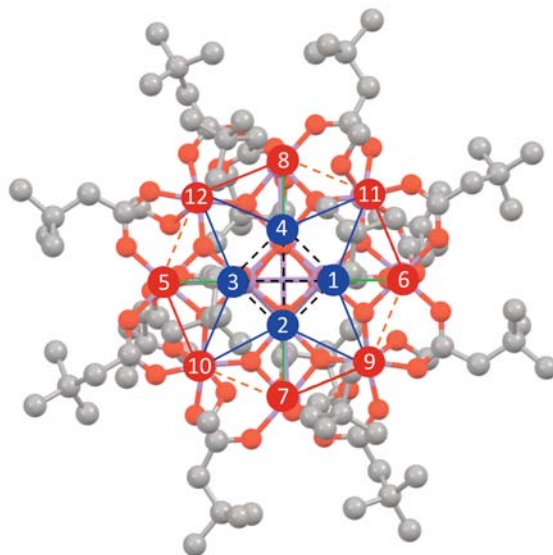
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**Keywords:** molecular magnetism, exchange interaction, neutron scattering

Inelastic neutron scattering (INS) is a very effective tool to study the spin correlations and dynamics in molecular nanomagnets and it allows to obtain the details of the microscopic interactions. The magnetic properties of complex polycentric molecules are often not completely understood due to the difficulty to determine the exchange interactions between the magnetic ions. I will show how neutron scattering measurements have been crucial to understand the magnetic behaviour of the prototypical Mn12 single molecule magnet. Despite the fact that Mn12 is the forefather and most studied of all molecular nanomagnets, an unambiguous determination of even the leading magnetic exchange interactions has been lacking for long time. We exploited four-dimensional inelastic neutron scattering to portray the spin precession patterns in Mn12, which are unambiguous fingerprints of the magnetic Hamiltonian. A thorough analysis of the INS data has allowed to fix the exchange couplings of Mn12 for the first time [1].



Structure of the Mn<sub>12</sub> cluster (Mn: purple; O red; C: grey; H omitted for clarity). The overlying schematic indicates the different exchange interactions (lines) between Mn<sup>4+</sup> (blue circle) and Mn<sup>3+</sup> (red circle) ions.

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## Entering the quantum Griffiths phase of a disordered superconductor



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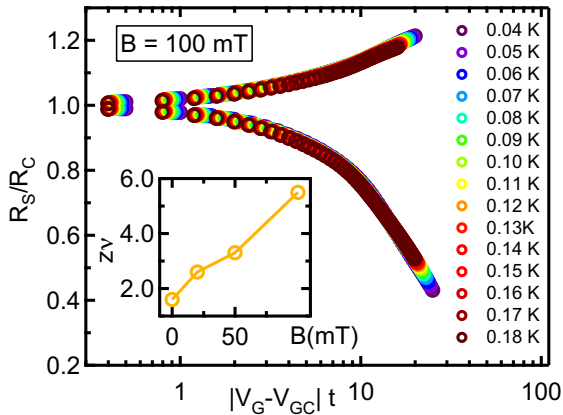
**Keywords:** oxide interface, quantum phase transition

A Quantum Phase Transition (QPT) from an ordered phase to a disordered one is described by critical exponents which characterize the divergence of the spatial and temporal coherence length when approaching the transition by tuning a parameter in the Hamiltonian [1]. These exponents characterize universality classes which depend of the physics of the system. Under certain circumstances, rare large fluctuations and the corresponding spatial regions, such as for instance large clusters of ordered phase in the disordered one, play an important role. They cause so-called Griffiths singularities which deeply change the phase diagram in the vicinity of the QPT [2]. The critical region, named Griffiths phase, extends, and the critical exponents themselves diverge at the critical point.

We studied the Superconductor-Insulator Transition that occurs in the two-dimensional electron gas (2-DEG) at  $\text{LaAlO}_3/\text{SrTiO}_3$  interface using two parameters: the carrier density electrostatically modulated by a gate voltage VG [3] and a perpendicular magnetic field B [4]. We showed that the critical exponents measured when the SIT is driven by VG, change with the mag-

netic field: they diverge when  $B$  is increased, as if the magnetic field controls the Griffiths character of the system (cf Figure). We analyzed the resistive transitions as a function of temperature for all possible VG and  $B$  values. We know from previous studies that the system is made of superconducting puddles embedded in normal regions [4]. When the magnetic field is turned on, we evidence the development of rare superconducting regions obeying a Levy statistics typical of rare events, accompanying the divergence of the critical exponents. Random Resistance Network simulations confirm this finding [5].

We report therefore for the first time the progressive transition from a non-Griffiths to a Griffiths phase in an experimental system, with a divergence of the critical exponents and the development of rare events.



Scaling of the resistance as a function of the gate voltage, under a magnetic field of 100 mT. Inset : critical exponent product as a function of the magnetic field.

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## STM/STS imaging of energy gaps and their related superstructures in high-Tc cuprate Bi2212



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STM/STS experiments have been performed in underdoped (UD) and optimally-doped (OP) crystals of Bi-based high-Tc cuprate Bi2212. In many cases of STM/STS experiments on UD Bi2212 crystals, the observed bias-dependences of tunneling conductance, the so-called “STS spectra,” are consistent with two-gap structure consisting of a d-wave SC gap (SCG) and a spatially inhomogeneous pseudogap (PG), whose size varies in nanometer scale over a wide range from an energy of the SCG amplitude to several times larger one. In such UD crystals, we confirmed that checkerboard modulation (CBM) [1-3] and unidirectional Cu-O-Cu bond-centered modulation (BCM) [4] are observed in conductance images at low energies around the SCG and high energies around the PG, respectively; the two electronic superstructures with different characteristic energies coexist with each other in real space [3].

On the other hand, no CBM and BCM are observed on some cleaved surfaces of OP Bi2212; STS spectra exhibit homogeneous single d-wave like SCG structure within the areas examined. In such OP crystals, we demonstrate that the overall SCG on the entire Fermi surface changes along the b-axis with an amplitude of ~6% of its average and the same period as in the one-dimensional superlattice, which has been predicted in theoretical studies to cause periodic modulation of the antiferromagnetic coupling between Cu-spins [5, 6].

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## Mechanism for pressure driven transitions between itinerant ferromagnetism and antiferromagnetism in correlated materials



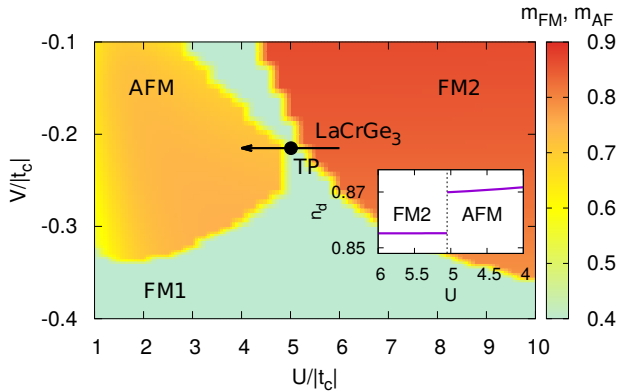
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**Keywords:** antiferromagnetism, ferromagnetism, phase transition

Recent discovery in itinerant ferromagnet  $\text{LaCrGe}_3$  of a pressure-induced phase transition to an antiferromagnetic state [1] raises a question of an underlying mechanism.



Magnetic phase diagram on the interaction - hybridization,  $U$ - $V$  plane. Color scale denotes total ordered magnetic moment in each phase. An arrow marks a direction (for  $V=-0.21$ ), associated with  $\text{LaCrGe}_3$  under pressure, encompassing FM to AFM transition accompanied with an increase of  $d$ -orbital filling (cf. inset).



We propose a novel theory for a switching between ferromagnetic and antiferromagnetic groundstates valid for  $d$ -electron magnets, a Stoner-like microscopic mechanism [2], that relies on a very generic electronic structure properties shared by a number of materials. We show that restricted mechanism is applicable also to f-electron USb<sub>2</sub> [3] where reverse transition has been observed [4].

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## **Coupling between dynamic magnetic and charge-order correlations in the electron-doped cuprate NCCO.**



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Charge order has now been observed in several cuprate high-temperature superconductors. We report a resonant inelastic x-ray scattering experiment on the electron-doped cuprate  $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$  that demonstrates the existence of dynamic correlations at the charge-order wave vector. Upon cooling we observe a softening in the electronic response, which has been predicted to occur for a d-wave charge order in electron-doped cuprates. At low temperatures, the energy range of these excitations coincides with that of the dispersive magnetic modes known as paramagnons. Furthermore, measurements where the polarization of the scattered photon is resolved indicate that the dynamic response at the charge-order wave vector primarily involves spin-flip excitations. Overall, our findings indicate a coupling between dynamic magnetic and charge-order correlations in the cuprates.

## **Ultrafast enhancement of charge density waves via laser-driven competition with superconductivity in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$**



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**Keywords:** charge density waves, superconductivity, cuprates, ultrafast , FEL, X-ray scattering

The use of ultrashort optical and X-ray pulses offers new opportunities to study fundamental interactions in materials exhibiting unconventional quantum states, such as stripes, charge density waves and high-temperature superconductivity. In this talk I will discuss recent ultrafast resonant X-ray scattering (RXS) experiments on  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  (YBCO) single crystals performed at the LCLS. Ultrashort infrared pulses produce a non-thermal quench of the superconducting state while X-ray detect the reaction of the charge density waves. A low fluences a transient enhancement of charge density waves is observed, directly revealing the interaction between the two order parameters on their natural timescales.

## **Thermodynamic quantum time crystals**



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Investigation of states with a periodic time dependence of observable physical quantities attracts a considerable interest now. Although it has been proposed initially that such states (coined Quantum Time Crystals) might be macroscopic and thermodynamically stable, results of a more careful study of the problem seemed to indicate that quantum time crystals could be realized only in systems out of equilibrium. Here we show that, in contrast to the general belief, thermodynamically stable macroscopic quantum time crystals can exist. The order parameter of this new state of matter is periodic in both real and imaginary time but its average over the phase of the oscillations equals zero. At the same time, certain correlation functions characterizing physical quantities oscillate periodically in time without any decay. An alternative interpretation of the results is based on a concept of an operator order parameter. Calculations are performed for a rather general microscopic model that may in particular be suitable for describing the pseudogap state in superconducting cuprates.

## A multi pulse optical study on anomalous nonequilibrium polarization dynamics above $T_c$ in organic superconductors



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**Keywords:** organic superconductor, time resolved pump-probe spectroscopy

Toward full understanding of high-temperature superconductivity (SC), unusual electronic properties in the normal state have been extensively studied in the organic superconductors. Recently, the optical time resolved pump-probe spectroscopy has shown that the anomalous nonequilibrium dynamics characterized by polarization anisotropy of probe photons appears well above the SC transition temperature ( $T_c$ ), implying emergence of pseudogap (PG). However, the origin of the PG is still unclear. In this study, to obtain further insight into the PG, the three-pulse pump probe spectroscopy has been carried out. In the measurement, by investigating the photoinduced carrier dynamics after irradiation of high-intensity pulses, we found that the recovery dynamics of the PG state is similar to that of the Mott insulating state, indicating that the origin of PG is involved with the Mott insulator.

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## Optical time-resolved studies of Bi-based cuprates with out-of-plane disorder



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**Keywords:** time-resolved spectroscopy; polarimetry; pseudogap.

Quasiparticle (QP) dynamics of high- $T_c$  cuprates observed by optical pump-probe technique have attracted attention because of the ability to identify the superconducting (SC) and pseudogap (PG) states. We have also demonstrated that polarized pump-probe scheme has the advantage of probing the rotational symmetry breaking of the states, where the polarization response with B<sub>2g</sub> symmetry can be identified as the PG state both in under-doped and over-doped Bi2212. In this work, we apply the technique to the study of nearly optimally doped samples. Here we measure the samples with different degrees of out-of-plane disorder induced by the Bi-Sr substitution. The results show gradual enhancement of the PG with increasing disorder, where the samples with large disorder show a well polarized transient response. On the other hand, the polarization responses of the less disordered samples show a mixture of the SC and PG states below  $T_c$ , suggesting an unstable relationship between the states in the homogeneous sample.

## Progress towards a universal approach for prediction of the superconducting transition temperature



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**Keywords:** Fermi energy; Fermi level; Fermi surface; k-grid; electronic topological transition; electron-phonon coupling; resonance.

To adequately relate electronic band structure and Fermi surface features to the superconductivity of materials, an appreciation of the role played by accurate, consistent and reliable values of calculated Fermi energies and positioning of Fermi levels [1] is required. In contrast to widespread practice that treat these values as arbitrary, they should be associated with the density of nearly free valence electrons. In addition, these values should be obtained using calculations with much finer k-grids than those typically reported in the published literature [1-4].

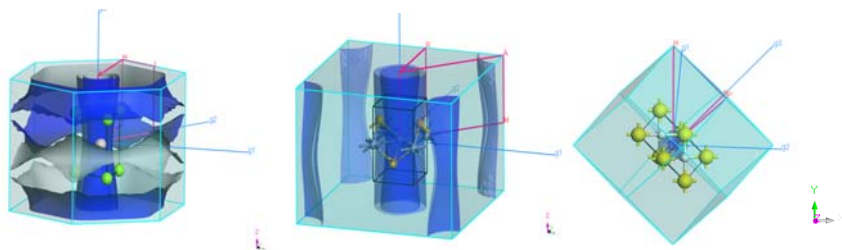
Many layered superconductor materials display Fermi surfaces with almost parallel tubular regions (in close, reciprocal space proximity), that are separated by a nearly constant reciprocal space vector (see Figure 1 left and centre). These parallel Fermi surfaces provide a suitable topology for a strong resonant coupling of electrons or quasiparticles to a dominant phonon mode, which can shift large sections of the corresponding electronic bands below and above the Fermi level at the frequency of the coupling phonon in nonadiabatic processes [1,5-9]. The coupling phonon is typically the most affected by external pressure, atomic substitutions, isotopes and other electronic effects.

Thus, the electron-phonon coupling works as an oscillatory deformation potential, which periodically breaks and restores the degeneracy of corresponding bands (at  $\Gamma$  for  $k=0$ ), and produces associated electron density re-

sponses between the adjacent bands with slightly different Fermi vectors  $k_F$  [5-6]. This electron-phonon coupling takes place via a prevalent phonon mode (which may also be degenerate) in layered structures and between bands involving primarily s and p electrons as is the case, for example, with  $MgB_2$  [4-8].

The structures and/or the orbital(s) character of the bands involved in this resonant coupling of highly covalent bonds increases in complexity, as d or f electrons with higher angular orbital momentum become involved. In this case, covalent bond coupling becomes effective via a multiplicity of phonons or between multiple bands. Under these conditions, the oscillatory patterns of Fermi surface connectivity become more complex and co-exist with periodic appearance and disappearance in reciprocal space of new electron or hole pockets. In addition, electron spin and conservation rules for total angular momenta become more important and influential.

We show how reliable Fermi energy and Fermi surface topology determinations can simplify interpretation of superconducting phenomena and assist  $T_C$  prediction. For example, the deformation potential(s) or changes in electronic bands and Fermi surfaces induced by vibrations along key phonon modes could be interpreted as resonant, dynamic, temperature-driven electronic topological transitions. In these transitions, connectivity of the Fermi surfaces is periodically lost and subsequently restored. Furthermore, we show that the separation between parallel Fermi surfaces for layered superconductors is commensurate with superconducting properties such as the coherence length and  $T_C$  for a range of different compounds.



Calculated Fermi surfaces (FS) for  $MgB_2$  (left),  $FeSe$  (middle) and  $H_3S$  [10] with primitive cell and selected branches of the FS at 200 GPa (right).



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## Hard x-ray photoemission study of $\text{Ca}_2\text{RuO}_4$ under electric field



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**Keywords:** Ruthenate, multi-orbital system, insulator-metal transition, hard x-ray photoemission spectroscopy

The strongly correlated insulator  $\text{Ca}_2\text{RuO}_4$  exhibits the insulator to metal (IM) transition by applying weak electric-field and a record-giant diamagnetism under electric current flow. Using hard x-ray photoemission spectroscopy, we report the electronic structure of  $\text{Ca}_2\text{RuO}_4$  under electric-field. We reveal the insulating gap suppression and the reduction of spectral weight of lower Hubbard band derived from Ru  $4d_{xz=yz}$  orbitals by applying electric-field. The observed insulating gap suppression causes the non-linear conductivity. Furthermore, we propose the scenario that the electric-field gives rise to the elongation of compressed  $\text{RuO}_6$  octahedra. Our findings provide a new basis of understanding the mechanism of unusual giant diamagnetism.

## Direct measurements of energy levels in next generation nitride phosphors



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**Keywords:**  $\text{Eu}^{2+}$  luminescence, soft X-ray scattering, absorption and emission spectroscopy

Highly efficient narrow-band red emitting phosphors are the most desired and requested materials for developing illumination grade phosphor-converted light emitting diodes (pcLEDs) [1].

This research presents direct measurements of RE energy levels, critical to the color and efficiency of LED phosphors. Modern phosphors use the  $5d^1$  to  $4f^{n+1}$  transition [2] of  $\text{Eu}^{2+}$ , which is an excited state since  $\text{Eu}^{2+}$  has no 5d electrons in the ground state. Unlike the relatively localized 4f states, the 5d states are very sensitive to the surrounding crystal and therefore key  $\text{Eu}^{2+}$  luminescence parameters like wavelength and efficiency can be tailored by the choice of host lattice. However, the problem is that the energetic position of the  $5d^1$  was not possible to be measured directly.

For the first time, we experimentally directly determine the energetic separation of the Eu 5d state and the conduction band [3], which is the key indicator of quantum efficiency. This was achieved for the three next-generation pcLED phosphors  $\text{Li}_2\text{Ca}_2[\text{Mg}_2\text{Si}_2\text{N}_6]:\text{Eu}^{2+}$ ,  $\text{Ba}[\text{Li}_2(\text{Al}_2\text{Si}_2)\text{-N}_6]:\text{Eu}^{2+}$ , and  $\text{Sr}[\text{LiAl}_3\text{N}_4]:\text{Eu}^{2+}$  using resonant inelastic soft X-ray scattering. Furthermore we directly observe conduction to valence band and 4f to valence band transitions in X-ray excited optical luminescence spectra of  $\text{Sr}[\text{LiAl}_3\text{N}_4]:\text{Eu}^{2+}$  and  $\text{Sr}[\text{Mg}_3\text{SiN}_4]:\text{Eu}^{2+}$ .

These techniques are widely applicable and create a comprehensive, experimental picture of the important  $\text{Eu}^{2+}$  energy levels in these compounds,

leading to a complete understanding of all pertinent electronic processes. This study forms the base needed for a detailed discussion of the structure – property relationships, such as specific atoms, coordination and density of states, underpinning phosphor color, efficiency and quenching [4].

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## Screening of pair fluctuations in superconductors with coupled shallow and deep bands: a route to higher temperature superconductivity



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**Keywords:** two-band superconductivity; pair fluctuations

A combination of strong Cooper pairing and weak superconducting fluctuations is of crucial importance to achieve and stabilize high- $T_c$  superconductivity. Here we demonstrate that a coexistence of a shallow carrier band with strong pairing and a deep band with weak pairing, together with Josephson-like pair transfer between the bands to couple the two condensates [1-4], realizes an optimal superconducting multicomponent system: it preserves the regime of strong pairing to generate large gaps and very high pairing temperatures but screens the detrimental superconducting fluctuations, thus suppressing the pseudogap in the normal state. Surprisingly, we find that the screening is very efficient even when the pair-transfer coupling is considerably small. Thus, a multi-band superconductor with a coherent mixture of condensates in the BCS regime (deep band) and in the BCS-BEC crossover regime (shallow band) exhibits a promising route to obtain higher superconducting critical temperatures.

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## Experimental evidence for broken time-reversal symmetry in multi-band superconductors



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**Keywords:** multi-band superconductors, broken time-reversal symmetry (BTRS), Lifshitz transition, s+is

In general, magnetism and superconductivity are antagonistic to each other. However, there are several families of superconductors, in which superconductivity may coexist with magnetism, and only a few examples are known, when superconductivity itself induces a spontaneous magnetism. The most known compounds are p-wave  $\text{Sr}_2\text{RuO}_4$  and some noncentrosymmetric superconductors. Here, we report the finding of a narrow dome of a novel s+is' superconducting (SC) phase with broken time-reversal symmetry (BTRS) inside the broad s-wave SC region of the centrosymmetric multiband superconductor  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$  ( $0.7 < x < 0.85$ ). Spontaneous magnetic fields inside this dome we observe using the muon spin relaxation ( $\mu\text{SR}$ ) technique. Furthermore, our detailed specific heat study reveals that the BTRS dome appears very close to a change in the topology of the Fermi surface (Lifshitz transition). With this, we experimentally demonstrate the emergence of a novel quantum state at topological changes of the electronic system.

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## Edge effect pinning in mesoscopic superconducting strips with non-uniform distribution of defects



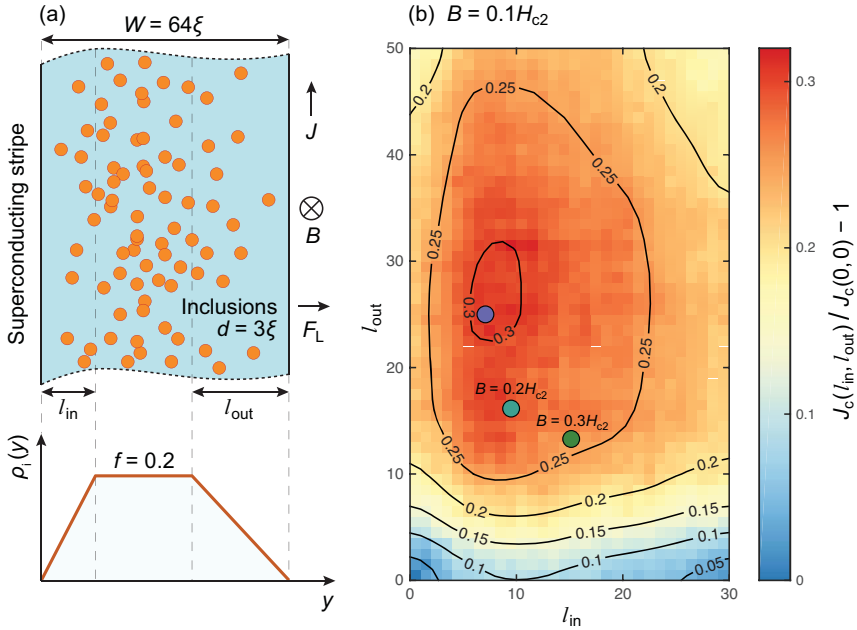
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Transport characteristics of nano-sized superconducting strips and bridges are determined by an intricate interplay of surface and bulk pinning. In the limiting case of a very narrow bridge, the critical current is mostly defined by its surface barrier, while in the opposite case of very wide strips it is dominated by its bulk pinning properties. Here we present a detailed study of the intermediate regime, where the critical current is determined, both, by randomly placed pinning and by the Bean-Livingston barrier at the edge of the superconducting strip in an external magnetic field. We use the time-dependent Ginzburg-Landau equations to describe the vortex dynamics and current distribution in the critical regime. Our studies reveal that while the bulk defects arrest vortex motion away from the edges, defects in their close vicinity promote vortex penetration, thus suppressing the critical current. We determine the spatial distribution of the defects optimizing the critical current and find that it is in general non-uniform and asymmetric: the barrier at the vortex-exit edge influence the critical current much stronger than the vortex-entrance edge. Furthermore, this optimized defect distribution has a more than 30% higher critical current density than a homogeneously disorder superconducting film.





(a) Defect distribution in the strip; (b) Map of the critical current as function of entrance and exit edges

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## Critical temperature enhancement from quantum confinement in niobium-doped strontium titanate thin films



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A precise solution of the quasi-2D problem for the mean-field critical temperature  $T_C$  at any electron density in a finite rectangular potential well reveals shape resonances induced by quantum confinement [1]:  $T_C$  oscillates as a function of well thickness and is enhanced compared to the bulk above a threshold confinement strength [2]. Such threshold is lower for low-density superconductors like doped strontium titanate (STO) thus favoring  $T_C$  enhancements in quasi-2D [3]. We fabricated niobium-doped STO thin films of different thickness at 1% doping, sandwiched between undoped STO, and performed transport experiments to measure the thin-film  $T_C$  and Hall carrier density.  $T_C$  is enhanced with decreasing thickness at constant 3D carrier density.

We analyze the system utilizing a two-band model for Nb-doped STO with pairing interaction reproducing the density-dependent bulk  $T_C$  [4,5]. We apply confinement in the square-well quasi-2D geometry and find a  $T_C$  enhancement in the thin-film limit. The theory quantitatively agrees with experiment, taking into account carrier density inhomogeneity in the films.

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## Nodeless superconductivity in type-II Dirac semimetal PdTe<sub>2</sub>: low-temperature London penetration depth and symmetry analysis

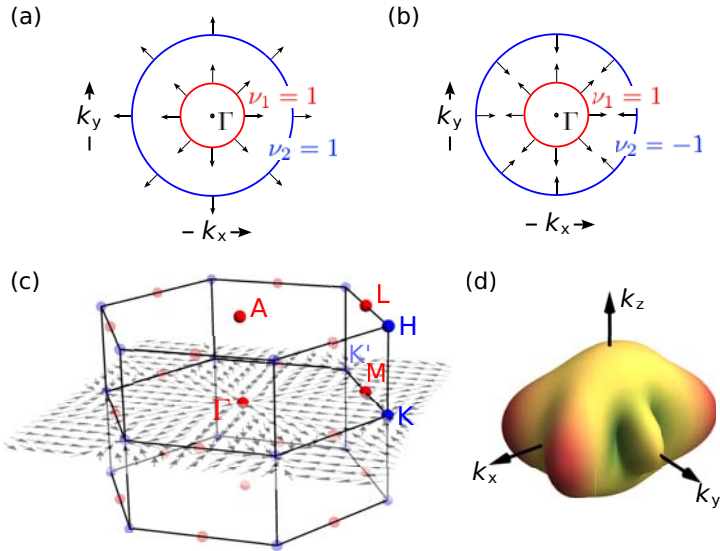


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**Keywords:** Dirac semimetals, multi-gap superconductivity, symmetry analysis, London penetration depth

Superconducting gap structure was probed in type-II Dirac semimetal PdTe<sub>2</sub> by measuring the London penetration depth using the tunnel diode resonator technique. At low temperatures, the data for two samples are well described by a weak-coupling exponential fit yielding  $\lambda(T = 0) = 230$  nm as the only fit parameter at a fixed  $(0)/T_c \approx 1.76$ , and the calculated superfluid density is consistent with a fully gapped superconducting state characterized by a single gap scale. Electrical resistivity measurements for in-plane and inter-plane current directions find very low and nearly temperature-independent normal-state anisotropy. The temperature dependence of resistivity is typical for conventional phonon scattering in metals. We compare these experimental results with expectations from a detailed theoretical symmetry analysis and reduce the number of possible superconducting pairing states in PdTe<sub>2</sub> to only three nodeless candidates: a regular, topologically trivial s-wave pairing, and two distinct odd-parity triplet states that both can be topologically nontrivial depending on the microscopic interactions driving the superconducting instability.



The triplet vector (black arrows) on the two Fermi surfaces (red and blue solid lines) enclosing the point is shown in (a), for the same sign of the order parameter on the two Fermi surfaces, and (b), for opposite signs, yielding a topologically non-trivial ( $\nu_1 + \nu_2 = 0$ ) and trivial state ( $\nu_1 + \nu_2 = 0$ ), respectively. In (c), we indicate the high-symmetry points, where the triplet vectors of the two candidate states,  $A1u$  and  $eu(1,0)$ , have to vanish as a consequence of inversion symmetry (red dots) and rotation symmetries (blue dots).

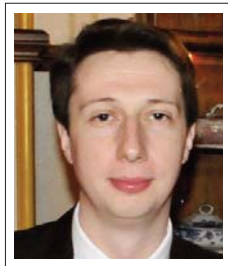
The gray arrows illustrate the (simplest) texture of the triplet vector of the  $A1u$  state in the  $k_z = 0$  plane (with minimal number of defects).

Panel (d) shows the directional dependence (i.e., anisotropy) of the gap of the  $eu(1,0)$  state on a Fermi surface enclosing the point. The distance of the surface to the origin is proportional to the magnitude of the gap. The state breaks the threefold rotation symmetry and its gap is, thus, generically anisotropic.

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## Dimensional Crossover and Topological Phase Ordering in Quasi-One-Dimensional Superconductors



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**Keywords:** Quasi-one-dimensional crystals, phase fluctuations, low-dimensional superconductivity, nanowire networks

Quasi-one-dimensional (q1D) materials composed of weakly-coupled one-dimensional (1D) filaments or stripes invariably undergo dimensional crossover to 2D or 3D behavior at sufficiently low temperature. If a q1D metal develops a superconducting instability, the phenomenology of its superconducting transition is determined by the relationship between the pairing temperature in the 1D filaments,  $T_p$ , and the crossover temperature  $T_x$  below which electrons can hop coherently between filaments. For  $T_x > T_p$ , a mean-field transition to anisotropic 3D superconductivity occurs. In contrast, for  $T_p > T_x$  a sequence of 1D pairing and phase fluctuations is anticipated, followed by a 2-particle dimensional crossover to long-range order mediated by Josephson coupling.

Identifying  $M_2Mo_6Se_6$  ( $M = Na, Tl$ ) crystals as exemplary q1D superconductors [1-3], we show that this 2-particle crossover robustly coincides with an exponential drop in the electrical resistivity and a jump in the superfluid density. Consequently, we argue that phase coherence is established by a topological process: binding vortex strings into 3D loops. Penetration depth data reveal a region of anomalously low phase stiffness persisting  $\sim 2K$  below the crossover [4], suggesting the survival of vortex loops within the superconducting state. We compare our results with data from superconducting nanowire networks and discuss possible mechanisms for suppressing  $T_x$  within q1D crystals.

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## Full statistics of voltage fluctuations in Quasi-1D superconductors



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**Keywords:** Quantum phase slips, Shot noise

In our talk we present a microscopic theory describing complete statistics of voltage fluctuations generated by quantum phase slips (QPS) in thin superconducting nanowires. We demonstrate that shot noise of the voltage as well as the third and all higher voltage cumulants differ from zero only due to the presence of QPS. As expected for tunneling-like problems in the zero-frequency limit voltage fluctuations in superconducting nanowires are described by Poisson statistics. However, at non-zero frequencies quantum voltage fluctuations in superconducting nanowires become much more complicated and are not anymore accounted for by Poisson statistics. Also we show our results for all finite-frequency voltage cumulants which were explicitly evaluated in the case of short superconducting bridges and Josephson junctions. In addition we discuss a non-trivial relation between these cumulants and the current-voltage characteristics of the system.

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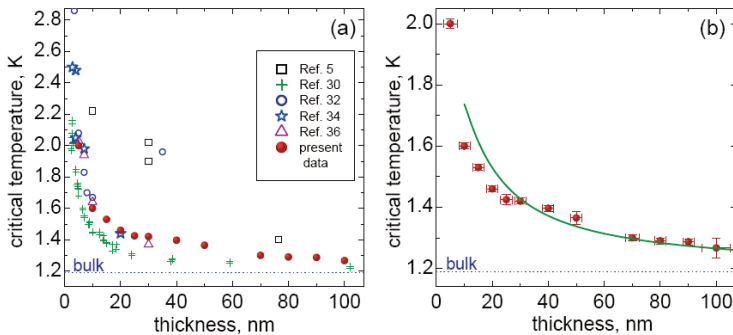
## Quantum Size Effects in Superconducting Thin Films



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Quantum confinement is known to affect a nanosized superconductor through quantum-size variations of the electronic density of states. Here we demonstrate that there is another quantum-confinement mechanism overlooked in previous studies. In particular, we find that the electron-electron attraction can be enhanced due to quantum-confinement modifications of electronic wave functions. The superconducting correlations are strengthened by such quantum mechanical effect, which creates a subtle interplay with surface-substrate phonon modifications. The combined effect depends on nanofilm thickness and can be controlled by nanoarchitecture. The calculations are in a reasonable agreement with experiments performed on high-quality aluminum films. Our findings shed light on the long-standing problem of the size dependence of the critical temperature in low-dimensional superconductors.



$T_c$  (thickness) for aluminum films

## Correlation Induced Capacitance Enhancement



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It is commonly accepted that strongly correlated electron systems entail a wealth of application oriented properties, such as superconductivity, transparent conducting oxides and high-temperature ferromagnets. To date, a lesser degree of attention has been paid to the possibility of using them in order to increase the capacitance of a capacitor [1,2].

This presentation focuses on capacitors consisting of a polar dielectric located between two strongly correlated plates. In the event where the isolated plates turn thermodynamically unstable because of electronic phase separation it will be shown that the capacitor geometry restores thermodynamical stability [3]. This additionally yields a capacitance enhancement as compared to weakly correlated plates. Such a phase separation may occur in the two-dimensional Hubbard model, augmented by nearest-neighbor attractive interaction [4]. Other geometries and microscopical models will be addressed as well [5].

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## **Fracton-elasticity duality**



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**Keywords:** topological matter, duality, quantum liquids

Motivated by recent studies of fractons, we demonstrate that elasticity theory of a two-dimensional quantum crystal is dual to a fracton tensor gauge theory, providing a concrete manifestation of the fracton phenomenon in an ordinary solid. The topological defects of elasticity theory map onto charges of the tensor gauge theory, with disclinations and dislocations corresponding to fractons and dipoles, respectively. The transverse and longitudinal phonons of crystals map onto the two gapless gauge modes of the gauge theory. The restricted dynamics of fractons matches with constraints on the mobility of lattice defects. The duality leads to numerous predictions for phases and phase transitions of the fracton system, such as the existence of gauge theory counterparts to the (commensurate) crystal, supersolid, hexatic, and isotropic fluid phases of elasticity theory. Extensions of this duality to generalized elasticity theories provide a route to the discovery of new fracton models. As a further consequence, the duality implies that fracton phases are relevant to the study of interacting topological crystalline insulators.

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## **Conformal phase transition in topological matter**



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**Keywords:** Topological states of matter in two dimensions; Chern-Simons theory; topological superconductor

Conformal phase transition is an unconventional type of quantum phase transition in strongly interacting systems. It is sometimes also said that conformality is lost in this case. The basic mechanism relies on the spontaneous breaking of conformal symmetry. The most well known example is the Berezinsky-Kosterlitz-Thouless (BKT) transition. We will consider examples of conformal phase transition in topological interacting systems. Particular focus will be given to a Higgs Chern-Simons superconductor. Such a system provides a description of a strongly coupled topological superconductor. We show that in this system conformality is lost for a given range of the Chern-Simons coupling, in which case a BKT scaling in  $2+1$  dimensions follows. As a consequence, we also show that the superfluid stiffness features a universal jump at the quantum critical point.

## Electrostatics of superinsulators: strings in the Lab



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**Keywords:** superinsulator, dual Meissner effect, string phenomenology

I will present the electrostatic properties of superinsulators, a new topological state of matter, which realizes a single-color version of QCD, with Cooper pairs linearly confined by electric field strings.

The response of a superinsulator to an applied dc electric field shows an electrostatic analogue of the Meissner effect in superconductors. Namely, electric fields below a first critical field,  $E_{c1}$  are expelled from a superinsulator, fields in the range  $E_{c1} < E < E_{c2}$ , superinsulation breaks down completely. Moreover measurements in NbTiN films reveal the field-theory-predicted transition from superinsulating to metallic behavior in sufficiently small systems, mimicking the asymptotically free behavior of quarks within mesons. We also find quantitative agreement between the measured and the predicted linear dependence of the threshold voltage. Our findings establish superinsulators as systems with zero dielectric permittivity and open the route to measurements of Polyakov's string tension as a function of the system parameters, enabling thus the exploration of strong coupling gauge theory concepts via desktop experiments.

## Superinsulating wires



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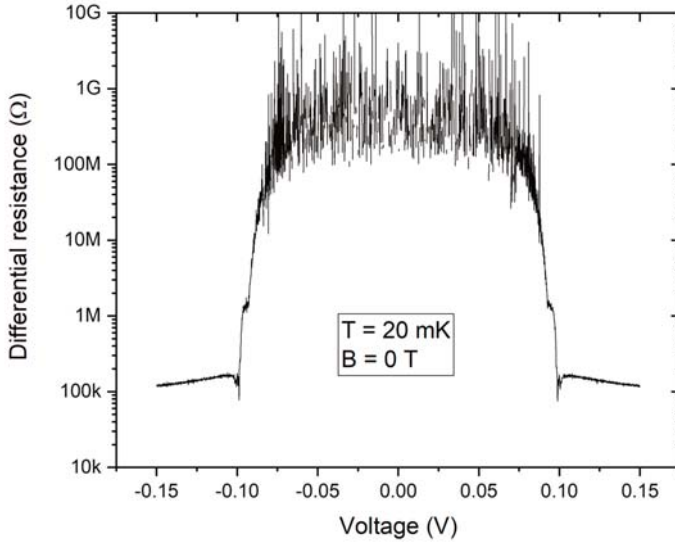
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**Keywords:** superinsulator, wires, photons detectors

We present the results of the study of low-temperature linear and non-linear transport properties of disordered NbTiN wires with thickness 100 – 300 nm based on superinsulating NbTiN films [1,2]. We show that all wires also are superinsulating. Appearance of the superinsulator is detected by the changes from the monotonic to threshold behavior of current-voltage characteristics evidencing formation of the zero-conducting state at finite temperature. It was found that superinsulating properties depends from length and width of wire. We demonstrate suppression of charge Berezinskii-Kosterlitz-Thouless transition with decreasing of wires width. Possibility of using such system for detecting single photons is discussed.

Experimental work was supported by the RSF # 18-72-10056 and. Theoretical work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.



Differential resistance of 200 nm wire at base temperature.

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## Non-equilibrium dynamics of superconductors: A Gutzwiller perspective



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**Keywords:** quench dynamics, superconductivity, Gutzwiller approximation

Recent advances in ultra-fast spectroscopy allow us to monitor the dynamics of electrons on a femtosecond scale. This is especially interesting for strongly correlated materials, such as high-temperature superconductors, since in their case the spectroscopic probe is able to investigate the intra-electronic redistribution of excitation energies before the relaxation via the lattice starts. From the theoretical point of view, this is obviously a challenging problem since it requires a method capable of treating the relaxation dynamics of a strongly correlated system out of equilibrium. In this regard the time-dependent Gutzwiller approximation is an effective approach which is based on a time-dependent variational principle for a variational wave-function where local electronic configurations are weighted differently by a time-dependent projector. For the attractive Hubbard model this approach leads to a dynamical crossover between weak and strong coupling limits where in the latter regime the pairing amplitude decreases with increasing attraction whereas the time-average of the dynamical gap increases.

Here we analyze in detail the differences with regard to the quench dynamics of BCS superconductors where exact analytical solutions exist. In addition we study the case of two coupled superconductors out-of-equilibrium. We consider both, interaction quench and an initial phase difference between the two SC's which allows to study the charge dynamics of the system.



## **Higgs spectroscopy of superconductors**



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**Keywords:** Higgs, non-equilibrium

Time-resolved pump-probe experiments recently attracted great interest, since they allow to detect hidden states and they provide new information on the underlying dynamics in solids in real time.

Recently, with the observation of a Higgs mode in superconductors it is now possible to investigate the superconducting order parameter, and thus the ground state, directly. By comparison with analytical calculations we now have a microscopic understanding of the Higgs mode in superconductors. After calculating the non-equilibrium response of s- and d-wave superconductors we show that such non-equilibrium Higgs spectroscopy opens a unique approach to distinguish between different symmetries of the condensate, even for new and unknown superconductors.

## DFT and DMFT study of rare-earth filled skutterudites



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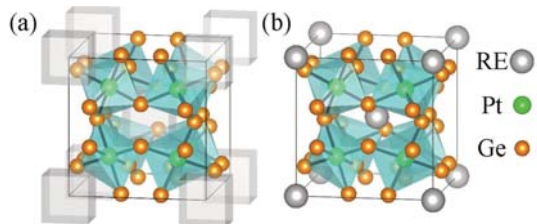
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**Keywords:** Skutterudites, f-electrons, spin-orbit, multi-band, DFT, DMFT, superconductivity

Recent experiments on rare-earth filled skutterudites have revealed an intriguing array of thermodynamic, transport and superconducting properties. They are also believed to be useful for thermoelectric applications. These materials have also brought to fore theoretical challenges posed, in particular, by the f electrons. Our state-of-the art DFT and DMFT calculations attempt to decipher these experimental findings and predict new results and properties. We explain RPES data on La and PrPt<sub>4</sub>Ge<sub>12</sub>, at finite-T and different photon energies; the temperature scale at which Kondo Fermi liquid-like behavior of CePt<sub>4</sub>Ge<sub>12</sub> sets in and the T-dependence of the observed resistivity and susceptibility. Our calculated spectral function can be compared with future ARPES experiments, and finite-T Fermi surfaces with future dHvA measurements, while also shedding light on the question of multi-band superconductivity. Another important result is the ability of our DMFT calculations to demonstrate that the Pr-skutterudite ground state is a singlet (as



deduced experimentally), by treating carefully f-electron spin-orbit and Hubbard-like correlations, and crystal field effects.

Crystal Structure of rare-earth filled Skutterudites

## Weyl States and the Dirac linear spectrum - a new point of view



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**Keywords:** topological, two-dimensional, Dirac, Weyl

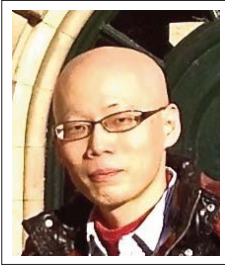
Electrons in conductors are basically free particles subject to residual collisions, according to the picture first proposed by Paul Drude in 1900 and later developed by Arnold Sommerfeld in 1927 with quantum concepts. Here I show that the same picture unfolds startling new results, such as the natural onset of Weyl states from parabolic bands provided that electrons are constrained to move in a layer. For this a Drude-Sommerfeld assumption must be reviewed, namely, the claim that in between any two residual collisions the electrons move freely. This is an approximation that ignores the magnetic field produced by the electrons, which although very small cannot be discarded in case of electronic motion along the layer, as shown here. The electric current creates a three-dimensional magnetic field around the layer which leads to topologically protected states independently of the strength of the field. This is because the magnetic field streamlines, created by the electronic motion form loops that pierce the layer twice and cannot be broken unless by a strong collision regime. The present results stem from the three term decomposition of the kinetic energy [1], from which it follows that the above mentioned magnetic field loops are a consequence that the electrons occupy Weyl states. The linear Dirac spectrum of such Weyl states arise in the limit of zero helicity and set up magnetic protectorates forbad to decay into the lowest energy states. Remarkably the residual magnetic interaction among electrons is shown to be attractive leading to the conjecture of the onset of a magnetic condensate. In summary the Drude-

Sommerfeld scenario for layers turns the electrons into skyrmions made stable by virtue of their own magnetic field. I also report here their non zero Chern index and obtain the electrical and the thermal conductivity of such states and compare to the Wiedemann-Franz law.

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## Higgs Spectroscopy of Nematic Topological Superconductors



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Nematic/chiral superconductivity accompanying the spontaneously broken rotational/time-reversal symmetry has been reported in doped topological insulators,  $M_x\text{Bi}_2\text{Se}_3$  ( $M=\text{Cu}, \text{Sr}, \text{Nb}$ ) and U- compounds. Here we propose that transverse electromagnetic wave response of long-lived massive bosonic (Higgs) excitations provide fingerprint spectroscopy of nematic/chiral superconductivity. Using quasiclassical Keldysh theory, we show the existence of characteristic bosonic modes in nematic/chiral superconductors [1,2]. There exist nematicity and chirality vibration modes in nematic superconductors. The former is the pseudo Nambu-Goldstone boson associated with the broken rotation symmetry. The latter can be identified as the fluctuation of the orbital angular momentum of Cooper pairs. We find that in  $M_x\text{Bi}_2\text{Se}_3$ , the mass gap of the chirality mode closes at the critical doping rate, signaling the dynamical instability of the nematic state towards the chiral state with broken time reversal symmetry [2]. We demonstrate that the spectral evolution of bosonic excitations can be clearly captured by the power absorption spectrum of electromagnetic waves.

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## **Exceptional nodal lines in topological semimetals and superconductors**



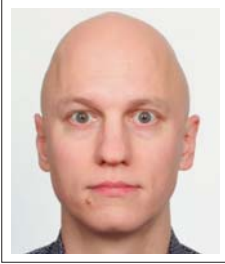
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We consider the impact of the disorder on the spectrum of three-dimensional Weyl and nodal-line semimetals. We show that the combination of disorder and a tilted spectrum leads to a non-Hermitian self-energy contribution that can split a Weyl node and nodal line into a single nodal ring and pair of exceptional lines, respectively. In nodal-line semimetals, these exceptional lines form the boundary of an open and orientable bulk Fermi ribbon in reciprocal space on which the energy gap vanishes. We find that the surface of such a disorder-induced bulk Fermi ribbon in general lies orthogonal to the direction of the tilt, which can be exploited to realize a bulk Fermi ribbon with nontrivial topology by means of a tilt vector that twists along a nodal loop.

We also consider the dispersion of the quasiparticles excitations in nodal superconductors in presence of weak disorder. Similarly to the semimetals, the complex self-energy correction to the Green function of quasiparticles due to disorder gives rise to the non-Hermitian BdG Hamiltonian describing the quasiparticle spectrum with exceptional points and lines.

## Newton-Cartan structures and anomalies in chiral p-wave Weyl superfluids and superconductors



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**Keywords:** topological superfluids and superconductors; chiral p-wave superfluids and superconductors; emergent gravity; Weyl fermions; chiral anomaly;  $^3\text{He-A}$ ; Newton-Cartan spacetimes

We consider emergent Newton-Cartan (NC) structures in Weyl superfluids and superconductors with chiral  $p+ip$  order parameter. We compute hydrodynamics and momentum space anomalies for the low-energy quasi-relativistic fermions. In particular, in the presence of superflow and order parameter textures, the non-trivial order parameter background fields lead to anomalous transport for the Bogoliubov-Majorana-Weyl fermions. For superconductors and superfluids, these are best understood as emergent Newton-Cartan gravitational fields coupling to the fermions.

The anomaly can be matched with the torsional Nieh-Yan (NY) term of the emergent NC space-time and includes a non-universal cut-off scale. Comparison of the anomaly and hydrodynamics suggests that the ultraviolet cut-off is determined by the non-relativistic uniaxial symmetry of the p-wave superfluid that follows from the normal Fermi-liquid state. It matches with the previous results found for superfluid  $^3\text{He-A}$  beyond the low-energy approximation and is Galilean invariant.

## Topological properties of multilayers and surface steps in the SnTe material class



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**Keywords:** SnTe, TCI, step states, atomic steps

Surfaces of multilayer semiconductors typically have regions of flat terraces separated by atom-high steps. We investigate the properties of the low-energy states appearing at such atomic steps in Sn(Pb)Te(Se) [1]. We identify the important approximate symmetries and use them to construct the topological invariants. We calculate the dependence of mirror- and spin-resolved Chern numbers on the number of layers and show that the step states appear when these invariants are different on the two sides of the step. Since the density of states is large at the step the system is susceptible to different types of instabilities, and we consider an easy-axis magnetization as one realistic possibility. We show that magnetic domain walls support low-energy bound states because the regions with opposite magnetization are topologically distinct in the presence of non-symmorphic chiral and mirror symmetries, providing a possible explanation for the zero-bias conductance peak observed in the recent experiment [2].

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## Phase Separation in the Vicinity of Fermi Surface Hot Spots in 1T-TiSe<sub>2</sub>



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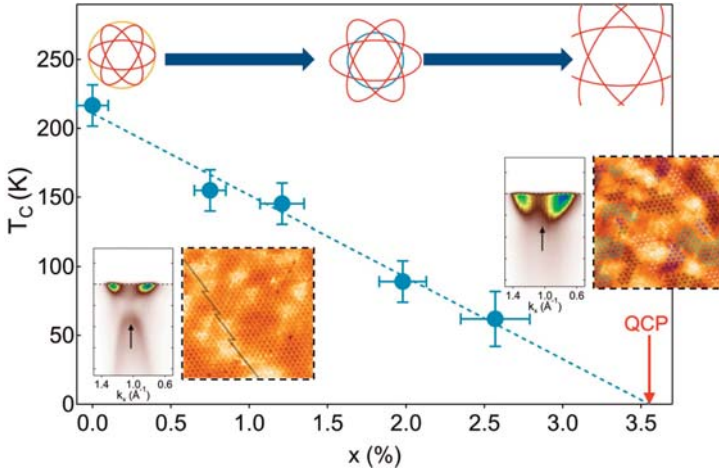
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**Keywords:** Charge-density-wave, phase separation, ARPES, STM

1T-TiSe<sub>2</sub> is a prototypical system hosting mixed CDW-superconducting phases under Cu intercalation, pressure or electrical gating [1-3]. It has been recently proposed that the emergence of superconductivity relates to CDW fluctuations and the development of discommensurations in a nearly-commensurate intermediate regime (NCCDW) separating commensurate and incommensurate CDW [4-5]. Similar NCCDW phases have been observed in Ti self-doped 1T-TiSe<sub>2</sub> without any sign of superconductivity yet [6]. Here, we report on the phase diagram of 1T-TiSe<sub>2</sub> as a function of Ti self-doping and focus on its charge density wave (CDW) using angle-resolved photoemission spectroscopy and variable-temperature scanning tunneling microscopy. We demonstrate that the spatial texturing of the CDW is an intrinsic property of doped 1T-TiSe<sub>2</sub> in the vicinity of Fermi surface hot spots,

i.e. electron-hole band crossing close to, but not at the Fermi level. Our study sheds light on the intimate relationship between Fermi surface topologies and the emergence of spatially textured electronic phases in electron-doped 1T-TiSe<sub>2</sub>.



T-x phase diagram of Ti-doped 1T-TiSe<sub>2</sub>. The CDW transition temperature  $T_c$  is linearly decreasing with the intercalated-Ti concentration towards a quantum critical point (QCP). Superimposed are STM images and corresponding ARPES spectra for low (1.21 %) and high Ti-doping (2.57 %). Added meshes on the  $x=2.57\%$  STM image and gray line on the  $x=1.21\%$  one highlight CDW domains and a phase shift between them, respectively. At the top of the image is shown the Fermi surface evolution of the high-temperature phase through the doping-driven Lifshitz transition at the QCP.

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## Neutron Studies on The Role of Iron-Vacancy to Superconductivity in $K_{2-x}Fe_{4+y}Se_5$



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**Keywords:** iron-based superconductors, iron-vacancy, magnon excitation

The crystal and magnetic structure of polycrystalline  $K_{2-x}Fe_{4+y}Se_5$  was examined through neutron powder diffraction (NPD). The magnetic structure showed checkerboard anti-ferromagnetic (AFM) superlattice in the parent compound  $K_2Fe_4Se_5$  sample, and  $\sqrt{5}\times\sqrt{5}\times 1$  iron-vacancy order was clearly observed. It has been demonstrated [1] that the iron-vacancy plays a crucial role in superconductivity (SC), ordered iron-vacancy in  $K_2Fe_4Se_5$  makes the material a Mott insulator; whereas disordered iron-vacancy results in the appearance of superconductivity in  $K_{2-x}Fe_{4+y}Se_5$  [2]. To further understand the interplay between the AFM and SC, a series of sample was prepared to for NPD and inelastic neutron scattering studies. The apparent differences of the phonon/magnon excitations were found for the annealed and the quenched  $K_2Fe_4Se_5$  samples, while the iron-vacancy turns to disorder state in the quenched sample. For the annealed  $K_2Fe_4Se_5$  sample, the broad peak at 60 K splitting into two peaks at 300 K, which separates Verwey-like transition temperature at 125 K. As for the quenched  $K_2Fe_4Se_5$  sample, the 27 meV shifts to 24 meV, indicating distinct behavior for the two samples. It was speculated that the 27 meV possibly be the magnon excitation. We shall present our experimental result and discuss its implication.

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## Electrochemical Synthesis of Iron Chalcogenide Superconductors



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Iron-based superconductors have great potential for high magnetic field applications such as superconducting wire and tapes because of their high superconducting transition temperature ( $T_c$ ), upper critical field ( $H_{c2}$ ), and irreversibility field (Hirr).

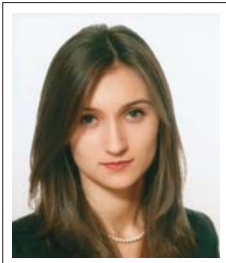
As a new route for synthesize the iron chalcogenide superconductors, we focused on an electrochemical reaction. The electrochemical reaction is widely used for electroplating metal chalcogenides and inter/deintercalating the ions into/from a host material.

To date, we have successfully synthesized FeSe superconductors by electrochemical reaction [1-4]. For more sophisticated conditions to obtain high quality samples, we focused on increase of solution temperature and verifying the applied voltage. The highest crystallinity sample was obtained at solution temperature of 70 °C. Finally, we have successfully observed the zero resistance in as-deposited FeSe sample [5]. This is the first report for the observation of zero resistance in electrodeposited FeSe without any heat treatment. This method will be the promising way for synthesis and coating of iron chalcogenide superconductors.

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## Charge density wave order in cuprates under extreme conditions



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**Keywords:** Charge Density Waves, uniaxial pressure, cuprates, pulsed field

The cuprates are known for having a rich variety of electronic orders that break the lattice symmetry. One of them, the two-dimensional (2D) charge density wave (CDW) order within the  $\text{CuO}_2$  planes, has been universally found in all families of cuprates [1]. The doping dependence of the CDW wavevector in  $\text{HgBa}_2\text{CuO}_{4+y}$  provides a strong evidence that these correlations are responsible for the Fermi-surface reconstruction, assuming these correlations are bi-directional [2,3]. In contrary, some measurements for  $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$  (YBCO) demonstrated that the CDW order is consistent with a local unidirectional “stripe” order [4]. As experiments in YBCO showed an additional three-dimensional (3D) charge order, triggered by external magnetic fields [5], it remains unclear whether the 2D or 3D order is responsible for the Fermi-surface reconstruction. I will present the results of the resonant X-ray scattering performed under uniaxial pressure (up to 250 N) and X-ray absorption spectroscopy in pulsed fields (up to 30 T), aimed to address these important issues.

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## Superconducting spin valve based on spiral magnet with broken inversion symmetry



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**Keywords:** superconducting spin valve, cryogenic magnetic memory, Josephson device

Superconducting spintronics has emerged in the last decade as a promising new field that seeks to open a new dimension for nanoelectronics by utilizing the internal spin structure of the superconducting Cooper pair as a new degree of freedom. Currently, the discipline finds itself at the crossroads for developing first-generation devices. Among the basic units of superconducting spintronics are the so-called superconducting spin valves. These are nanodevices in which the superconducting current is controlled through the spin degree by changing the magnetization of magnetic elements.

We propose a superconducting spin-triplet valve, which consists of a superconductor and an itinerant magnetic material, with the magnet showing an intrinsic non-collinear order characterized by a wave vector that may be aligned in a few equivalent preferred directions under the control of a weak external magnetic field. Re-orienting the spiral direction allows one to controllably modify long-range spin-triplet superconducting correlations, leading to spin-valve switching behavior.

Our results indicate that the spin-valve effect may be noticeable [1-3]. This bilayer may be used as a magnetic memory element for cryogenic nanoelectronics. Josephson superconducting spin valve based on the same principle is also considered. Such spin valves have the following advantages in comparison to superconducting spin valves proposed previously: (i) it contains only one magnetic layer, which may be more easily fabricated and controlled; (ii) its ground states are separated by a potential barrier, which solves the “half-select” problem of the addressed switch of memory elements.

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## **Measuring coherence length $\xi$ in zero magnetic induction B.**



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When a long current-carrying solenoid pierces a superconducting cylinder, the magnetic induction  $B$  experienced by the superconductor (SC) is ideally zero anywhere apart from an edge with thickness of penetration depth at the interior of the cylinder. Consequently, vortices are not expected to flow, or even form, in the SC. Nevertheless, the SC will experience a vector potential  $A$  set by the solenoid, and, according to the London equation, supercurrent will flow in the SC cylinder. Thus, by driving the solenoid current, the critical-current of the SC can be measured in the absence of vortices and with no leads. This critical-current places an upper limit on the Ginzburg-Landau coherence length  $\xi$ . We performed such a measurement using a NbTi SC solenoid and optimally doped LSCO single crystal cylinder. We found that  $\xi$  is smaller than 7 nm. Future improvements in the experimental setup will allow us to place a tighter upper limit.



## Hidden antipolar order parameter and charged Néel-type domain walls in hybrid improper ferroelectrics



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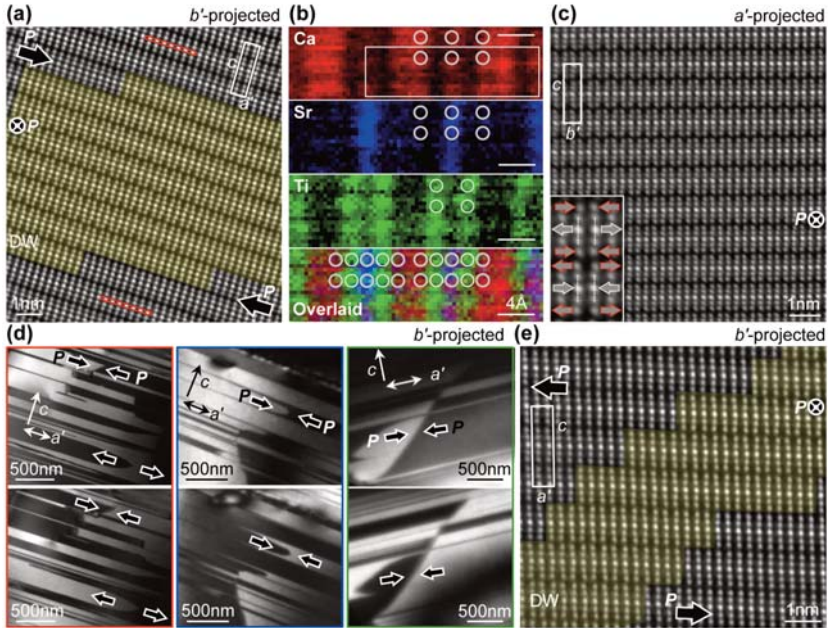
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Hybrid improper ferroelectricity (HIF) denotes a new class of polar instability by the mixture of two octahedral-distortion modes and can feature the coexistence of abundant head-to-head and tail-to-tail polar domains, of which the domain walls tend to be charged due to the respective screening charges with an opposite sign. However, no such coexisting carriers are available in the materials. Using group-theoretical, microscopic, and spectroscopic analyses, we established the existence of hidden antipolar order parameter in model HIF  $(\text{Ca,Sr})_3\text{Ti}_2\text{O}_7$  by the condensation of a weak, previously unnoticed antipolar lattice instability, turning the order-parameter spaces to be multicomponent with the distinct polar-antipolar intertwining and accompanied formation of Néel-type twin-like antipolar domain walls (few nm) between the head-to-head and tail-to-tail domains. The finite-width Néel walls and correlated domain topology inherently lift the polar divergences between the domains, casting an emergent exemplification of charged domain-wall screening by an antipolar ingredient [1]. Comparisons to topological defects in improper-ferroelectrics hexagonal manganites were discussed.



(a) The HAADF imaging of HH domains revealing a different feature in the DW (yellow). The Ca1/Sr1 (red rectangle) was used for determining the P direction. (b) The STEM-EELS chemical mapping. Gray (white) circles, Ca/Sr (Ti) omitting the off-center distortions for simplicity. (c) The  $a'$ -projected HAADF image. Lower-bottom inset, an uc blow-up showing the accentuated antipolar Ca1/Sr1 (white-margined) and Ca2/Sr2 (red-margined arrows) displacements. Dashed white lines, the centered anchors for guiding the eyes. (d) The various DF images (red, blue, and green) exploiting inversed reciprocal-lattice vectors, with the contrast reversal in each set unveiling the domain polarity. (e) The HAADF imaging of TT domains, with the DW structure (yellow) mimicking the HH counterpart in (a) and  $a'$ -projected (c). P in the DWs and (c), pointing in or out. White rectangles, projected uc.

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## Majorana multipole response of topological superconductors



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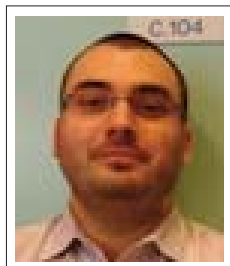
**Keywords:** Topological superconductor

We developed a general theory of magnetic multipoles for surface helical MFs on time-reversal invariant superconductors [1]. The results show that the multipole response is governed by crystal symmetry, and that a one-to-one correspondence exists between the symmetry of Cooper pairs and the representation of magnetic multipoles under crystal symmetry. The latter property provides a way to identify nonconventional pairing symmetry via the magnetic response of surface MFs. We also find that most helical MFs exhibit a magnetic-dipole response, but those on superconductors with spin  $3/2$  electrons may display a magnetic-octupole response in leading order, which uniquely characterizes high-spin superconductors. Detection of such an octupole response provides direct evidence of high-spin superconductivity, such as in half-Heusler superconductors

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## Superconducting stiffness of $\text{LaAlO}_3/\text{SrTiO}_3$ interfaces



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The achievement of high-quality epitaxial interfaces involving transition metal oxides gives a unique opportunity to engineer artificial materials where new electronic phases take place. The discovery of a high mobility two-dimensional electron gas (2-DEG) confined in a quantum well at the interface between two insulating oxides such as  $\text{LaTiO}_3$  and  $\text{SrTiO}_3$  or  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$ , is probably one of the most prominent examples in the field. Unlike more conventional semiconductor based quantum wells, conducting electrons in  $\text{SrTiO}_3$  fill 3d-bands, which gives a favourable ground for the emergence of complex electronic phases. In particular, 2D superconductivity [1] and strong spin orbit coupling [2] have been reported in such interfaces.

A key feature of these electronic systems lies in the possibility to control their carrier density by electric field effect. In this talk, I will present recent resonant microwave transport measurements on  $\text{LaAlO}_3/\text{SrTiO}_3$  interfaces that allows extracting the superfluid stiffness  $J_s$ , i.e. the energy scale that controls the phase rigidity of the superconducting condensate. We find that the competition between  $J_s$  and  $\Delta$  controls the superconducting phase diagram obtained by plotting the superconducting  $T_c$  as a function of gate voltage. Whereas a good agreement with the Bardeen-Cooper-Schrieffer (BCS) theory is observed at high carrier doping, our data suggest that the suppression of  $T_c$  at low doping is controlled by the loss of macroscopic phase coherence instead of electron pairing as in standard BCS theory [3]. In (110)-oriented  $\text{LaAlO}_3/\text{SrTiO}_3$  interfaces, we evidence a transition from single-band to two-band superconductivity driven by electrostatic doping,

which we relate to the filling of the different 3d-orbitals in the quantum well [4,5].

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## Non-locality of Majorana Bound States low dimensional hybrid structures



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**Keywords:** Majorana bound states, low dimensional physics, topological edge states.

In condensed matter physics in order for Majorana Bound States to emerge we need interaction between superconductivity, spin-orbit coupling and magnetic field in the system composed of low dimensional structures [1]. In finite 1D Rashba nanowires those states are manifested by emergence of a pair of zero-energy Majorana bound states [2]. On the other hand, in 2D systems spin currents contributed by the edge states might appear. If we are to conjoin these two ingredients a vast, new possibilities for probing the behaviour of Majorana Bound States present itself. Therefore, we investigate properties of such bound states in multi-dimensional hybrid structures [3] consisting of 1D Rashba nanowire and bounded 2D surfaces, by means of distribution of Majorana wave function as well as theoretical analogue of spin polarised tunnelling technique [4].

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## Multiferroicity of domain walls in magnetic oxides



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**Keywords:** multiferroics, domain walls, magnetoelectric effect

Recently there were a number of reports on ferroelectricity localized on the magnetic domain walls in rare earth iron garnets and orthoferrites [1-5]. These multiferroic properties of the domain walls manifest themselves as the electric field induced domain wall motion and transformation [1] and even the nucleation of it from the single domain state [5] in the gradient electric field from the tip electrode. The electric polarization of domain walls can be the result of several microscopic mechanisms: (i) the Dzyaloshinskii-Moriya-like interaction [1] (ii) the local decompensation of the antiferroelectric structure in the domain wall [6] (iii) the nonrelativistic interaction due to the exchange striction [3].

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## Doping driven 2x2 charge-density-wave in $(\text{LaSe})_{1,14}(\text{NbSe}_2)_2$



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**Keywords:** quasi-2D, charge-density-wave, unconventional superconductivity, doping, misfit, ising spin-orbit coupling

Transition metal dichalcogenide (TMD) 2H-NbSe<sub>2</sub> presents superconducting and 3x3 charge density wave (CDW) orders [1] which are also observed in monolayer (ML) NbSe<sub>2</sub> [2]. However, ML NbSe<sub>2</sub> breaks inversion symmetry which combined with the presence of large spin-orbit interaction give rise to out-of-plane spin-momentum locking and unconventional Ising pairing. This pairing leads to strong magnetic in-plane critical fields, well beyond the paramagnetic limit [3]. In the parent superconducting misfit TMD  $(\text{LaSe})_{1,14}(\text{NbSe}_2)_2$ , with alternation of bilayers of NbSe<sub>2</sub> and LaSe, similar features are observed [4]. Here, we report UHV-STM/STS and DFT results suggesting that  $(\text{LaSe})_{1,14}(\text{NbSe}_2)_2$  behaves like an electron-doped ML NbSe<sub>2</sub> exhibiting a transition to a 2x2 CDW order. Moreover, our quasiparticle interferences measurements depict clear signatures of unconventional superconductivity. Our study opens the possibility to use misfit exotic TMD heterostructures to thoroughly tune doping to unprecedented values and thus considerably modify the electronic properties of quasi-2D NbSe<sub>2</sub>.

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## Quantum thermalization in holography and the laboratory



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**Keywords:** Quantum matter, High Tc superconductivity, Holographic duality.

The simple moral of eigenstate thermalization is that what we think is the rattling of classical things producing heat is a delusion caused by our incapacity to keep track of the flow of quantum information in the enormous many-body Hilbert space. Are there circumstances where it is impossible to construct such a consistent classical metaphor? Helped by holography we stumbled recently into a number of cases. Even in the elementary physics of expanding cold atom clouds a vivid example has been identified [1] Planckian dissipation is in this regard a no-brainer but its ultimate consequence for experiment turns out to be stunningly weird (unpublished). Finally, the holographic incarnation of optical pump-probe experiments predicts that strange metals should invariably exhibit the phenomenon of instantaneous thermalization. I will argue that this suggests a critical test of the UV independence notion by mobilizing condensed matter experiment [2].

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## Confinement and asymptotic freedom with Cooper pairs



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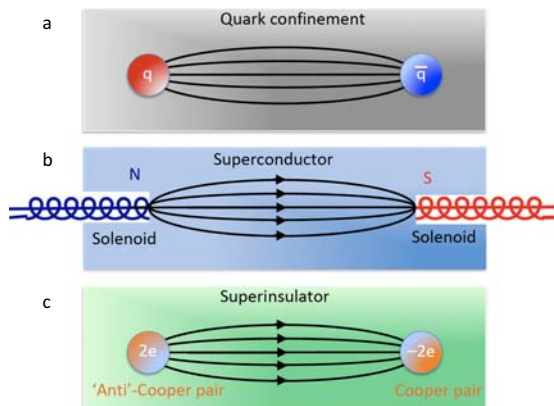
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**Keywords:** Disordered BKT transition, gauge theories, superinsulators

One of the most profound aspects of the standard model of particle physics, the mechanism of confinement binding quarks into hadrons, is not sufficiently understood. The only known semiclassical mechanism of confinement, mediated by chromo-electric strings in a condensate of magnetic monopoles still lacks experimental evidence.

Here we show that the infinite resistance superinsulating state, which emerges on the insulating side of the superconductor-insulator transition in superconducting films offers a realization of confinement that allows for a direct experimental access. We find that superinsulators realize a single-color version of quantum chromodynamics and establish the mapping of quarks onto Cooper pairs.

We reveal that the mechanism of superinsulation is the linear binding of Cooper pairs into neutral “mesons” by electric strings. Our findings offer a powerful laboratory for exploring and testing the fundamental implications of confinement, asymptotic freedom, and related quantum chromodynamics phenomena via the desktop experiments on superconductors.



Dual Mandelstam–’t Hooft–Polyakov confinement. a: quark confinement by chromo-electric strings. b: magnetic tube (Abrikosov vortex) that forms in a superconductor between two magnetic monopoles. c: electric string that forms in a superinsulator between the Cooper pair and anti-Cooper pair. The lines are the force lines for magnetic and electric fields respectively. In all cases the energy of the string (the binding energy) is proportional to the distance between either the monopoles or the charges.

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## Enhanced critical temperature, pairing fluctuation effects, and BCS-BEC crossover in a two-band Fermi gas



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**Keywords:** Lifshitz transition, high-T<sub>c</sub>, shape resonance, multigap superconductivity, isotope effects, organic materials, BCS-BEC crossover

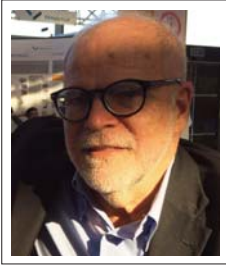
We study the superfluid critical temperature in a two-band attractive Fermi system with strong pairing fluctuations associated with both interband and intraband couplings [1-6]. We focus specifically on a configuration where the intraband coupling is varied from weak to strong in a shallow band coupled to a weakly-interacting deeper band. The whole crossover from the Bardeen-Cooper-Schrieffer (BCS) condensation of largely overlapping Cooper pairs to the Bose-Einstein condensation (BEC) of tightly bound molecules is covered by our analysis, which is based on the extension of the Nozieres-SchmittRink (NSR) approach to a two-band system. In comparison with the single-band case, we find a strong enhancement of the critical temperature, a significant reduction of the preformed pair region where pseudogap effects are expected, and the entanglement of two kinds of composite bosons in the strong-coupling BEC regime.

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## Room temperature Superconductivity by Fano shape resonances near Lifshitz transitions in superlattices of hydrogen wires in pressurized hydrides



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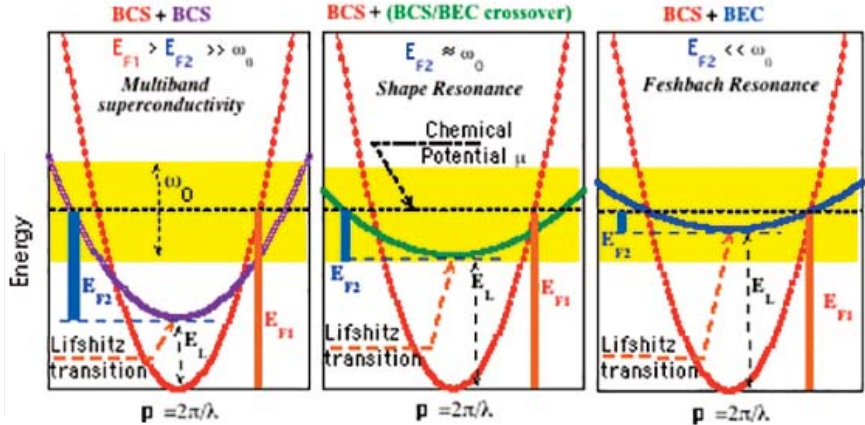
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Using the numerical joint solution of Bogoulibov gap equations and the density equation for anisotropic multigap superconductors the Bianconi-Perali-Valletta (BPV) theory [1-6] has been used to predict non-BCS superconductivity driven by the ++ attractive Majorana or +- repulsive Heisenberg exchange interaction between condensates (not considered in the conventional BCS theory) in a variety of systems predicting room temperature superconductivity by tuning the chemical potential near a Lifshitz transition. The idea was first developed in 1993-1998 [1-6] focusing on the 1D incommensurate lattice modulation of Bi2212 cuprate forming a superlattice of weakly interacting quantum stripes. The external physical stimulus to reach a Lifshitz transition could be doping, pressure or strain [7] in different materials going from cuprates, organics to pressurized hydrides. The BPV theory has predicted first the Fano Feshbach resonance at the Lifshitz transition with a first BCS condensate gap resonating with a second appearing BEC condensate which gives a dip of the critical temperature. Moreover it has predicted the Fano shape resonance where the new appearing superconducting gap is in the BCS-BEC crossover regime (see Fig. 1) which gives the maximum of the dome for the critical temperature as a function of the external tuning physical variable.



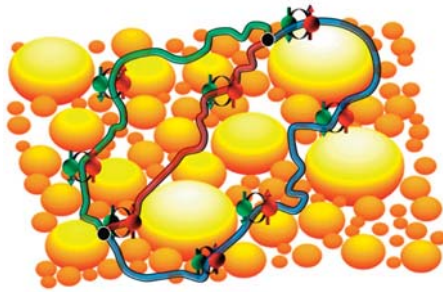
**Fig. 1** Three typical cases of non-BCS multigap superconductivity near a Lifshitz transition with a new appearing Fermi surface: left, in the BCS regime, center, in the BCS-BEC crossover giving the Fano shape resonance, right: in the BEC regime giving the Fano Feshbach resonance of Fermi-Bose models.

The BPV theory has predicted the doping dependent superconducting gaps near the Lifshitz transitions in  $Mg_{1-x}Al_xB_2$  [8-11] and in iron based superconductors [12-14] where the Lifshitz transitions tuned by strain and doping have been clearly conformed experimentally in these last years [15]. The theory of phase separation in the multi-band-Hubbard model near the Lifshitz transition predicts the arrested phase separation or nematic phase, observed by local probes [15,16]. Today our experimental research is focusing of on determination of emergent hyperbolic geometry for the filamentary interface pathways [16-18] which promote quantum coherence at high temperature. In this scenario interface superconducting filaments run in a hyperbolic space shown in Fig. 2 forming a complex network with mixed Bose and Fermi statistics.

The 200K superconductivity in  $H_3S$  [19] has been assigned to the tuning of the chemical potential in a superlattice of interacting hydrogen wires [20,21] like in A15 intermetallics giving an electronic topological transition with the appearing a tubular 2D Fermi surface. The BPV theory clearly predicts the dome of the critical temperature with a maximum of  $T_c=200$  K superconductivity in  $H_3S$ . Recently 260 K superconductivity was discovered in the  $LaH_{10}$  [22-26] clathrate made of metallic hydrogen nanotubes



embedded in the cubic crystallographic structure with La ions at its vertex. This crystallographic structures is therefore formed by modular atomic units, metallic hydrogen nanotubes. The BPV theory [1-6] for room temperature superconductors has predicted a very high critical temperature in the similar architecture of carbon nanotubes [27] where the pressure tunes the chemical potential near an electronic topological Lifshitz transition and the fermi level crosses a van Hove singularity in the Density of States.



**Fig. 2.** The filamentary pathways of interface superconductivity connecting two points in the superstripes landscape of striped puddles which can be mapped to a hyperbolic space providing a case of supersolid driven by strain and doping near a critical point of a Lifshitz transition and of large zero point lattice fluctuations

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## High-resolution XRD and EXAFS/XANES structural study of yttrium hydrides



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Up to date experimental results and theoretical calculations have revealed the most promising candidates for high  $T_c$  are metal hydrides [1-3]. The group of M. Eremets has already studied  $YH_n$  by optical microscopy, Raman spectroscopy and electrical measurements. In parallel, the XAFS experiments with unprecedented accuracy and under extreme conditions can nowadays be performed [4]. Here we present a high resolution XAFS and XRD study under extreme conditions of  $YH_3$  at ESRF. We use advanced Reverse Monte Carlo (RMC-EXAFS) approach [5] to extract the information on the local structure and its changes directly from the XAFS spectra of  $YH_3$  under extreme conditions of high pressure up to 180 GPa. We compare the XAFS results with Raman spectroscopy, electrical resistivity and SQUID measurements.

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## Intrinsic spatial and temporal destabilization of incommensurate stripes at low temperatures<sup>+</sup>



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**Keywords:** Stripes, Nickelates, XPCS

In superconducting cuprates as well as in non-superconducting layered nickelates stripe order has been found to decay towards low temperatures. While in cuprates this denotes the suppression of stripes by the onset of superconductivity, the mechanism behind the similar behavior in the absence of superconductivity in nickelates has remained unclear. Here we show the low-temperature decay of incommensurate nickelate stripes to occur via a loss of spatial correlations [1] and to involve spin-stripe fluctuations on time scales of tens of minutes over a wide temperature range. Fluctuation times and spatial correlation[1] are directly connected: Fluctuations slow down at intermediate temperatures where stripe correlations are largest and speed up upon cooling and heating. Low-temperature decay appears to be an intrinsic property of incommensurate stripe order. In turn, this mechanism may also play a role in the competition between stripes or density waves and superconductivity in cuprates.

This work was performed in collaboration with A. Ricci, N. Poccia, G. Campi, S. Mishra, L. Mueller, B. Joseph, Bo Shi, A. Zozulya, M. Buchholz, C. Trabant, J. Lee, J. Viehhaus, J. B. Goedkoop, A. A. Nugroho, M. Braden, S. Roy, M. Sprung.

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## Intermediate Magnetic Phase of Charge-Stripe Ordered La<sub>2</sub>NiO<sub>4.11</sub> and the probable trigger for static magnetic ordering



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**Keywords:** Charge-stripe order, neutron scattering, muSR

In La-based cuprates the partial gapping of the magnetic excitation spectrum [1], allows the magnetic excitations to be studied to lower energies than in other cuprate materials. These excitations are often compared to those of charge-stripe ordered La<sub>2-x</sub>Sr<sub>x</sub>NiO<sub>4+δ</sub>[2,3].

Recently two striking in La-based cuprates have been observed, a low energy kink in the magnetic excitation spectrum [4], and an offset between the centring of low energy magnetic excitations and the magnetic Bragg peaks [5]. A combined neutron scattering and  $\mu$ SR study of charge-stripe ordered La<sub>2</sub>NiO<sub>4.11</sub>, shows similar effects as in La-based cuprates[4,5]. In La<sub>2</sub>NiO<sub>4.11</sub> there is an offset between the wave vectors of the magnetic Bragg reflections and the low energy magnetic excitations in the ordered phase. Whilst the temperature evolution identifies an intermediate magnetic phase, and the probable trigger to static magnetic order in La<sub>2-x</sub>Sr<sub>x</sub>NiO<sub>4+δ</sub>.

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## Pulsing normal and collective counter-currents driven by the Hall voltage in a sliding charge density wave

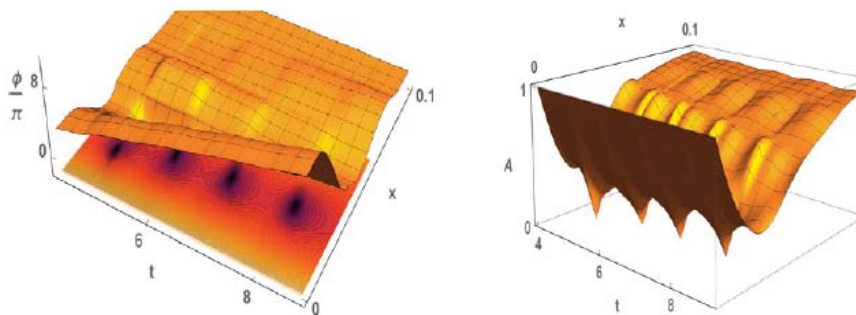


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**Keywords:** high magnetic field, charge density wave, sliding state, phase slip, phase vortex, Shapiro steps, quantum Hall effect, mesa junction

Remnant pockets of carriers left over after formation of a charge density wave (CDW) could be brought to a current-carrying state at quantized Landau Levels. The generated Hall voltage polarizes and puts to sliding the flexible CDW background. The screening from the CDW allows for a so strong redistribution of normal electrons density under the action of the Lorentz force alone, that an integer filling of the lowest Landau level might be reached at one edge at the expense of the full depletion at another edge of the Hall bar. With the Hall field exceeding the sliding threshold, the regime of exactly compensated collective and normal counter-currents develops in the open-circuit direction across the bar. The annihilation of the two currents proceeds via a regular sequence of phase slips which are the space-time vortices of the CDW phase around the enforced nodes of the CDW amplitude (the simulations are shown in the figure below). The resulting spontaneous generation of coherent high  $\sim$ GHz frequency signals was detected by observations of multiple Shapiro steps. This picture results from experiments on micron-sized Hall bars in crystals of NbSe<sub>3</sub> prepared by means of focused ion beams [1]. The interpretation is confirmed and illustrated by a numerical solution of equations coupling normal and collective subsystems and the electrostatic potential [1,2].



Evolution with periodic phase slips as spatiotemporal vortices: the 3D plot of the CDW phase  $\phi(t,x)$  on top of the density plot showing the vorticity (left); the CDW amplitude  $A(t,x)$  with nodes at the vortex centers (right).

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## **Soft modes and nonanalyticities in Dirac metals**



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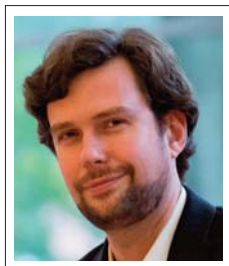
**Keywords:** Non-Fermi-liquid behavior, quantum magnets

We study the bulk electronic properties of a clean Dirac metal, i.e., a Dirac system with the chemical potential not tuned to the Dirac point. The soft two-particle excitations in such a Dirac Fermi liquid (DFL) are qualitatively different from the corresponding excitations in a conventional, or Landau, Fermi liquid (LFL) [1]. They lead to nonanalytic dependencies of observables, including the spin susceptibility, the density of states, and the specific heat, on the wave number, the temperature, and an external magnetic field. We discuss these nonanalyticities in a DFL, and their consequences for magnetic quantum phase transitions in Dirac metals, and compare them with the corresponding effects in a LFL.

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## **Rational design of low-dimensional electronic phenomena at Mott interfaces**



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**Keywords:** spintronics, standing-wave photoemission spectroscopy, oxide interfaces, epitaxial strain, oxygen vacancies

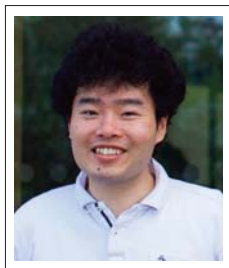
Rational design of low-dimensional electronic phenomena at Mott oxide interfaces is considered to be one of the most promising schemes for realizing new energy-efficient logic and memory devices. As an effective tuning parameter, coherent epitaxial strain in such films and their heterostructures has been widely utilized to control key functional properties, such as the metal-insulator transition temperature in vanadates [1] and magnetotransport in manganites [2]. Similarly, local strains and superlattice misfit strains have been shown to be key physical variables controlling the superconducting critical temperatures in the cuprate [3], diboride [4], and pnictide [5] single crystals. In this talk, I will discuss three recent studies, in which we utilized a combination of advanced x-ray spectroscopic and electron imaging techniques to investigate the electronic-structural origins of the emergent ferromagnetism at the atomically-abrupt coherently-strained  $\text{CaMnO}_3/\text{LaNiO}_3$  interface [6]. Starting with the building blocks of this heterojunction, we used a combination of hard x-ray photoemission (HAXPES) and x-ray absorption spectroscopy (XAS) to establish a direct link between the in-plane strain and the oxygen-vacancy content in  $\text{CaMnO}_3$  [7]. Then, by using a combination of XAS and scanning transmission electron microscopy, we examined the nature of the metal-insulator transition in coherently-strained  $\text{LaNiO}_3$  in the ultrathin limit [8]. Finally, we utilized a combination of HAXPES and standing-wave photoemission spectroscopy

to demonstrate a depth-dependent charge reconstruction at the  $\text{CaMnO}_3/\text{LaNiO}_3$  interface [9].

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## Superconducting spin transport in magnetic Josephson junctions



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**Keywords:** Spin triplet superconductivity, proximity effect, Josephson junctions

Electron pairing at a superconductor / ferromagnet (S/F) interface is controllable through the alignment of the magnetic exchange field. Over the past decade, it has been established that a non-uniform magnetic exchange field at a S/F interface converts spin-singlet pairs (antiparallel spins) to a triplet state in which the spins are parallel and triplet supercurrents are long-ranged in Fs[1-4]. Here we demonstrate that spin-polarised triplet supercurrents can transfer spin angular momentum from one F to another without dissipation. The spin-polarised supercurrents are generated via Cr/Fe spin-glass interfaces and are controlled through a spin-filtering effect through a Fe/Cu/Fe pseudo spin-valve barrier: an antiparallel alignment of the Fe moments suppresses the Josephson current (10%) with respect to the parallel state, analogues to giant magnetoresistance. The results are promising for the development of superconducting spintronic devices in which read and write operations are achieved via spin-polarized triplet states.

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## Identification of chiral Majorana edge states in chiral $p$ -wave superconductors



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**Keywords:** Spin triplet superconductivity (I5)

Finding a smoking-gun signature of chiral Majorana edge states is an urgent issue in physics of  $\text{Sr}_2\text{RuO}_4$ , which is a promising candidate material of intrinsic chiral  $p$ -wave superconductors. In this work, we demonstrate that the chiral nature of Majorana edge states is drastically manifested in “nonlocal” conductance in a junction consisting of a chiral  $p$ -wave superconductor and two ferromagnetic leads. The nonlocal conductance in the present junction is insensitive to the distance between the two leads and is sensitive to the chirality of the pair potential. These two drastic features enable us to identify the moving direction of the chiral Majorana edge states in the single experimental setup only by changing the lead wire to which the bias voltage is applied. We propose a smoking-gun experiment for identifying the chiral Majorana edge states in the chiral  $p$ -wave superconductor [1].

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## Visualizing polaron formation in $\text{EuB}_6$



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**Keywords:** magnetic polarons, colossal magnetoresistance, electronic inhomogeneities, hexaborides

Magnetic polarons are objects encountered frequently in nature, particularly in magnetic semiconductors and colossal magnetoresistive manganites. Magnetic polarons are quasiparticles resulting from the exchange interaction, and hence a spin alignment, between the spin of the conduction carriers with the localized spins of magnetic ions in the material. Their presence can strongly influence the material properties near phase transitions (an example here are metal-insulator transitions) and therefore, they have enormous potential for applications, e.g. in spintronics devices. Here we present direct evidence for polarons in  $\text{EuB}_6$  by visualizing their locally enhanced density of states combined with magnetic characterization of the cluster formation near its metal-insulator transition.

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## Phase separations and nematicity in dilute magnetic materials



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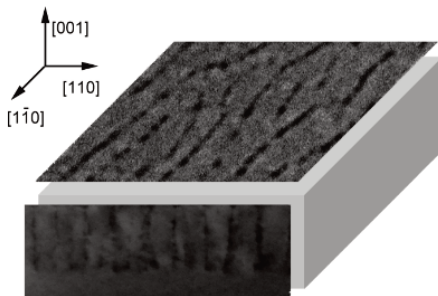
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**Keywords:** phase separation, nematicity, magnetic semiconductors

Semiconductors and topological materials doped with magnetic impurities show fascinating physics and nonspintronic functionalities associated with exchange coupling between band carries and localized spins [1]. However, d-shells of magnetic impurities contribute also to bonding, which can affect their spatial distribution and modify key properties, such as magnetic ordering temperature [2]. It has recently been demonstrated that in a class of dilute magnetic semiconductors the resulting phase separation is anisotropic and results in rotational symmetry breaking [3]. This finding shed a new light on a possible origin of nematicity in other systems, such as unconventional superconductors

and modulation doped semiconductor quantum wells, in which rotational symmetry breaking has so far been assigned to unidirectional spontaneous ordering of spin, orbital or charge degrees of freedom.



Non-uniform and anisotropic distribution of Fe cations (dark regions) in a zinc-blende (In,Fe)As layer visualized by electron microscopy. An average distance between Fe-rich lamellae is 10 nm. After ref. 3.

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## Atomic-scale imaging of strain-controlled emergent electronic states



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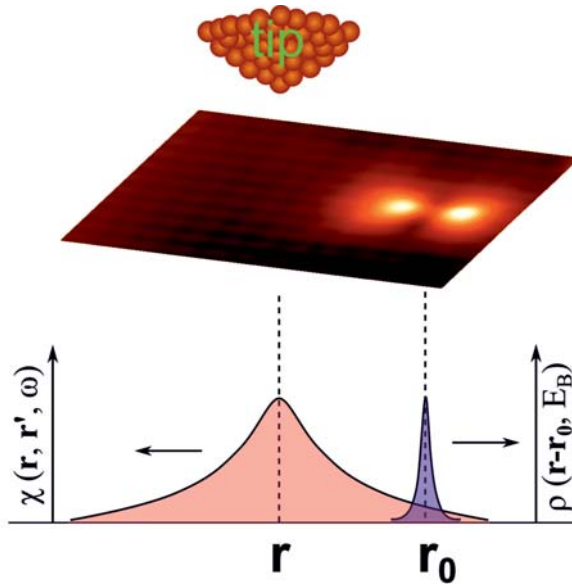
**Keywords:** iron-based superconductors, inelastic excitations, spin-polarized scanning tunneling microscopy and spectroscopy

Here we present new STM results on strain effect in strongly correlated electron materials, in particular iron-based superconductors like LiFeAs where the lattice symmetry is reduced from four-fold ( $C_4$ ) to two-fold ( $C_2$ ) [1]. Here we image by STM the influence of strain-tuned lattice distortions on the correlated electronic states in the iron-based superconductor LiFeAs, which in its ground state is tetragonal, with  $C_4$  symmetry while in a strained  $C_2$  symmetry phase exhibits a unidirectional charge density wave (CDW). In this electronic state the strain not only breaks rotational symmetry but also reduces translational symmetry through a long-range stripe-like modulation of the electronic density of states. The superconducting gap changes from the unstrained material with  $C_4$  symmetry to a phase with  $C_2$  symmetry and CDW order. The results show similarities with the effect of strain in reduction of lattice symmetry and in the formation stripes puddles in cuprates [2-3] and iron based superconductors [4-6].

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## Temporal holography of electromagnetic fields in ultrafast electron microscope



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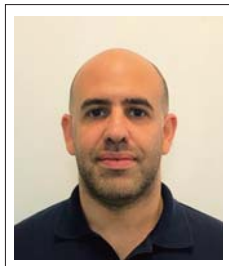
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**Keywords:** holography, ultrafast electron microscopy, imaging, plasmons, Rabi oscillations

Holography relies on the interference between a known reference and a signal of interest to reconstruct both the amplitude and phase of that signal. Commonly performed with photons and electrons, it finds numerous applications in imaging, cryptography and arts. With electrons, the extension of holography to the ultrafast time domain remains a challenge, although it would yield the highest possible combined spatio-temporal resolution. We will show that holograms of local electromagnetic fields can be obtained with combined attosecond/nanometer resolution in an ultrafast transmission electron microscope (UEM). Unlike conventional holography, where the signal and the reference are spatially separated and then recombined to interfere, in our method we use electromagnetic fields to split an electron wave function in a quantum coherent superposition of different energy states. In the image plane, spatial modulation of the electron-energy distribution reflects the phase relation between reference and signal fields, which we map via energy-filtered UEM. Beyond imaging applications, this approach allows implementing optically-controlled and spatially-resolved quantum measurements in parallel, providing an efficient and versatile tool for the exploration of electron quantum optics.

## The nature of the phase transition in the cuprates as revealed by a magnetic field free stiffness meter



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**Keywords:** superconductivity, stiffness, penetration depth, phase transition, cuprates

A new method to measure the superconducting (SC) stiffness tensor  $\bar{\rho}_S$ , without subjecting the sample to external magnetic field, is applied to  $\text{La}_{1.875}\text{Sr}_{0.125}\text{CuO}_4$  (LSCO). The method is based on the London equation  $\mathbf{J} = -\bar{\rho}_S \mathbf{A}$ , where  $\mathbf{J}$  is the current density and  $\mathbf{A}$  is the vector potential.  $\mathbf{A}$  is applied in the SC state, once the phase of the order parameter is constant; it remains so as long as  $\mathbf{A}$  is smaller than some critical value. Using rotor free  $\mathbf{A}$  and measuring  $\mathbf{J}$  via the magnetic moment of superconducting rings, we extract  $\bar{\rho}_S$  at  $T > T_C$ . The technique, named Stiffnessometer, is sensitive to very small stiffness, which translates to penetration depth on the order of a few millimeters. We apply this method to two different LSCO rings: one with the current running only in the  $\text{CuO}_2$  planes, and another where the current must cross planes. We find different transition temperatures for the two rings, namely, there is a temperature range with two dimensional stiffness. The Stiffnessometer results are accompanied by Low Energy  $\mu\text{SR}$  measurements on the same sample to determine the stiffness anisotropy at  $T < T_C$ .

## Enhancing Superconductivity by Disorder

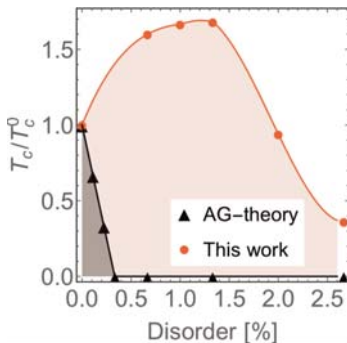


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**Keywords:** superconductivity, disorder, enhancing  $T_c$

We study two mechanisms for enhancing the superconducting mean-field transition temperature  $T_c$  by nonmagnetic disorder in both conventional (sign-preserving gaps) and unconventional (sign-changing gaps) superconductors (SC). In the first scenario, relevant to multi-band systems of both conventional and unconventional SC, we demonstrate how favorable density of states enhancements driven by resonant states lead to significant enhancements of  $T_c$  in the condensate formed by the near-Fermi-level bands. The second scenario focuses on systems close to localization where random disorder-generated local density of states modulations causing a boosted  $T_c$  even for conventional single-band SC. We analyze the basic physics of both mechanisms within simplified models, and discuss the relevance to existing materials.



Superconducting transition temperature versus disorder concentration

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## Charge vs. Spin Disorder in a Correlated Electron System



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**Keywords:** many body localisation, sub-diffusion, t-J model, correlated electron systems

In the first part [1] I will show that electron-magnon interaction delocalizes the particle in a system with strong charge disorder. The analysis is based on results obtained for a single hole in the one-dimensional t-J model. Unless there exists a mechanism that localizes spin excitations, the charge carrier remains delocalized even for a very strong charge disorder and shows subdiffusive motion up to the longest accessible times.

In the second part [2] I will present a study of dynamics of a single hole in one dimensional t-J model subject to a random magnetic field. Strong disorder that couples only to the spin sector localizes both spin and charge degrees of freedom. While we cannot precisely pinpoint the threshold disorder, we conjecture that there are two distinct transitions. Weaker disorder first causes localization in the spin sector.

Finally I will discuss the problem of a single electron in a random potential, coupled to different bosonic degrees of freedom [3].

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## Hidden order of Cooper pairs in striped cuprates at high magnetic fields



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**Keywords:** cuprates, stripes, novel states

The magnetic-field-tuned interplay of superconductivity with charge-ordered states in underdoped cuprates has been of great interest, but it remains an open question. We report the observation of an unanticipated, insulator-like ground state with strong superconducting phase fluctuations that emerges with field ( $H$ ) in underdoped Eu-LSCO and Nd-LSCO with striped charge order, suggesting an unprecedented freezing (i.e. “the hidden order”) of Cooper pairs. This novel state starts to develop already at temperatures comparable to the zero-field  $T_c$ , suggesting that it competes with the  $H=0$  superconductivity. The presence of stripes appears to play a crucial role in the freezing of Cooper pairs in this novel regime. Our findings offer a qualitatively new test of theoretical proposals for dominant orders in the charge-ordered region of the pseudogap phase in cuprates, and establish striped cuprates as a promising platform for exploring the long-standing problem of the field-tuned suppression of 2D superconductivity.

## **In situ ultrafast electronic thermometry via combined TR-ARPES and TR Raman scattering**



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**Keywords:** pump-probe experiments, in situ thermometry, XFEL, time-resolved ARPES, time-resolved Raman scattering

Do we or don't we have "thermal" hot electrons after a pump? How do the hot electrons relax? In recent work, we show that electrons coupled to phonons can never exactly fulfil the hot-electron paradigm, because once they have an equilibrium distribution, they no longer relax any further [1,2]. But how close can they be to a hot-electron model, and how can we determine these approximate temperatures? We discuss a number of issues related to ultrafast thermometry including how one can combine probes like photoemission and electronic Raman scattering to directly test for thermalization, which requires the fermionic and collective bosonic temperatures to be the identical [3]. We also describe how the strong temperature dependence in core-level x-ray photoemission spectroscopy sidebands or x-ray absorption spectroscopy satellites can be employed as an in situ ultrafast measure of the temperature (or total energy) of the electrons [4]. Interestingly, similar ideas employing rf spectroscopy are used in ultracold atomic physics to show how systems go from the quantum transport regime to the hydrodynamic regime [5]. Will XFELs enable similar experiments for solids in the ultrafast time domain?

**Acknowledgments** The formal work on relaxations, combining PES and Raman scattering probes, and the proposal to use XPS or XAS for in situ thermometry was supported under grant number DE-FG02-08ER46542 funded by the Department of Energy, Office of Science. The ongoing work



to implement this with XFELs is supported under grant number DE-SC0019126 funded by the Department of Energy, Office of Science.

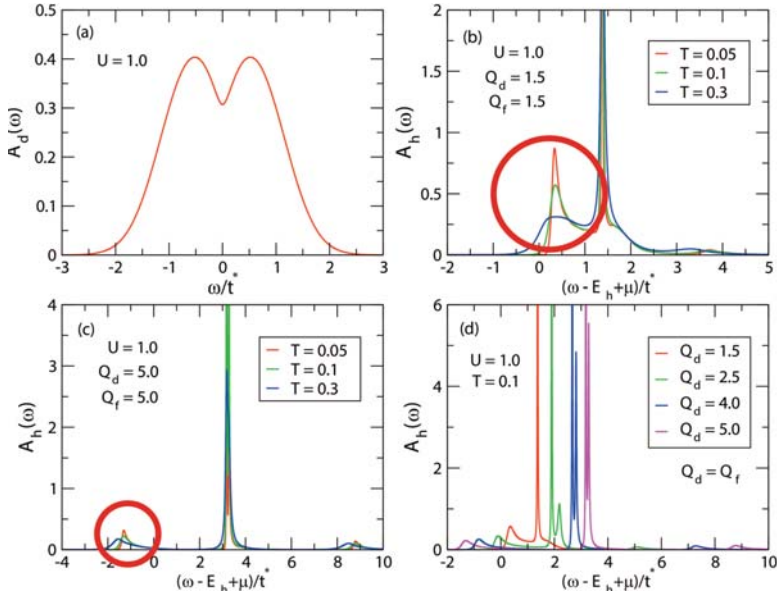


Image showing the conduction electron DOS (a) and the core-hole XPS signal (b-d). The red circle highlights the satellite peak features which depend strongly on temperature.

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## Photo-induced new collective modes and metastable states in cuprate superconductors



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We present near and mid-infrared pump c-axis terahertz probe measurement on hole and electron doped 214 superconducting single crystals (La<sub>1.905</sub>Ba<sub>0.095</sub>CuO<sub>4</sub> with  $T_c=32$  K and Pr<sub>0.88</sub>LaCe<sub>0.12</sub>CuO<sub>4</sub> with  $T_c=22$  K). The measurement reveals that the pump-induced change occurs predominantly at the Josephson plasma edge position below  $T_c$ . Upon excitation by the intense near- or mid-infrared pulses, the superconducting state is disturbed and incoherent quasiparticle excitations develop in frequency regime above the static plasma edge. However, within very short time delay we observe the reappearance of a very sharp Josephson plasma edge at frequency lower than the static Josephson plasma edge and the emergence of a new light-induced edge at higher energy. Then the effect keeps almost unchanged up to the longest measurement time delay 210 ps. The results suggest that the intense pump drives the system from a superconducting state with a uniform Josephson coupling to a new metastable superconducting phase with modulated Josephson coupling strengths.

## **Lattice-driven nonequilibrium magnetic dynamics in rare earth orthoferrites**



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Selective optical excitation of the crystal lattice can drive phase changes in materials with competing ground states. In this talk we will review the experimental technique of resonant excitation of infrared active phonon modes and its non-linear coupling to low-energy collective modes including magnons, polarons and Raman active phonons. We will discuss ultrafast lattice control of the magnetic insulating oxide DyFeO<sub>3</sub> whose energy landscape hosts competing anti- (AFM) and weak-ferromagnetic (wFM) orders. Resonant pumping of a lattice vibration promotes an ultrafast coherent transition from the AFM to the wFM state. Coherent ballistic switching between competing magnetic phases is demonstrated by resonant phonon pumping and accounted for by ultrafast control of the magnetic energy landscape.

## Nolinear change of semiconductors by THz-FEL irradiation



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**Keywords:** THz, FIR, FEL

A free electron laser (FEL) is constructed by an electron gun, a linear accelerator, and an undulator. There are several wavelength ranges from infrared to x-ray for FEL. The characteristics of FEL are; short pulse time structure, high intensity, variable wavelength, monochromatic, and high coherency in both time and space scales. Terahertz (THz) and/or far-infrared (FIR) is an electromagnetic wave located on the boundary between radio waves and lights. It behaves as a high-frequency oscillating electric field and also as a low-energy photon. Thus, by using the THz-FEL as a pump light source for the solid state electrons, novel excited states can be expected in the electronic materials. Recently, nonlinear interactions between semiconductors and intense THz wave (frequency: 2.5-7.5 THz, electric field:  $\sim 3$  MV/cm) have been investigated [1]. Under high photon flux irradiation by focused THz-FEL, a periodic structure formation was observed on the surface of semiconductor Si [2]. The structure, LIPSS in case of NIR region has been known soon after the invention of the ruby laser [3], but the experiments and theories were limited for nm wavelength scale up to now. The new results in THz-FIR region can give the break through for this situation including application development.

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## **Non-Hermitian properties of dissipative quantum gases with correlation**



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**Keywords:** Cold atoms, Nonequilibrium, Correlation

We study non-Hermitian properties of dissipative quantum gases with correlation. As a prototypical example, we address the Kondo effect in an open quantum system [1] motivated by recent experiments with ultracold alkali-earth(-like) atoms. Due to inelastic collisions and the associated atom losses, this system is described by a non-Hermitian extension of the Kondo problem. We show that the non-Hermiticity induces anomalous reversion of renormalization-group, leading to a unique quantum phase transition. Furthermore, by exactly solving the non-Hermitian Kondo Hamiltonian, we obtain the critical line consistent with the renormalization-group flow. If time allows, we also address a related but slightly different non-Hermitian phenomenon with strong correlation [2].

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## Higher-order topology in stacked graphene layers



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**Keywords:** Topological states of matter; higher-order topological insulators; multilayer graphene

Higher-order topological insulators are  $d$ -dimensional systems which feature  $d-n$  dimensional gapless states where  $n > 1$ . For example, a 3D system may feature protected 1D states on its hinges. In this talk I will introduce the  $Z_2$  topological invariant protecting such hinge states in the cases of four-fold rotoinversion and inversion symmetry, which will be defined in terms of symmetric hybrid Wannier functions of the filled bands, and can be readily calculated from the knowledge of the crystalline symmetry labels of the bulk band structure.

Using this invariant we prove the existence of higher-order topological insulators with protected chiral hinge modes in quasi-two-dimensional systems made out of coupled layers, stacked in an inversion-symmetric manner. In particular, we show that an external magnetic field drives a stack of alternating  $p$ - and  $n$ -doped honeycomb layers into a higher-order topological phase, which provides a strategy to construct such phases of matter.

## Electron-number density as a new dimensionless coupling constant in superconductivity



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**Keywords:** Boson-fermion models; BCS-Bose crossover; Two-hole Cooper pairs

The generalized Bose-Einstein condensation (GBEC) theory [1] is essentially an fully-interacting boson-fermion ternary gas made up of unbound electrons as fermions, two-electron Cooper pairs (2eCPs) and explicitly two-hole Cooper pairs (2hCPs), both as actual, real bosons. Subsumed in GBEC is the BCS-Bose crossover theory[2] extended with 2hCPs. For the extended crossover we find that its dimensionless electron-number density  $n/n_f$  plays the role of a new dimensionless coupling constant, where  $n$  is the total electron-number density and  $n_f$  that of unbound electrons at  $T = 0$ . For  $n/n_f = 1$  one recovers the weak-coupling or BCS regime, while for  $n/n_f \rightarrow \infty$  (with, e.g.,  $n_f \rightarrow 0$ ) one has the strong-coupling regime, e.g., an ideal Bose gas of 2eCPs. We calculate the energy gap, the critical temperature  $T_c$  and the gap-to- $T_c$  ratio. By slightly varying  $n/n_f$  one can reproduce the gap-to- $T_c$  ratio of several elemental superconductors—including the BCS-theory “bad actors” [3]. Moreover, using  $n/n_f$  one can determine the superfluid density  $n_s(T)$  which agrees well with empirical data [4,5].

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## Composite quasiparticles in strongly-correlated two-dimensional dipolar Fermi liquids



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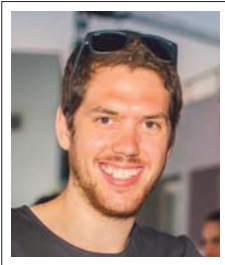
**Keywords:** Ultracold Fermi gases, quasiparticle properties, plasmarons

Strong particle-plasmon interaction in electronic systems can lead to composite hole-plasmon excitations. We investigate the emergence of similar composite quasiparticles in ultracold dipolar Fermi liquids originating from the long-range dipole-dipole interaction.

We use the G0W technique with an effective interaction obtained from the static structure factor to calculate the quasiparticle properties and single-particle spectral function.

We first demonstrate that within this formalism a very good agreement with the quantum Monte Carlo results could be achieved over a wide range of coupling strengths for the renormalization constant and effective mass. The composite quasiparticle-zero sound excitations which are undamped at long wavelengths emerge at intermediate and strong couplings in the spectral function and should be detectable through the radio frequency spectroscopy of nonreactive polar molecules at high densities.

## Detecting 2D Stiffness



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2D superconductors obey the London equation in the sense that their surface current  $J$  is proportional to the vector potential  $A$  via  $J = -r_{2D} * A$ , where  $r_{2D}$  is known as the stiffness. However, these superconductors cannot produce macroscopic currents, and are unable to expel magnetic fields. In other words, they lack the Meissner effect. Consequently, measuring their stiffness is no trivial. We present a new method, which bypass the Meissner effect, to determine  $r_{2D}$  based directly on the London equation.

## On the electronic structure in hydrogen superhydride $H_3S$



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The sulfur superhydride  $H_3S$  [1,2] has attracted enormous interest since the discovery of the 200K superconductivity in this material under extreme pressure. According to the previous studies, its  $T_c$  is boosted by the peaked structure in the density of states (DOS) [2-6] and its presence is robust against substitution of sulfur atoms to phosphorus etc. Its persistence has been thought to emerge through some complicated interplay of the sulfur 3s, 3p and hydrogen 1s orbitals but clear explanation on it has yet been established. We disentangle the “complicated interplay” to clarify how the DOS peak emerges.

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## Metallic Weyl ferromagnet in a kagome lattice



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**Keywords:** Weyl nodes, ferromagnet, spin reorientation

While several Weyl semimetals with broken centro-symmetry have been predicted and confirmed using ARPES technique, the search for Weyl semimetals with broken time-reversal symmetry has not been as fruitful. In this talk, I will present our recent work on a room temperature kagome ferromagnet that is magnetically and electronically interesting; it undergoes a spin reorientation, exhibits a large anomalous Hall effect, has attracted a large amount of interest due to the prediction of flat bands and associated fractional quantum Hall effect, has a skyrmion state at room temperature, and is predicted to have Weyl nodes at the Fermi level<sup>1</sup>.

Using local probes MFM and XMCD-PEEM, we directly imaged the nucleation and growth associated with the spin reorientation and show how the low temperature phase emerges and self organizes to coexist with the high temperature phase. Our band structure calculations using DFT predict the presence of Weyl nodes at or near the Fermi level which move depending on the magnetization direction. Although the predicted Weyl nodes cannot be confirmed in ARPES measurements, other features of the band structure calculation, such as Dirac-like points are consistent with our ARPES data validating our DFT calculations.

The band structure calculations can account for the so far mysterious spin reorientation transition and dramatic evolutions in electrical properties depending on the temperature and magnetic field. The dense magnetic domain patterns and phase coexistence in a ferromagnetic Weyl metal imply a complex inhomogeneous electronic structure, which will yield anomalous con-

tributions to the magnetic field and temperature-dependent electrical conductivity.

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## Quantum critical density-wave fluctuations in an optically doped iron oxypnictide

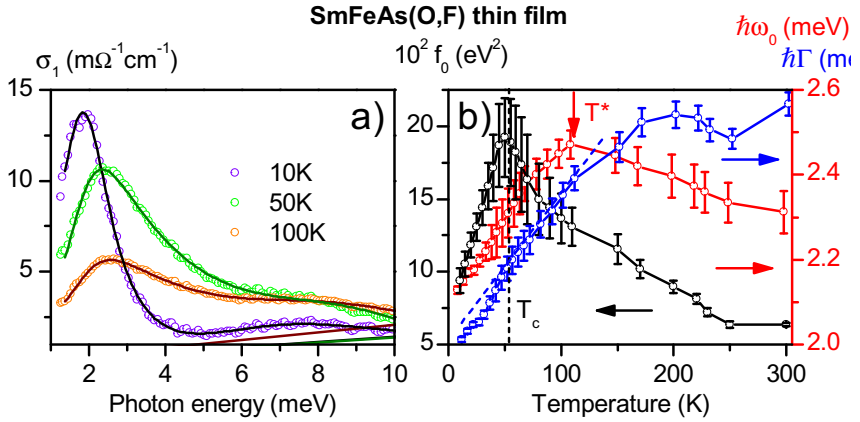


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**Keywords:** superconductivity, iron pnictides, quantum criticality, density wave, optical spectroscopy, time-domain THz spectroscopy, ellipsometry

We report the first determination of the in-plane complex optical conductivity of 1111 high- $T_c$  superconducting iron oxypnictide single crystals  $\text{PrFeAs}(\text{O},\text{F})$  and thin films  $\text{SmFeAs}(\text{O},\text{F})$  by means of conventional and microfocused infrared spectroscopy, ellipsometry, and time-domain THz transmission spectroscopy. A strong itinerant contribution is found to exhibit a dramatic difference in coherence between the crystal and the film. Using extensive temperature-dependent measurements of THz transmission, we identify a previously undetected 2.5-meV collective mode in the optical conductivity of  $\text{SmFeAs}(\text{O},\text{F})$ , which is strongly suppressed at  $T_c$  and experiences an anomalous T-linear softening and narrowing below  $T^* \approx 110\text{K} \gg T_c$ . The suppression of the infrared absorption in the superconducting state reveals a large optical superconducting gap with a similar gap ratio  $2\Delta/kBT_c \approx 7$  in both materials, indicating strong pairing.



(a) THz conductivity at three different temperatures revealing the thermal evolution of the density-wave collective mode. (b) Temperature dependence of the collective-mode oscillator strength (black symbols and line), energy (red symbols and line), and width (blue symbols and line) extracted from the fit in panel (a).

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## Topology in crystalline lattices



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**Keywords:** topology, crystal symmetry, time reversal symmetry

Topology has in the past decades become an organizing principle in the classification and characterization of phases of matter. While all possible topological phases of free fermions in the presence of external symmetries have been fully worked out, the inclusion of lattice symmetries relevant to any real-life material provides for an active research area.

In this seminar, I will present a classification of all possible gapped topological phases of non-interacting insulators with lattice symmetries, both in the absence and presence of time-reversal symmetry. This is done using a simple and intuitive counting scheme based on the symmetries of electronic band structures. Despite the simplicity of the procedure, it matches all predictions of the more mathematically involved K-theory where available, and goes beyond these known results by predicting new topological phases as well as a new type of topological invariant in symmetry classes that have not yet been successfully analysed within the context of K-theory.

The same straightforward counting can also be used to study transitions between crystalline topological phases. This allows us to list all possible types of such transitions for any given crystal structure, and accordingly stipulate whether or not they give rise to intermediate Weyl semimetallic phases. The presented procedure is ideally suited for the analysis of real, known materials, as well as the prediction of new, experimentally relevant, topological materials.

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## **Chiral anomaly phenomena in Weyl superconductors**



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**Keywords:** Weyl fermions, chiral anomaly, Weyl superconductors, chiral magnetic effect

We discuss chiral anomaly phenomena associated with Weyl quasiparticles in Weyl superconductors. We particularly focus on three phenomena; (i) superconducting analogue of chiral magnetic effect, (ii) negative thermal magnetoresistivity, and (iii) torsional chiral magnetic effect induced by skyrmion textures of superconducting order parameter.

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## Intrinsic low-energy magnetic excitations and bulk in-gap states in the candidate topological Kondo insulator $\text{SmB}_6$



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**Keywords:** Topological insulator, spin exciton, muon spin rotation

$\text{SmB}_6$  is a well-known Kondo insulator, believed to develop into a topological insulator at low temperatures. Yet while a true Kondo insulator is nonmagnetic, low-temperature magnetism is clearly present in the real material. By means of new muon spin relaxation/rotation measurements, we have disentangled extrinsic and intrinsic sources of low-temperature bulk magnetism. In particular, our measurements reveal intrinsic magnetism from apparently two different sources. Our findings suggest that there are thermally-activated magnetic excitations that hinder surface conductivity in  $\text{SmB}_6$  above  $\sim 4.5$  K. In addition, we detect underlying low-energy ( $\sim 100$  neV) weak magnetic moment fluctuations that are very similar to observations in the topological Kondo insulator candidate  $\text{YbB}_{12}$ . Potential sources of the intrinsic magnetism and open questions concerning the true ground state of  $\text{SmB}_6$  will be discussed.

## Topological phases by combining superconductivity and magnetism



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**Keywords:** topological superconductivity, correlated oxides, topological antiferromagnetic semimetals

After the great impact of topological insulators, there has been a significant expansion towards metals and semimetals (SMs) as well as quantum materials combining topological and conventional forms of order. The search for new variants of SMs recently highlighted the interplay of Dirac fermions physics and magnetism. Indeed, while most of the currently known SMs are non-magnetic, antiferromagnetic (AFM) SMs can be obtained where both time and inversion are broken while their combination is kept [1] or due to chiral- [1] and time-symmetry [1] combined with non-symmorphic transformations [1]. We discuss specific materials, i.e.  $t_{2g}$  oxide systems, that can exhibit AFM-SM phase due to emergent orbitally directional double-exchange effects. Due to the orbital directionality, the competition between antiferromagnetic (AF) and ferromagnetic (FM) correlations uniquely makes antiferromagnetically coupled FM zigzag stripes and checkerboard clusters the dominant patterns in the phase diagram over a large range of doping. [2] Such zigzag AF states are representative of a class of non-symmorphic antiferromagnets with glide reflection symmetry. [1] As a result of the non-symmorphic symmetry, topological gapless phases with Dirac points/lines as well as semimetals with triple and quadruple band-crossing points are shown to occur.

Apart from the large variety of fundamental aspects related to Dirac systems, the combination with other type of conventional orders (e.g. mag-

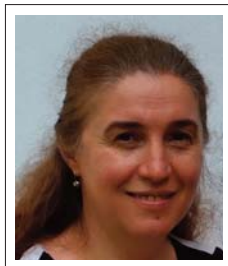
netism or superconductivity) represents an ideal testbed for achieving new phases of matter and single out materials for future technologies. In this talk we will discuss mechanisms and potential materials for achieving antiferromagnetic semimetals. Then, we consider the impact of s-wave spin-singlet pairing on AFM-SMs with Dirac points or nodal loops at the Fermi level [3]. The electron pairing is generally shown to convert the semimetal into a tunable nodal superconductor. The changeover from fully gapped to gapless phases is dictated by symmetry properties of the AFM-superconducting state that set the occurrence of a large variety of electronic topological transitions. We provide a general criterion for predicting a series of transitions between nodal and fully gapped superconducting phases. Different types of antiferromagnetic patterns are then employed to explicitly demonstrate the microscopic mechanisms that control the character of the quasiparticle spectrum [3].

Finally, I will review some quantum platforms marked by spin-singlet or triplet pairing interfaced with non-trivial magnetic patterns and discuss the nature of the emerging topological superconductors [4,5,6].

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## Common trends in the electronic behaviour of $\text{FeSe}_{1-x}\text{S}_x$ tuned by pressure



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**Keywords:** fermiology, superconductivity, pressure

Quantum oscillations studies on the nematic superconductors  $\text{FeSe}_{1-x}\text{S}_x$  under applied pressure are reported. We show the common trends in the Fermi surface behaviour and the unusual changes in the electronic correlations across the nematic phase transitions [1,2].

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2. P. Reiss, D. Graf, A. A. Haghighirad, et al. Quenched nematic criticality separating two superconducting domes in an iron-based superconductor under pressure arXiv preprint arXiv:1902.11276

## Quantum-oscillation Fermiology of 1111 and 11 iron-based superconductor (parent) compounds



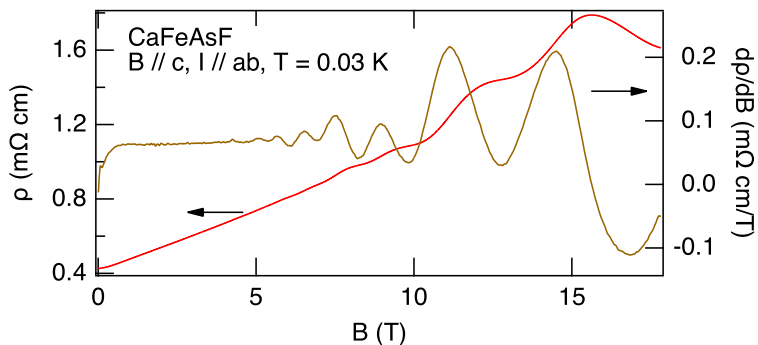
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**Keywords:** Iron-based superconductor, quantum oscillation, Fermi surface

I report on quantum oscillation measurements on CaFeAsF [1] and FeS [2]. CaFeAsF, a variant of the 1111 iron-pnictides, is paramagnetic at room temperature and exhibits a structural and an antiferromagnetic transition at  $T_s = 121$  K and  $T_N = 110$  K, respectively. We have performed Shubnikov-de Haas measurements on high-quality single crystals of CaFeAsF grown by Ma et al. [3] in the antiferromagnetic state and determined that the Fermi surface consists of a hole and a symmetry-related pair of electron cylinders. Analyses of oscillation phases indicate that the electrons are Dirac fermions.

Hydrothermally-synthesized tetragonal FeS is paramagnetic and exhibits superconductivity below  $\sim 5$  K. We have performed de Haas-van Alphen measurements on single crystals of FeS [4]. Combining the dHvA data and quasiparticle self-consistent GW calculations, we have determined the Fermi surface with accuracy better than 0.2% of the Brillouin zone area.



Resistivity and its oscillatory part as a function of magnetic field in CaFeAsF

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## Nematic fluctuation and nematic resonance in iron based superconductor via Raman scattering spectroscopy



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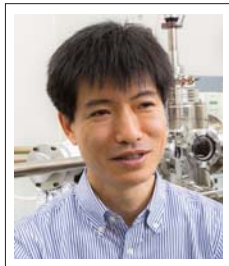
**Keywords:** Iron based superconductors, nematic fluctuation, Raman scattering spectroscopy

Various iron-based superconductors show the in-plane anisotropy of the electronic properties, so-called “electronic nematicity” above the structural/magnetic transition temperature. [1-3] In this work, we have investigated the doping dependence of the nematic Raman response for P-doped Ba122 system. The nematic susceptibility has been estimated from the B1g Raman scattering spectra, and its temperature dependence can be fitted by the Curie-Weiss law. [4,5] The Curie-Weiss temperature is the bare nematic transition temperature  $T_0$ .  $T_0$  decreases with P doping and becomes 0 K very near the magnetic/structural quantum critical point (QCP), indicating that the nematic QCP exists near magnetic/structural QCP in this system. In the optimally doping region, the pair breaking peak and the nematic resonance one appear below  $T_c$  in B1g spectra. The existence of nematic resonance peak suggests the correlation between the superconductivity and the nematic fluctuation.

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## **On the zero-energy bound state in the vortex cores of Fe(Se,Te)**



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**Keywords:** Majorana bound state, topological superconductivity, vortex, SYM/STS

We will present our recent STM/STS results on the vortex cores of the possible topological superconductor Fe(Se,Te). We will argue the relevance of the Majorana state as the origin of the zero-energy bound state in the vortex core.

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## Size restricted magnetotransport in the non-magnetic delafossite metals PdCoO<sub>2</sub> and PtCoO<sub>2</sub>



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**Keywords:** Electron hydrodynamics, high-conducting oxides

Ultra-pure delafossite metals can present bulk mean free paths as long as tens of microns, long enough such that the momentum conservation of the electron fluid might play a role in electrical transport. As the signatures of this are most prominent in the mesoscopic limit, we use focussed ion beam (FIB) techniques to thin down bulk samples, down to widths as small as submicron, much smaller than the bulk mean free path. In this talk I will present magnetotransport measurements in these highly-conducting delafossites at the mesoscopic limit. Magnetic field introduces a variable length-scale, the cyclotron radius, in the system which can be used to tune through different transport regimes. I will discuss the ballistic and hydrodynamic signatures in the transport that becomes accessible through magnetic field tuning in the mesoscopic samples of the non-magnetic delafossites PdCoO<sub>2</sub> and PtCoO<sub>2</sub>.

## High pressure direct synthesis of some superhydrides: magnetic and structural studies



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The study of superhydrides under pressure holds great promises to approach ambient temperature superconductivity. Though many ab initio calculations have predicted the existence of such materials, only a few experiments have succeeded in synthesizing them, and while the recent results on H<sub>3</sub>S [1,2] and LaH<sub>10</sub> [3] - with T<sub>c</sub> measured as high as 260 K - give credit to these predictions, the experimental picture is not as clear as the numerical one. It is indeed of utmost importance now to fully characterize both the structure and the superconducting properties of a given pristine sample as to confirm or disprove theoretical calculations.

We elaborated a miniature diamond anvil cell (mDAC) allowing both x-ray diffraction structural characterization and SQUID magnetic measurements [4]. Several hydrides were synthesized from the reaction of hydrogen with metallic elements, and XRD data were obtained on pristine samples in regular DAC and mDAC. Our work on various polyhydrides such as CrH<sub>x</sub>, YH<sub>x</sub> and UH<sub>x</sub> will be presented, together with the principle of our mDAC.

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## **Photo-excited dynamic superfluid density, vortex-like Nernst effect and role of competing order in unconventional superconductors**



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Since the discovery of high- $T_c$  cuprate superconductors, the present author has proposed a few pictures based on phenomenological considerations of energy scales obtained by experimental measurements of muon spin relaxation, neutron scattering and other methods. The linear relationship between  $T_c$  and the effective Fermi temperature, derived from the equilibrium superfluid density, were discussed as a behavior which cannot be expected for BCS condensation, which favors Bose Einstein condensation of preformed charge pairs. Another linear correlation between  $T_c$  and the energy of the magnetic resonance mode observed by neutron scattering was discussed as representing the effect of competing antiferromagnetic order in reducing  $T_c$  from the BE condensation temperature of ideal non-interacting Bose gasses.

We now introduce two additional phenomena into this energy scale phenomenology. Since several years ago, Andrea Cavalleri and co-workers have observed emergence of transient superconducting-like signal in photo-excited optical conductivity measurements of cuprates and  $A_3C_{60}$  superconductors. The photo-induced measurements provide transient superfluid density and onset temperature of transient  $T_c$ . Since the early 2000's N.P. Ong and co-workers reported observation of the vortex-like Nernst effect signals and diamagnetic susceptibility well above  $T_c$  in cuprate superconductors, and this observation was followed by similar results in organic

BEDT and heavy fermion superconductors including URu<sub>2</sub>Si<sub>2</sub>. The onset temperature of the Nernst effect has not yet been compared to the density of paired and unpaired carriers above  $T_c$ .

The present author recently attempted to plot points for the onset temperatures of the photo-induced optical conductivity, vortex-like Nernst effect and diamagnetic responses in the plot of  $T_c$  versus the effective Fermi temperature derived from the equilibrium and transient superfluid density and relevant phase diagrams. This consideration has revealed that the onset temperatures of these effects can be identified as the point where the local phase coherence emerges among pre-formed bosonic charges in the normal state well above  $T_c$ . The actual superconducting condensation occurs well below this temperature due to the existence of the competing order.

In this talk, we present this picture with additional data of equilibrium and transient optical responses near the 400 cm<sup>-1</sup> frequency and the intensity comparison of this mode and the magnetic resonance mode in underdoped cuprates. Previously, vortex-like responses of pre-formed pairs in the normal states, associated with phase fluctuations of the order parameter, have been discussed based on two energy scales: pair formation energy  $T^*$  and the actual condensation temperature  $T_c$ . The present author proposes that the new concept of “local phase coherence” should be introduced, and the relevant energy scale  $T_{LPC}$  should be introduced as the third energy scale when superconductivity is competing with antiferromagnetic or other order. The transient superconducting responses in photo-excited studies and the vortex-like Nernst effect are observed not between  $T^*$  and  $T_c$  but between  $T_{LPC}$  and  $T_c$ .

## Quantum confinement and superconductivity



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**Keywords:** granular superconductivity, Mott transition , BCS to BEC crossover, Mott triggered BCS to BEC crossover in granular aluminum films.

A key prediction of modern theories of the Mott metal to insulator transition is that the electronic density of states remains finite up to the transition while the effective Fermi energy decreases towards zero. In the case where the metal is a superconductor and superconductivity subsists up to the transition, the superconducting gap and the effective Fermi energy will become necessarily of the same order. The strong coupling ratio should then rise above the BCS weak coupling limit. The Mott transition occurs when the Coulomb energy becomes of the order of the band width. This is difficult to achieve starting from a metallic state.

We have studied how the superconducting gap and the upper critical field of nano-scale granular aluminum films vary as the Al grains, a couple of nanometers in size, are progressively decoupled by increasingly thick  $\text{Al}_2\text{O}_3$  dielectric barriers between them. The idea is that the coherence length can then reduce up to the point where the number of pairs in a coherence volume is of order unity, electron confinement being enhanced by the electrostatic charging energy of the grains, and resulting in a The Mott transition [1] and to a BCS to BEC crossover. The films consist of about 10 grain layers, and should therefore be considered as 3D. Up to very high normal state resistivity values, of the order of 10,000 micro-ohm-cm, the gap structure as determined from the optical conductivity, remains well defined. As expected, the strong coupling ratio increases well beyond the BCS



weak coupling value. The values that we have measured are consistent with those calculated by Pisani et al. [2,3], The temperature dependence of the upper critical field varies from that of a conventional dirty limit Type II superconductor for well coupled grains metallic samples in which  $kF_l$  is larger than unity, to a behavior where it is limited by a combination of the orbital and of the Pauli critical fields. We will show that this behavior is also consistent with a BCS to BEC crossover. By contrast, near an Anderson metal to insulator transition superconductivity is quenched before the BCS to BEC crossover is reached, and the behavior that we report here cannot be observed [4].

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## **The evolution from BCS to BEC superfluidity in multi-band systems: Applications to two-band superconductors and ultra-cold Fermi gases**



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**Keywords:** Multi-band superfluids, BCS to BEC, unconventional pairing.

In the first part of the talk, I review some early work about the evolution from Bardeen-Cooper-Schrieffer (BCS) to Bose-Einstein Condensate (BEC) superfluids in the context of multiband systems. I focus primarily on three-dimensional s-wave two-band superfluids with a possible Josephson coupling between bands and discuss how collective modes evolve during the crossover from BCS to BEC superfluidity [1]. I also review the case where the Josephson interaction is tuned from negative to positive values leading to a quantum phase transition. In addition, I show that population imbalances between the two bands can be created by tuning intraband or interband interactions. Furthermore, I discuss the critical temperature of two-band superfluids, obtain the resulting coupled Ginzburg-Landau equations and show that they reduce to coupled Gross-Pitaevskii equations for two types of bosons in the BEC limit [2, 3]. In the second part of the talk, I present unpublished results on the evolution from BCS to Bose superfluidity for two-band fermions in two dimensions, including the cases of two particle (two hole) bands or of one particle and one hole bands. In these cases, I discuss also the critical temperature, the superfluid density tensor of the system and the resulting vortex-antivortex structures in connection to the Berezinskii-Kosterlitz-Thouless (BKT) transition [4]. For the two-dimensional case, possible connections are made to experimental systems

consisting of two-band ultra-cold fermions such as 6Li or 40K, as well as, of two-band superconductors such as FeSe.

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## **Accounting for the experimental fraction of preformed pairs in the BCS-BEC crossover**



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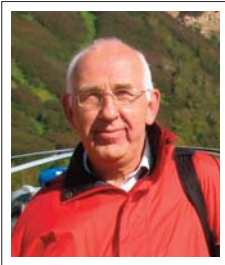
**Keywords:** degenerate Fermi gases, quantum fluids, BCS-BEC crossover, pairing in the normal phase

In a recent manuscript [1] the total number of fermion pairs in a spin-balanced two-component Fermi gas of  $6\text{Li}$  atoms was experimentally investigated in the normal phase above the superfluid critical temperature, in order to distinguish between the sectors of pseudogap and preformed-pair in the temperature-coupling phase diagram. Here, we present a theoretical account of these experimental results in terms of an ab-initio self-consistent t-matrix calculation, which emphasizes the role of the pair-correlation function between opposite-spin fermions at equilibrium. Excellent agreement is found between the available experimental data and the theoretical results with no adjustable parameter.

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## Temperature dependent electronic structure of cuprates



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**Keywords:** strong electron correlations, cluster perturbation theory, polaron band structure

The generalized tight binding (GTB) method to calculate the electronic structure of strongly correlated electrons in cuprates is modified to incorporate also strong electron-phonon interaction. By exact diagonalization of the p-d- Holstain model Hamiltonian for a separate CuO<sub>6</sub> unit cell we find the multielectron and multiphonon local eigenstates that are used to construct a set of local Hubbard operators. Then we treat the intercell electron hopping  $t$  by the perturbation approach over small ratio  $t/U$ , where  $U$  is the charge transfer excitation energy. Without electron-phonon interaction we obtain the band of spin polaron and a set of local multiphonon Franck-Condon excitations. The electron-phonon interaction results in the hybridization of spin polaron and Franck-Condon excitations that forms the polaronic band structure with strong temperature dependence. The temperature dependence of the polaronic band structure and Fermi surface is discussed. The peak of a spectral function at the top of the valence band has large width typical to the ARPES data and determined by a large number of the multiphonon excitations.

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## Critical pattern formation at the Mott metal-insulator transition



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**Keywords:** strongly correlated electronic systems pattern formation fractal scale-free

We discuss the critical pattern formation of metallic and insulating nanoscale domains observed in  $\text{NdNiO}_3$  [1] and  $\text{VO}_2$  [2] which undergoes a reversible metal-insulator-transition (MIT) near room temperature [3] via scanning near-field optical microscopy. The electronic phase transitions of these materials hold promise for novel ways to encode and process information, of interest for developing memristors and neuromorphic devices. Using theoretical tools from fractal mathematics and disordered statistical mechanics, we use the rich spatial information of this scanning probe in order to diagnose criticality from the spatial structure alone, without the need of a sweep of temperature or external field. The observed pattern formation points toward a combination of quenched disorder and interactions as the driving mechanism of the power law spatial organization of the domains.

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## **Landau Theory of Disorder-Driven Metal-Insulator Transitions**



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**Keywords:** Correlations and Disorder

We formulate a Landau theory of disorder-driven metal-insulator transitions, for electrons coupled to generic bosonic collective modes, which becomes exact in the limit of large spatial dimensions. This formulation is able to capture non-perturbative, disorder-enhanced polaronic effects, that provide a new driving force for the transition. In contrast to traditional approaches to interaction-localization, our new saddle point formulation suggests a finite upper critical dimension for the transition, also allowing for systematic studies of fluctuation corrections in finite dimensions.



## Complex nanoscale phase separation in quantum materials as seen by synchrotron x-ray micron beam techniques



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**Keywords:** Topology, complex quantum materials, fluctuations, spatial statistics

Complex quantum materials present structural units kept together by weak interactions giving rise to different spatio-temporal configurations at nanoscale and mesoscale [1]. These units are due to different order degrees due to electronic charge and spin connected with lattice distortions and quenched disorder [2-7] where the functionality is driven by doping and strain as shown in cuprates [8] diborides [9] and iron based superconductors [10]. The spatial fluctuations of these configurations play a crucial role in the complex quantum materials functionality. In order to visualize the fluctuations between these configurations we have used advanced methodologies based on spatial scanning using focused X-ray synchrotron beam and statistical tools for data analysis [11]. Here we present recent results on the connections between the nanoscale and mesoscale geometry and the functionality in cuprates and nickelates. Focusing in  $\text{La}_{1.72}\text{Sr}_{0.28}\text{NiO}_4$ , [12] we find the coexistence of different spin and charge striped puddles with a complex nanoscale phase separation. At low temperature, we distinguish the quantum fluctuations from the thermal fluctuations. Finally, we discuss the similarity of complexity of conformational fluctuations in this complex quantum matter and fluctuations in biological and supramolecular assembly [13-16].

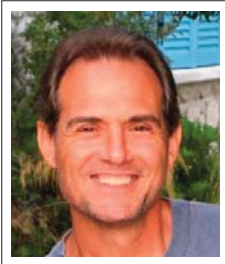
I thank my collaborators Alessandro Ricci, Nicola Poccia, Bobby Joseph, Markus Braden, Christian Schussler-Langeheine, Alexey Zozulya, Michael

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## **From Mott to not: phenomenology of overdoped cuprates**



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New experimental data on superfluid density and terahertz conductivity of overdoped LSCO have exhibited behavior incompatible with a clean BCS superconductor. Many of the properties observed are however compatible with “dirty d-wave theory” assuming weak scattering by dopant atoms. Here we test these ideas by comparing to specific heat and thermal conductivity data on LSCO, showing that the theory works extremely well across the overdoped region for similar disorder parameters. We then study the same properties in another overdoped cuprate, Tl-2201, thought to be quite “clean” since it exhibits quantum oscillations, low residual resistivities and small superconducting state Sommerfeld coefficients. Our results are consistent with the Tl-2201 system being  $\sim 3$  times cleaner due in part to the dopant atoms’ being located further from the  $\text{CuO}_2$  plane. We conclude that overdoped cuprates can be described semiquantitatively by dirty d-wave theory, subject to significant Fermi liquid renormalizations, without introducing physics beyond the Landau-BCS paradigm.

## Electronic properties of monolayer MoS<sub>2</sub> and MoS based heterostructures



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Layered atomically thin materials, including graphene, hexagonal boron nitride and layered transition metal dichalcogenides, have been a revolution in condensed matter physics and they are at the forefront of recent scientific research. They are being explored for their unusual electronic, optical and magnetic properties with special interest in their potential uses for sensing, information processing and memory. Among the semiconducting two-dimensional (2D) transition metal dichalcogenides, MoS<sub>2</sub> is the prototypical material due to its stability, relatively low cost, and unique electronic, optical and mechanical properties. An interesting property of 2H-MoS<sub>2</sub>, and in general of 2D materials, is the huge flexibility in tuning of their electronic properties.

A change in the nature and size of the band gap has been reported as a function of the numbers of layers and explained in terms of a redistribution of the band structure with a downshift of states at the G point and a transition from indirect to direct band gap at K point of the Brillouin zone when the thickness is reduced from two to one unit cell [1]. Using high resolution

scanning tunneling microscopy and spectroscopy (STM/STS), coupled to Green's function based calculations, we investigated the electronic properties of MoS<sub>2</sub> as a function of the number of layers at the nanoscale and highlighted the nature of the shift of the valence band edge and the role of the interfacial Sulphur atoms [2]. Furthermore, STM/STS, Kelvin probe force microscopy, and transmission electron microscopy were used to obtain quantitative measurements of the local density of states, work function and nature and mobility of defects (vacancies, film edges and grain boundaries) [3].

The ability to control nanoscale electronic properties by strain has been proposed long ago for layered cuprates [4] diborides [5], iron-based superconductors [6] and it is of critical importance for the implementation of 2D materials into next generation strain engineering devices. Single-layer MoS<sub>2</sub>, like graphene, exhibits flexibility out of plane coupled with a high intrinsic tensile strength allowing the film to sustain up to 11% strain before rupturing [7,8]. This intrinsic property not only produces a large range for tuning in possible strain engineering applications but also elects these materials as prime candidates for components in future flexible devices such as mountable physiological monitoring devices, touch screens and flexible energy storage systems [9]. We used STM/STS to correlate the atomic-scale lattice deformation with local electronic properties as a function of systematic macroscopic bending of monolayer MoS<sub>2</sub> films and characterized nanoscale strain [10]. We are able to induce strains of up to 3% before slipping effects take place and relaxation mechanisms prevail. We find a reduction of the quasiparticle bandgap of about 400 meV per percent local strain measured with a minimum gap of 1.2 eV [10].

Heterostructures based on MoS<sub>2</sub> offer another viable possibility to further tune its electronic properties [11]. In these heterostructures, interactions between the planes of different materials are indeed expected to modify the electronic properties of the constituent materials and open unprecedented possibilities of combining them for technological use.

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## Current progress in high temperature superconducting nano-devices using novel “van der Waals technologies”



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The strong variations in superconducting critical temperature among complex cuprate perovskites, that have identical hole density, indicates the importance of lattice modulation effects. The one-dimensional incommensurate lattice modulation of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+y}$ , [1] where the average atomic positions are perturbed beyond the unit cell, is an ideal case where to study the interplay between superconductivity and the one-dimensional incommensurate lattice fluctuations. Here we report nano X-ray diffraction imaging of incommensurate lattice structure in a bulk  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+y}$  ( $T_c = 90\text{K}$ ) down to a 2 u.c van der Waals heterostructure [2,3]. Despite the atomically thin heterostructure, the superconducting critical transition temperature is identical

to the bulk devices and the long- and short range incommensurate lattice modulations are still detected. The incommensurate lattice modulations are spatially correlated and fluctuate respect the average wavevector, showing a strain dependence with the substrate. Which is in agreement with the key role of strain in quantum materials at atomic limit [4-6]. We correlate the structural and transport data by measuring the Hall-effect down to two unit cells. We establish quantitative agreement between theory and data through the observation of the the Hall sign reversal far above  $T_C$  [3]. We have thus bridged the gap between low temperature superconducting films (where Hall sign reversal occurs above  $T_c$  due to superconducting fluctuations) and cuprates (where Hall sign reversal was previously believed to occur below  $T_c$  and as the result of vortex dynamics). The newly developed techniques that allow the atomically thin incorporation of BSCCO into van der Waals heterostructures opens the possibility of a new generation of extremely sensitive nanodevices for the search and study of high temperature superconductivity and their interplay with other van der Waals crystal systems.

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## Pressure driven superconductivity in topological materials



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Pressure-dependence of electric transport and crystal structure of topological insulator,  $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$ , in which the Fermi level and Dirac point are well controlled with  $x$  and  $y$  [1], is systematically investigated. These compounds showed no superconductivity down to 2.5 K at ambient pressure, and the crystal showed rhombohedral structure (space group of  $R\bar{3}m$ , No. 166), called as ‘phase I’. The  $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$  crystal showed two structural phase transitions, such as rhombohedral structure (phase I) to monoclinic one (phase II), and the phase II to the other monoclinic structure (phase III). Moreover, the additional monoclinic phase (phase II’) was often present with phase II and phase III. Exactly saying, the Phase II’ was observed in  $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$  at  $x \neq 0$ . Interestingly, the pressures causing the first and second structural phase transitions increased with increasing  $x$ . The superconductivity appeared when applying pressure. Actually, the superconductivity of all  $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$  samples emerged in phase I, and the pressure at which the superconductivity appears monotonically in-

creased with increasing  $x$ . The detailed research on superconductivity under pressure was achieved in this study, and the topological nature of superconductivity was clarified.

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## AgFBF<sub>4</sub>: possibly the most strongly coupled and nearly one-dimensional quantum antiferromagnet



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For about two decades it has been known that silver(II) fluorides exhibit pronounced similarities to undoped copper(II) oxides, particularly in terms of crystal and electronic structure including strong hybridization of metal and nonmetal states. [1] A decade ago similarity in terms of magnetic superexchange has been theoretically predicted, [2] which was confirmed in subsequent theoretical[3,4] and experimental studies. [5] Here, following theo 3,4] we have experimentally investigated AgFBF<sub>4</sub> which is a rare example of one-dimensional[6] antiferromagnet with d(z<sup>2</sup>)[1] ground state (“inverse” Jahn-Teller effect). Its crystal structure features nearly ideally linear infinite chains [AgF<sub>2/2</sub>]<sup>+</sup> with very short Ag–F separations of *ca.* 2.0 Å, *i.e.* several % shorter than for alkali metal fluoroargentates(II). Within the framework of the Goodenough-Kanamori rules, both features that very strong antiferromagnetic intra-chain coupling is expected, which was indeed suggested in recent theoretical studies.[3,4] with the predicted superexchange constant of *ca.* 300 meV.

Since the inelastic neutron scattering (INS) study at ISIS-RAL failed to detect spin wave excitations,[7] and the muon spin rotation (μSR) spectroscopy showed that this system is not ordered above 75 mK,[8] the lowest temperature reached in our experiments, we have turned to optical spectroscopy, which has previously proved useful for detection of spinon + phonon absorption in Sr<sub>2</sub>CuO<sub>3</sub>. [9] Using an absorption spectrometer operating in 3,500–12,000 cm<sup>-1</sup> range, and equipped with the integration

sphere for minimization of scattering and reflectivity losses, we have been able to detect a broad band centered at *ca.*  $4300\text{ cm}^{-1}$  ( $533\text{ meV}$ ). This band is absent for an  $\text{AgF}_2$  reference sample (a two dimensional and much less coupled antiferromagnet) which suggest its magnetic origin.[10] Since the wavenumber of the assisting Ag–F intra-chain stretching optically active phonon, which is strongly coupled to spin excitations, is  $575\text{ cm}^{-1}$ , one may deduce that intra-chain  $J$  equals  $294\text{ meV}$  (theoretical value  $298\text{ meV}$ )[3]. Thus, it is 20% larger than the corresponding value for  $\text{Sr}_2\text{CuO}_3$  ( $241\text{ meV}$ )[10]. Simultaneously, the very low ordering Néel point (below  $75\text{ mK}$ ) suggests huge anisotropy,  $J'/J$ , of  $6 \times 10^{-6}$  at most, *i.e.* two orders of magnitude more pronounced than for  $\text{Sr}_2\text{CuO}_3$  ( $7 \times 10^{-4}$ )[13], and rendering  $\text{AgFBF}_4$  *the* model one-dimensional system.[12]

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## Extremely anisotropic $(\text{LaSe})_{1.14}(\text{NbSe}_2)$ misfit layer superconductors



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Extremely anisotropic  $(\text{LaSe})_{1.14}(\text{NbSe}_2)$  [1] and  $(\text{LaSe})_{1.14}(\text{NbSe}_2)_2$  misfit layer superconducting single crystals with the superconducting transition  $T_c$  around 1 K and 5 K, resp., are studied by means of the transport measurements and scanning tunneling microscopy and spectroscopy at very low temperatures and in high magnetic fields. The in-plane upper critical fields strongly exceed the Pauli limit reminding the Ising superconductivity in monolayer of  $\text{NbSe}_2$  [2]. The tunneling density of states indicate non-conventional superconductivity. Fourier transform of the surface topography maps shows besides the Bragg peaks due to hexagonal  $\text{NbSe}_2$  lattice also a long range modulation in the misfit direction and additional structures. Spectroscopy Imaging STM conductance maps at energies close to Fermi level are recorded to get quasiparticle interference patterns for study of the electronic structure in the systems.

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## FeSe under uniaxial strain



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**Keywords:** FeSe, Uniaxial Strain, Resistive Anisotropy, Nematicity

In many high-temperature superconductors the rotational symmetry is broken as a precursor of the superconducting state [1,2]. In FeSe this broken symmetry, the electronic nematic order, leads to an anisotropy in the electronic transport and a spontaneous lattice distortion. In our experiment we are using uniaxial strain to continuously tune the crystal structure and its nematic order. With a sample-on-platform technique compressive and tensile stresses can be applied up to 0.6% of this very ductile material. This allows us to access the phase diagram from the completely twinned to the fully detwinned state. We show the non-monotonic elastoresistance in the low temperature regime, the contribution of domains to electrical transport and the dependence of  $T_C$  to strain applied along the Fe-Fe bond direction. This results old works showing the key role of strain to control functionality of quantum matter [3-5].

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## **Strongly interacting Weyl semimetals**



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We examine the impact of Coulomb interactions on the electronic structure of Weyl semimetals using a combination of analytical methods and diagrammatic Monte Carlo simulations. In particular, we address the stability of the semimetallic phase, qualitative changes to quasiparticle behaviour due to many-body effects, and whether nodes of higher topological charge survive strong interactions.

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## Complex ground state evolution and charge ordering following sub-mesoscale oxygen ordering in non-stoichiometric $\text{Pr}_2\text{NiO}_{4+d}$



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Like an oxygen sponge,  $\text{Pr}_2\text{NiO}_{4+d}$  can reversibly uptake oxygen in the range  $0 < d < 0.25$  via a topotactic intercalation reaction performing at ambient temperature. We report here on single-crystal synchrotron diffraction experiments on  $\text{Pr}_2\text{NiO}_{4+d}$ , uncovering unprecedented oxygen ordering up to the meso-scale. The corresponding commensurate unit cells show an increase of the parent unit cell by 3 orders of magnitude.

A full description of the complex oxygen ordering is given here for the first time, allowing to further evidence related charge ordering. For both phases we found the segregation into a mixed checkerboard and stripe charge ordering at 80K, the different modulation vectors of the stripe charge ordering being directly scaled with the respective incommensurate oxygen ordering.



## **Second critical temperature in the Bardeen-Cooper-Schrieffer superconductors**



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Bardeen-Cooper-Schrieffer (BCS) theory describes superconducting transition as a single critical point where the gap function or, equivalently the order parameter vanishes uniformly in the entire system. We demonstrate that in a superconductor described by a BCS model, superconducting gap should survive at surfaces at higher temperatures than superconductivity in the bulk. Therefore conventional superconductors have multiple critical points associated with separate phase transitions at surfaces and bulk. We show that by revising the Caroli-De Gennes-Matricon theory of a superconductor-vacuum boundary and finding robust inhomogeneous solutions of the BCS gap equation near boundaries, which asymptotically decays in the bulk. The analytical results are confirmed by numerical solutions of the microscopic model. This resolves the long standing question about the origin of the discrepancies between the critical temperatures observed in calorimetry and transport probes and provides a geometric design principle for achieving more robust superconductivity in devices.

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## Observation, control, and understanding of coupled multiferroic domains in conical spiral magnetoelectrics



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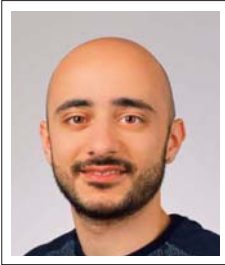
**Keywords:** magnetoelectric, multiferroics, noncollinear magnetic order

In this presentation, we show selective observations, control, and understanding of coupled magnetic domains which coexist in conical spiral multiferroics. Examples of such multiferroics are hexaferrites (e.g.,  $\text{Ba}_{1.3}\text{Sr}_{0.7}\text{CoZnFe}_{11}\text{AlO}_{22}$ ) showing the so-called alternating longitudinal conical structure [1] and olivine-type manganese germanate  $\text{Mn}_2\text{GeO}_4$  showing canted antiferromagnetic conical spin chains [2,3]. For the observations, we adopted single-crystal measurements of scanning resonant x-ray microdiffraction for the hexaferrites or (un)polarized neutron scattering and optical second harmonic generation for the manganese germanate. These techniques clarify multiple magnetic order parameters and domain structures and their manipulations by external stimuli such as magnetic and electric fields in these peculiar multiferroics. This work has been done in collaboration with H. Ueda, Y. Tanaka, Y. Wakabayashi, T. Honda, J. S. White, M. Kenzelmann, A. B. Harris, N. Leo, and M. Fiebig.

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## Probing spin and orbital degrees of freedom in quantum materials with time-resolved Resonant Inelastic X-ray Scattering



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The capability of Resonant Inelastic X-ray Scattering (RIXS) of probing elementary excitations involving different degrees of freedom makes this technique a powerful tool for the study of quantum materials [1,2]. The advent of FEL sources enables pump-probe schemes, extending its capabilities to the time domain [3].

In  $V_2O_3$ , it is of great interest disentangling the role of different degrees of freedom in driving the metal-to-insulator (MIT) transition [4]. We use an infrared pump to transiently induce the MIT and V L-edge RIXS to unveil the resulting ultrafast dynamics of the orbital structure, encoded in the evolution of the dd-excitations.

In the spin-chain  $CuGeO_3$ , the relation between charge, spin and lattice degrees of freedom, giving rise to the Spin-Peierls transition, is still unclear. With time-resolved RIXS, we study the interplay between non-local charge excitations and spin correlations: we use a UV laser pulse to excite carriers across the charge gap and O K-edge RIXS to probe the resulting evolution of the Zhang-Rice singlet excitations, connected to the dynamics of the short-range magnetic correlations.

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## Ultrafast THz and ARPES Studies of Electronic Correlations in Quantum Materials



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**Keywords:** Ultrafast Dynamics, Strongly Correlated Materials, Terahertz Spectroscopy, Angle-resolved Photoemission, Excitons

In the study of complex materials, ultrashort light pulses provide a powerful means to both interrogate perturbative ground-state interactions and to induce non-thermal transient phases. I will discuss our experiments using ultrafast THz and ARPES spectroscopies to capture transient correlations across the electronic and vibrational Brillouin zones in quantum materials. In stripe-phase nickelates, tracking zone-folded resonances of the THz-frequency bending-mode vibrations provides direct insight into the dynamic coupling between atomic-scale electronic and lattice order during stripe melting and formation [1]. In turn, time-resolved ARPES (tr-ARPES) is of great interest to track dynamics of electronic bands and quasiparticles directly in momentum space via the single-particle spectral function. Our capability for extreme-ultraviolet tr-ARPES at high repetition rates and its application to studies of transition-metal dichalcogenides will be discussed [2]. In particular, this allowed us to observe the momentum-space photoelectron signatures of Coulomb-bound band-gap excitons [3]. Such access to electronic dynamics across the full Brillouin zone with high sensitivity opens up novel opportunities for ultrafast measurement and control of superconducting and charge-ordered systems.

Work performed in jointly with G. Coslovich, J. H. Buss, F. Joucken, J. Maklar, H. Wang, Y. Xu<sup>1</sup>, A. Lanzara, Z. Hussain, S. Tongay, T. Sasagawa, and A. F. Kemper.

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## **Photo-induced skyrmion dynamics studied by ultrafast Lorentz electron microscopy**



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**Keywords:** Ultrafast electron microscopy; skyrmion;

Magnetic skyrmions are topologically nontrivial spin texture in chiral magnets which would be stable carriers of information in future spintronics and memory devices [1]. Various external stimuli have been applied to realize a precise control of the skyrmion dynamics. However, benefits of the topological stability at short time scales have not been experimentally confirmed. Here we report a real-space visualization of ns-ms skyrmion dynamics in a chiral magnet thin film by employing ultrafast Lorentz electron microscopy. The initially helical stripes are converted into distorted skyrmions via supercooling by ns laser irradiation. By employing this metastable state for the pump-probe experiment, we observe the division of the skyrmions in ns-scale and subsequent slower dynamics such as expansion, drift motion and recombination. We will discuss the possible contribution of the topological protection to the skyrmion dynamics.

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## Higgs spectroscopy for periodically driven unconventional superconductors



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**Keywords:** Superconductivity, Nonequilibrium, THz-spectroscopy, Third-harmonic generation, Higgs spectroscopy

Higgs spectroscopy for superconductors in nonequilibrium is a new method to obtain phase-sensitive information about the underlying gap symmetry. One experimental setup to observe the Higgs mode is third-harmonic generation (THG), where the driving frequency of a multicycle THz pulse is brought in resonance with the Higgs mode. This was already successfully demonstrated for s-wave superconductors.

We show that THG can be used to observe also additional Higgs modes predicted to occur in d-wave superconductors. They show up as a second resonance in the THG response. Such an additional resonance was found in recent THG experiments on cuprates and can be explained by our theory. This theory is not limited to d-wave superconductors but applies in general to any gap symmetry where multiple Higgs modes are possible. Thus, THG experiments extend the repertoire of Higgs spectroscopy experiments and can be used for the identification of gap symmetries of unconventional superconductors.



## Time-resolved reflectivity and Raman studies of the interplay of enigmatic orders in $\text{Mo}_8\text{O}_{23}$



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**Keywords:** ultrafast optical spectroscopy, charge density waves, metal-insulator transitions

Monoclinic semi-metallic  $\text{Mo}_8\text{O}_{23}$  shows multiple ordering phenomena with diverse characteristics.[1,2,3] An incommensurate order appears at  $T_{\text{IC}}=350$  K, followed by a structural cell-doubling transition to commensurate order at  $T_{\text{IC-C}} \sim 283$  K. In addition, an enigmatic resistance hump is observed at  $T_{\text{el}} \sim 150$  K, whose origin has so far proved elusive. Aiming to disentangle the multiple orders in  $\text{Mo}_8\text{O}_{23}$  single crystals we use the polarization-resolved ultrafast transient optical spectroscopy supplemented by Raman spectroscopy to study the single-particle relaxation and lattice vibrational modes. Remarkably, both the coherent vibrational mode response and single particle response display extrema of damping/relaxation times close to  $T_{\text{el}}$  with the concurrent appearance a few new coherent/vibrational modes. The single-particle relaxation data analysis shows the appearance of a temperature-independent gap in the electronic excitation spectrum below  $T_{\text{IC}}$  and another BCS-like gap opening near  $T_{\text{el}}$ . Concurrently a low frequency vibrational mode shows anomalous softening around  $T \sim 200$  K, far below  $T_{\text{IC-C}}$  and  $T_{\text{IC}}$ . The observations are interpreted in terms of the appearance of a hidden gapped state below  $T_{\text{el}}$  that has so far eluded detection by structural analyses.

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## **Photoinduced spin dynamics in correlated magnets**



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Ultrafast photinduced spin dynamics in correlated electron magnets are examined theoretically. By analyzing the double exchange model using the exact numerical simulation methods, it is shown that the magnetic structure is converted from the ferromagnetic order to the antiferromagnetic one by photoirradiation. This is highly in contrast to the standard double exchange scenario. This phenomenon is confirmed by the analytical method based on the Floquet Keldysh Green's function method. We also found that the topological spin textures appear in the transient photoinduced dynamics during the ferromagnetic and antiferromagnetic orders.

## Ultrafast electron vortex beam generation by scattering with a chiral near field

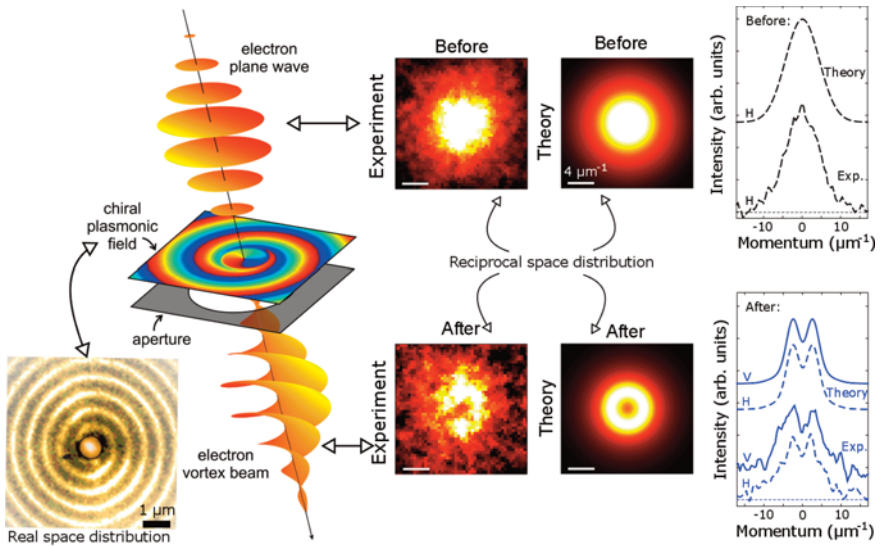


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**Keywords:** Electron-photon interaction, ultrafast, vortex electron beam, orbital angular momentum, ultrafast electron microscopy

The addition of orbital angular momentum (OAM) to massless and massive wave functions has opened new perspectives in fundamental and applied science [1,2]. Here we report the first generation of ultrafast electron vortices, i.e. femtosecond electron pulses with nonzero OAM [3]. The vortex generation has been developed with a novel photonic-based approach for imprinting phase profiles onto charged matter waves [3]. A circularly-polarized ultrafast laser pulses is used to create a chiral plasmonic field at the edge of a metallic nanohole, thanks to a spin-to-orbital angular momentum conversion mechanism. Nearly-relativistic free-electron wave packets are made to interact with the chiral near field, which stimulates the electrons to absorb and emit photons. In such a way, each electron wave packet acquires a net OAM from the interaction. We characterized the spatial distribution of the chiral plasmon by holographic ultrafast microscopy [4,5], and the transverse momentum electron distribution by small-angle electron diffraction. Furthermore, two pump pulses can be employed to precisely control the handedness of the plasmonic field.



Ultrafast electron vortex beam generation. A chiral surface-plasmon polariton is created around a hole. An electron plane wave (dome-shaped reciprocal space map) gains and cedes photons to the field, exchanging energy, linear and angular momentum. The orbital angular momentum is transferred to the electron wave function, whose wavefronts acquire a spiral distribution (doughnut-shaped reciprocal space map).

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## A nodal line semimetal state in a single-component molecular crystal



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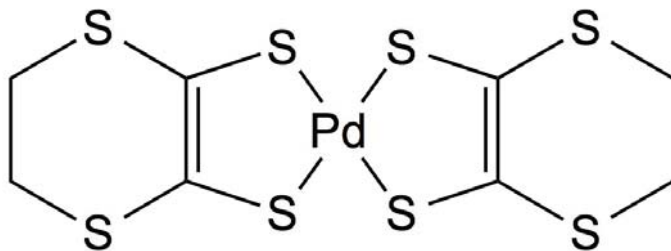
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**Keywords:** nodal line semimetal; single-component molecular conductors; metal dithiolene complex

Single component molecular conductors belong to the multiple-band system where both HOMO and LUMO bands that originate from the same molecule are located near the Fermi level. Metal dithiolene complexes are characterized by a small energy gap between HOMO and LUMO and suitable for the formation of the single component molecular conductors. In order to induce the band overlap that generates charge carriers, the application of high pressure is very useful because a molecular system has a soft lattice. We developed a diamond anvil cell technique that enables four-probe resistivity measurements under high-quality hydrostatic pressure up to 42 GPa.

Under such high pressure, molecular crystals show drastic changes. We found the emergence of the Dirac points in neutral [Pd(dddt)<sub>2</sub>] (dddt = 1,4-dithiin-2,3-dithiolate) at 12.6 GPa. This originates from the crossing band structure and the two-step HOMO-LUMO interactions. Notably, the Dirac point forms a loop in the three-dimensional k-space. A slight variation of the energy on the loop gives an electron pocket and a hole pocket, which implies that the system is a nodal line semimetal.

This work has been done in collaboration with H.B. Cui (RIKEN), T. Tsumuraya (Kumamoto Univ.), and Y. Suzumura (Nagoya Univ.).



[Pd(dddtdt)<sub>2</sub>]

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## Ultrafast spin dynamics in ferrimagnets with compensation point



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Ultrafast spin dynamics and all-optical magnetic switching in ferrimagnetic films with compensation temperature have been studied. A possibility of ultrafast non-thermal magnetization switching in garnet and orthoferrite films was shown in the recent experimental works [1,2]. Understanding all-optical switching in magnetic films is an important step towards realization of ultrafast magnetic memory with record low energy per bit writing.

The theoretical model is based on the nonlinear Landau-Lifshitz-Gilbert equations for a magnet film with uniform magnetization. The effect of the femtosecond laser pulse is described as an additional optical spin-torque, which is quadratic in laser electric field. We conducted simulations of the magnetization dynamics after the impact of a single femtosecond linearly polarized laser pulse in cases of different polarizations of the light and THz radiation. As a result, different switching patterns were obtained in agreement with the recent experimental works [1]. By changing the polarization of the laser pulse different outcomes of the magnetization dynamics were studied, which include repeatable magnetization reversal under alternation of different laser pulse polarizations.

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## Superconducting hybrids for quantum interfaces



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**Keywords:** Hybrid Josephson junctions, quantum devices, nanoscale

An integrated quantum device can be better than the sum of its ingredients. Only a smart combination of different platforms can provide transformational solutions, useful for a variety of quantum applications. A key issue is to make use of the best characteristics of different quantum systems. Photons can efficiently and durably transmit quantum information (QI), superconducting qubits can be rapidly manipulated to enable fast QI processing, while solid-state spin ensembles are particularly suited for long-lived quantum memories. The various quantum modules operate on very different energy scales at different temperatures with different spatial mode structures. Interfacing is crucial, is one of the real challenges to face and inspires the approach we are following to design superconducting circuits and their basic Josephson cells. We will report on some special properties of hybrid junctions, which make possible alternative layouts for the superconducting modules and relative interfaces inside the more complex general architecture. We refer to the capability of an all-RF drive of ferromagnetic Josephson junctions which is expected to allow novel tuning mechanisms that are not susceptible to flux noise, and permit alternative control schemes. These may open up new avenues in coupling schemes between the qubit processor and SC waveguide cavities. We classify some significant behaviors of hybrid and unconventional junctions through a comparative study of fluctuations and electro-dynamical properties.

## Oxygen induced electronic structure modification of VO<sub>x</sub> nanostructured thin films



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**Keywords:** VO<sub>x</sub>, nanodomains

Gas phase synthesis of nanoparticles is of high scientific relevance for technological applications, since it is the most eligible candidate to integrate nanostructured materials into micro-electronic devices [1]. Our interest has been devoted to vanadium oxides which exhibit fascinating and technologically relevant properties. As an example, because of their planar structure, both V<sub>2</sub>O<sub>5</sub> [2] and V<sub>6</sub>O<sub>13</sub> have been deeply investigated for possible applications as Li ion battery cathode materials [3,4]. VO<sub>2</sub> is instead investigated since its discovery because it undergoes a reversible metal-insulator-transition (MIT) near room temperature [5,6]. Many foreseen applications are also enhanced going to nanoscale. Indeed, the electronic and structural properties of these materials may strongly differ from the bulk analogue. We report preliminary results on oxygen induced changes in electronic structures of VO<sub>x</sub>. Our samples have been investigated via in-situ XPS, UPS and XANES spectroscopies. Exploiting these techniques, it is possible to probe the presence of quantum size effects and evaluate their influence on electronic and structural properties [7].

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## The Universal Fermi-Liquid Scaling in $\text{Sr}_2\text{RuO}_4$ thin films



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**Keywords:**  $\text{Sr}_2\text{RuO}_4$ , Terahertz ellipsometry, Fermi liquid

$\text{Sr}_2\text{RuO}_4$  is a transition-metal oxide compound which is iso-structural to  $\text{La}_2\text{CuO}_4$ . It is an unconventional superconductor in its parent form with a  $T_c$  of 1.5K and most experiments indicate a p-wave pairing symmetry, in contrast to the High- $T_c$  cuprates which exhibit a d-wave symmetry [1]. Depending on tuning of pressure or doping, both Fermi-liquid as well as non Fermi-liquid behavior has been observed in unconventional superconductors such as cuprates, heavy fermions and pnictides.

At low temperature, resistivity measurements in  $\text{Sr}_2\text{RuO}_4$  show a  $T^2$  dependence which is a signature of Fermi-liquids [2]. A previous optical study of  $\text{Sr}_2\text{RuO}_4$  single crystal material has provided the first evidence for the universal Fermi-liquid scaling law for the optical scattering rate  $1/\tau \propto (\hbar\omega)^2 + (2\pi K_B T)^2$  [3]. These studies were based on Kramers-Kronig analysis of reflectivity. The reflectivity value close to 100 percent carries over to relatively large systematic and statistical error bars, and it puts a lower limit of 20  $\text{cm}^{-1}$  on the accessible frequency window.

A new opportunity for extending the frequency range and improving the sensitivity for the optical scattering rate  $\tau$  has arisen due to two factors: (i) The availability of high quality epitaxial  $\text{Sr}_2\text{RuO}_4$  thin films (RRR about 50 and thickness 18.5 nm) on  $\text{NdGaO}_3$  substrates, and (ii) the construction in our laboratory of a time-domain THz ellipsometer which allows the measurement of the real and imaginary part of the optical conductivity directly, providing the most direct way to obtain the optical scattering rate  $\tau$  for fre-

quencies down to  $20 \text{ cm}^{-1}$ . Details and conclusions of this ongoing investigation will be presented in this presentation.

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## Charge configuration memory devices switching correlated electron states



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**Keywords:** Ultra-fast memory, charge configurational memory, charge density wave

Metastable states in correlated electron systems may be useful for various devices, such as sensors and particularly memory devices. All-electronic switching mechanisms promise very fast response and low programming energies and are therefore of great current interest. The current favourite material, tantalum disulfide is a quasi-two-dimensional transition metal dichalcogenide that exhibits many different states, including superconductivity, charge density waves (CDW), a Mott state and concurrent quantum spin liquid state<sup>1</sup>. A metastable ‘hidden’ state is reached by optical excitation<sup>2</sup> or injection of charge carriers<sup>3,4</sup> which breaks the perfectly ordered commensurate charge pattern into commensurate patches separated by domain walls<sup>5</sup>. The state is easily erased, is reached very rapidly (0.5 ps), is reversible and is also topologically protected which causes it to have extremely long lifetime<sup>3,6</sup>. The transition mechanism is based on a topological quantum charge reordering process, but from a device viewpoint, it shows a large drop in resistivity which in combination with its non-volatility properties can be used as an ultra-fast memory element. Here we report on the scaling of the programming energy with dimensions, pulse length and temperature, finding that such a charge configurational memory

(CCM) is a serious contender among the next generation memory technologies.

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## Study of electron density of states and electronic heat capacity of high temperature cuprate superconductor: $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$



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**Keywords:** Defects, anharmonicities, Born-Mayer-Huggins potential, electron density of states, electronic heat capacity, cuprate superconductors.

The renormalized electron density of states (REDOS) has been studied using quantum dynamical many body theory of electron Green's functions via model Hamiltonian and Born-Mayer-Huggins potential [1,2]. Different leading contributions due to harmonic phonons and electrons, their interactions, anharmonicities and defects are included in the Hamiltonian. The cuprate superconductor  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  has been taken up for numerical investigation purposes. Fig. 1(a) shows a 3-dimensional view of REDOS which explores the modified scenario of REDOS and displays strong dependence on temperature [3]. The results of REDOS have been utilized to investigate the electronic heat capacity (EHC). EHC  $C_{el}(T)$  has been plotted as a function of temperature along with experimental result of total heat capacity  $C(T)$  in Fig. 1(b) concluding that amplitude to EHC is very small as compared to the experimental results [4] because the rest of the contribution comes from phononic heat capacity. The REDOS and EHC are resolved into the isolated contributions coming from point impurities, electron-phonon interactions and anharmonic modes [5]. Thus, the considered effects show a substantial role in the study of REDOS and EHC and reveal some fascinating features.

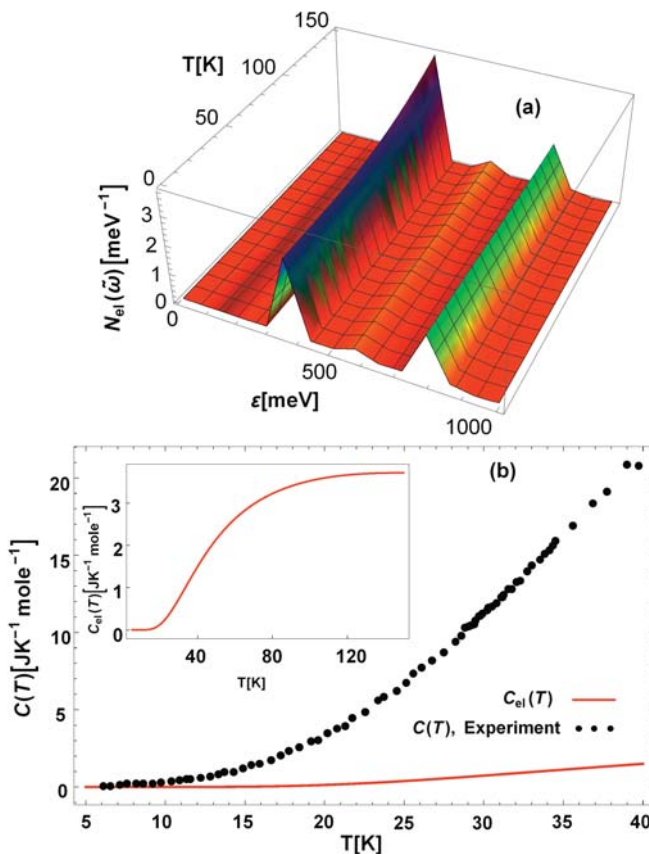


Fig. 1(a) Three dimensional view of renormalized electron density of states of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  cuprate in [110] direction and 1(b) variation of electronic heat capacity versus temperature along with experimental result at doping  $x=0.2$  and temperature  $T_c=37.5\text{K}$  for  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  cuprate.

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## High-Tc cuprates – story of two electronic subsystems



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We have performed a thorough experimental study of  $\text{HgBa}_2\text{CuO}_{4+\delta}$ , which in many respects is a model cuprate compound. From the comparison with data for other cuprates we are able to separate universal behavior from compound-specific features. The most remarkable finding is the existence of an underlying Fermi-liquid scattering rate [1] that remains essentially unchanged across the phase diagram [2,3]. Guided by established universalities, and by the knowledge that the cuprates are inherently inhomogeneous, we propose a simple model in which exactly one localized hole per planar copper-oxygen unit is gradually delocalized and becomes itinerant with increasing doping and temperature [4]. The model is percolative in nature, with parameters that are nearly compound- and doping-independent and experimentally constrained. It comprehensively captures pivotal unconventional experimental results, including the temperature and doping dependence of the pseudogap phenomenon, the strange-metal linear temperature dependence of the planar resistivity, and the doping dependence of the superfluid density.

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## Disorder-Driven Transition from $s_{\pm}$ to $s_{++}$ Superconducting Order Parameter in Proton Irradiated $\text{Ba}(\text{Fe}_{1-x}\text{Rh}_x)_2\text{As}_2$ Single Crystals



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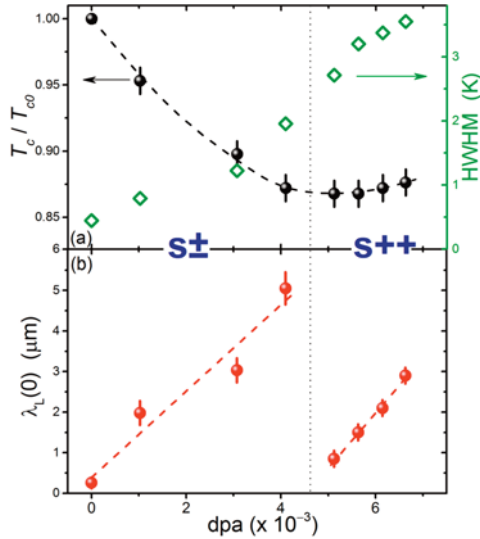
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**Keywords:**  $s_{\pm}$  to  $s_{++}$  Superconducting Order Parameter Transition, Iron Based Superconductors, Disorder, Multi Gap Superconductors, Eliashberg

A microwave technique [1-2] that allows us to determine the London penetration depth and the critical temperature  $T_C$  is used to show evidence of disorder-driven  $s_{\pm}$  to  $s_{++}$  order parameter symmetry transition in  $\text{Ba}(\text{Fe}_{1-x}\text{Rh}_x)_2\text{As}_2$  single crystals, where disorder was induced in the form of defects generated by 3.5-MeV proton irradiation.

This transition is expected in the presence of high levels of disorder that drives the system toward the convergence of the gaps values, and its signature was found as the predicted [3], but not yet observed [4], discontinuity in the low-temperature values of the London penetration depth.

These experimental observations are validated by multiband Eliashberg calculations in which the effect of disorder is accounted for in a suitable way. Our model reproduced exactly the experimental  $T_c$ s and semi-quantitatively the superfluid densities, with the  $s_{\pm}$  to  $s_{++}$  symmetry transition at the expected disorder level [5].

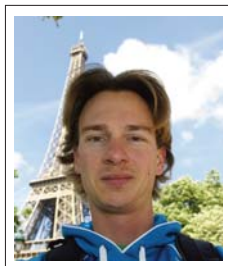


Experimental evidence of the  $s_{\pm}$  to  $s_{++}$  disorder driven phase transition: (a) Critical temperature of the irradiated crystal normalized to its value for the pristine crystal, as a function of the irradiation-induced disorder, expressed by the average displacement per atom. The width of the superconducting transition unaltered increase testifies that disorder continuously increases. (b) Low-temperature values of the London penetration depth. The transition between the  $s_{\pm}$  to  $s_{++}$  phases is identified in the predicted London penetration depth value drop.

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## Detection and manipulation of dopants in a cuprate superconductor



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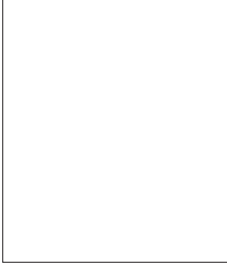
**Keywords:** Cuprates, Charge dynamics, Scanning tunnelling microscopy, Current noise

Dopants and impurities are crucial in shaping the ground-state of host materials: semiconducting technology is based on their ability to donate or trap electrons, and they can even be used to transform insulators into high temperature superconductors. Due to limited time resolution, most atomic scale studies of the latter materials focussed on the effect of dopants on the electronic properties averaged over time. In this talk I will present our observation of remarkable charge dynamics at select dopant sites in the high- $T_c$  superconductor  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ . The ionization and local environment of these dopants leads to a strong enhancement of the current-noise, signalling correlated tunnelling events. I will further discuss new routes to control doping at the atomic scale and visualizing its effect on high- $T_c$  superconductivity.

## **Majorana zero modes and skymion-like-strings on the domain wall and the d-brane-like dot**

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One (I.K) of the present authors has reported the importance of hole-induced domain wall and the hedge-hog-like magnetic soliton in diluted magnetic semiconductors [1,2], and doped manganites [3]. Kanazawa and coworkers [4,5] have proposed that there might be emergent quasiparticles and fractional electronic charge such as dyons on the domain wall between topological insulators and spin ice compound through the Witten effect. In this study, we shall consider the Majorana zero modes and skyrmion-like-strings on the domain wall and the D-brane-like dot, and the relation to low-energy hadron in QCD, from the viewpoint of a field-theoretical formula.

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## Superexponential wave function decay: a fingerprint of strings in doped antiferromagnets



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We determine the spectral function of a hole for the one-dimensional (1D) Ising  $t$ - $J_z$  model using the magnon language and obtain an exact result only when the magnon-magnon interactions are included. Interestingly, the magnon-magnon interactions completely cancel the string potential in 1D and the hole wave function has coefficients which decay exponentially with the increasing length of hole path. This stays in contrast with the two-dimensional (2D) case, for which the hole is always confined in a string potential and a superexponential decay of the hole wave function coefficients is predicted. The latter behavior is a fingerprint of the existence of strings in doped antiferromagnets, that can be observable in the numerical or cold atom simulations of the 2D doped Hubbard model.



## Photo-induced carrier relaxation dynamics in glassy electronic state of geometrically frustrated organic conductor

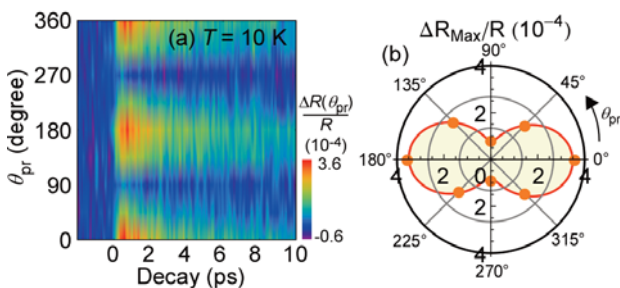


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**Keywords:** organic conductors, time-resolved spectroscopy

Glass transition, which is one of the critical issues in condensed matter physics, has been studied in atomic and molecular systems. Recently, a glassy state with charge-clusters has been suggested in the organic compound  $\theta$ -(BEDT-TTF)<sub>2</sub>RbZn(SCN)<sub>4</sub>[1]. In the state, charge-cluster freezes randomly without structural disordering, suggesting a nontrivial electronic structure in k-space. In this study, we carry out the optical pump-probe spectroscopy to investigate the electronic structure. By measuring probe polarization dependence of the transient change of reflectivity, we find that carrier dynamics of the glassy state can be characterized by polarization anisotropy for the probe beam as shown in Figure, indicating that k-space anisotropy of electronic excitations is induced in the glassy state. In the conference, the result will be discussed in detail.



(a) Density plot of probe polarization dependence of transient reflectivity change  $\Delta R(\theta_{pr})/R$  at  $T=10$  K. (b) Polar plot of probe polarization dependence of amplitude  $\Delta R_{Max}/R$ .

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## Statistical measurements of arrays of Josephson junctions and field effect transistors embedded into quantum integrated circuits



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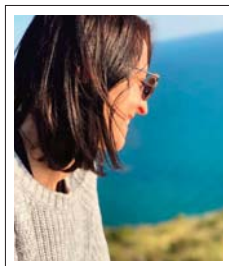
**Keywords:** Two-dimensional Josephson junctions, Quantum integrated circuits, Hybrid superconducting-semiconducting circuits, Josephson field effect transistors

Quantum integrated circuits on a chip with arrays of Josephson junctions (JJs) and field effect transistors (JoFET) will be demonstrated. We will discuss the statistics, quantum yields, and reproducibility of the differential conductance vs. temperature and magnetic field for these devices of identical or different geometries. Our study could be very important for hybrid qubit optimisation and realisation of scalable topological quantum processors.

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## Numerical solution of Bogoliubov equation in a superlattice of superconducting wires in organics superconductors: the effect of electron hopping between wires



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**Keywords:** Lifshitz transition, non-BCS superconductivity, Shape resonance, BPV Theory, anisotropic strain

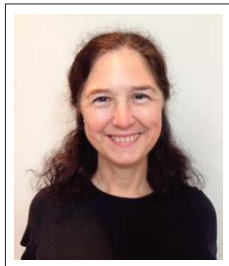
Non-BCS high-temperature superconductivity emerging by tuning the chemical potential near a Lifshitz transition [1] has been described by solution of Bogoliubov equation in order to describe the multi-gap superconductivity driven by Majorana exchange interaction between condensates beyond the standard BCS approximations has been able to predict and explain fine details of superconductivity in anisotropic organic conductors [2], interfaces [3], iron-based perovskites [4,1], pressurized sulfur hydrides [5-7], striped phase in doped cuprates [8-10] made of weakly interacting quantum wires which are controlled by anisotropic strains [11,12]. In this work we study the multigap scenario by joint solution of Bogoliubov and density equations as a function of the variable electron hopping between wires in a superlattice of stripes induced by variable anisotropic strain or pressure. We show how near the Lifshitz transition the coupling term in the

appearing band and the ratio between the energy cut off and the band dispersion in the transversal direction control the BCS-BEC cross-over regime and the emerging high temperature superconductivity.

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## Stripes and Nematicity in a hole-doped three-orbital spin-fermion model for superconducting cuprates



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**Keywords:** Charge- transfer insulators, numerical methods, multi-orbital systems

Numerical studies of a spin-fermion model that captures the charge-transfer properties of Cu-based high critical temperature superconductors [1] reveal the spin and charge order in the parent compound and under hole doping. In clusters of dimension  $16 \times 4$ , that break the rotational symmetry, half-filled stripes are observed upon hole doping, i.e.,  $n$  stripes of length 4 develop when  $2n$  holes are introduced in the system. The antiferromagnetic order observed in the parent compound develops a  $\pi$ -shift across each stripe and the magnetic structure factor peaks at momentum  $k=(\pi-\delta,\pi)$  with  $\delta=2\pi N_h/2L$  where  $L=16$  and  $N_h$  is the number of doped holes. The electronic charge is also modulated and the charge structure factor peaks at  $k=(2\delta,0)$ .

In addition, orbital nematicity with  $\langle n_{px} \rangle - \langle n_{py} \rangle \neq 0$  develops as electrons are removed from the system. These results indicate that the spin and charge distribution experimentally observed in hole-doped cuprates is captured by unbiased Monte Carlo studies of a doped charge-transfer insulator. [2]

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## **Spin-orbit Coupling: impact on the hole mechanism for Superconductivity**



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Spin-orbit coupling is known to generally decrease the superconducting critical temperature for a superconducting material. We discuss a model interaction where this is not the case, on the contrary, spin-orbit coupling leads to a significant increase in superconducting  $T_c$ . We also examine a class of lattice models where the symmetry of the order parameter varies as a function of temperature. This turns out to be the norm rather than the exception. Understanding the nature of these transitions may be important for assessing the symmetry of many superconductors known to exhibit unconventional superconductivity.

## A “coherent” picture of some Quantum Materials



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**Keywords:** Coherent scattering, electronic ordering, time and space correlations

Electronic properties of quantum materials inherently depend on their time and space correlations and their possibility of emerging to macroscopic scales are investigated by coherent x-ray diffraction [1,2]. Phase coexistence, segregation and their dynamics can be accessed from a preferential point of view, offering crucial key for understanding macroscopic properties of relevance.

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## Effect of the isoelectronic substitution of selenium with sulfur in superconducting $\text{Rb}_{0.8}\text{Fe}_{1.6}\text{Se}_2$



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

The origin of superconductivity in iron pnictides and selenides is still an open question [1]. Structurally the semiconducting  $\text{Rb}_{0.8}\text{Fe}_{1.6}\text{S}_2$  and superconducting  $\text{Rb}_{0.8}\text{Fe}_{1.6}\text{Se}_2$  are very similar [2]. Both compounds crystallize in the tetragonal space group  $I4/m$  and order antiferromagnetically (AFM) at  $T_N$  above 500 K. The  $^{57}\text{Fe}$ -Mössbauer spectra of both samples are strikingly similar. They have the same components, reflecting the intergrown antiferromagnetically ordered and paramagnetic fractions. These are associated with the majority AFM phase and the minority metallic phase responsible for superconductivity [3,4].

In principle, the possibility of “tuning” magnetism and superconductivity by doping and/or hydrostatic pressure application allows clarification of the interplay between them in iron-based superconductors. For example,

the isoelectronic substitution of selenium with sulfur in  $\text{Rb}_{0.8}\text{Fe}_{1.6}\text{Se}_{2-x}\text{S}_x$  leads to the reduction of the superconducting transition temperature from  $T_c = 32$  K ( $x = 0$ ) to 22 K ( $x = 1.0$ ), and the total suppression of superconductivity at  $x = 1.4$  [2].

The main issue of our study can be summarized as follows: why is superconductivity affected by a substitution of FeSe by FeS layers in  $\text{Rb}_{0.8}\text{Fe}_{1.6}\text{Se}_2$ ? A thorough analysis of Mössbauer hyperfine parameters might resolve the issue. Obviously, magnetic fluctuations and steric effects associated with the effective chemical pressure caused by substitution should be taken as the primary factors into consideration.

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## Superconductivity and magnetic and nonmagnetic mesoscopic phase separation in superconducting selenides



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**Keywords:** superconductivity, phase separation, high- $T_c$  superconductors, iron based superconductors

Layered iron selenides have attracted a lot of attention in the last few years. The issues concerning the nature and the role of inhomogeneities in those materials are addressed. It was shown that the inhomogeneous spatial distribution of ions with nanoscale phase separation enhances the superconductivity in superconducting Fe-Te-Se chalcogenides. It has been demonstrated that thermally induced modifications of  $\text{Rb}_x\text{Fe}_{2-y}\text{Se}_2$  microstructure together with mesoscopic phase separation, leads to an improvement of the superconducting properties and an enhancement of transition temperature ( $T_c$ ). Moreover, the magnetic and nonmagnetic mesoscopic phase separation, found in iron selenides intercalated with organic molecules, opened discussion on the nature of superconducting phase and the role of organic intercalants in tuning of superconducting properties. It is suggested that appearance of superconductivity in iron selenides intercalated with organic molecules at the temperatures higher than  $T_c$  of  $\text{A}_x\text{Fe}_{2-y}\text{Se}_2$  ( $A = \text{K}, \text{Rb}, \text{Cs}$ ) is related to magnetic inhomogeneity in that system.

## Fluctuations in $s+is$ superconductors. Applications to iron-based materials

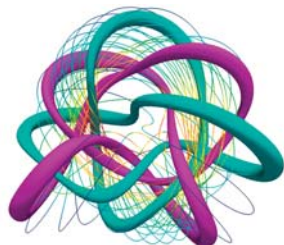


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**Keywords:** multicomponent superconductors, type-1.5 superconductivity

The basic topological excitation in an ordinary superconductor is a vortex line, which topological invariant is the phase winding. A number of multicomponent superconducting states are known to support stable excitations characterised by different topological invariants: domain walls and Skyrmion lines. By contrast, attempts to identify whether there are superconducting states which topological excitations are stable closed three dimensional objects, such as Hopfions, were not successful. Although, in a number of superconducting and superfluid models, one can attribute a Hopf topological index to closed vortex loops and knots, such objects are not stable because the kinetic energy of a superflow and the magnetic energy is expected to be smaller the smaller a vortex loop is. We demonstrate that in multicomponent



superconductors, under certain conditions, such as proximity to pair-density-wave instabilities, the property of vorticity and nature of topological excitations changes dramatically: the excitations acquire the form of stable vortex loops and knots characterized by Hopf topological indices.

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## Negative thermal expansion in spin-orbital systems



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**Keywords:** spin-orbital physics, negative thermal expansion, hybrid bond

Strong Coulomb interactions in transition-metal oxides lead to low-energy superexchange with entangled spin-orbital states [1]. Neutral doping of ruthenium oxides, as e.g. in  $\text{Ca}_2\text{Ru}_{1-x}\text{Cr}_x\text{O}_4$ , shows surprising negative volume thermal expansion. Such doping introduces hybrid  $d^4-d^{4-n}$  bonds in correlated insulators with:

- (i) orbital dilution for  $n=1$  realized by  $3d^3$  impurities, and
- (ii) hole-doublon pairs in case of  $n=2$  and  $3d^2$  doping.

In case of orbital dilution superexchange favors doubly occupied active orbitals along the hybrid bond leading to orbital polarons [2]. For doublon dilution the derived spin-orbital interactions on the hybrid bonds contain  $T_i^+T_j^+$  terms responsible for double hole-doublon excitations which generate enhanced quantum fluctuations [3]. We show that electron correlations lead in a class of transition-metal oxides with active orbital degrees of freedom to negative thermal expansion, using both the degenerate Hubbard and spin-orbital model.

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## **Magnetic torque measurements in high $T_c$ cuprates**



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**Keywords:** Cuprates, magnetic torque

The nature of the pseudogap state and the role it plays in the rich phase diagram of cuprate superconductors is yet to be fully understood. It is still an open question whether the transition to this state is a true phase transition or a slow crossover. A further question is whether the phase transition terminates at a zero temperature quantum critical point and what influence this has on the superconductivity. Recently, measurements of in-plane magnetic torque have suggested an abrupt transition close to the estimated edge of the pseudogap phase; suggesting a thermodynamic transition to an electronically nematic state. Here we further investigate these effects in different high  $T_C$  cuprates and in particular how extrinsic effect can influence the signals seen.

## Local strain determination in superconducting $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$ using scanning XANES microscopy



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$\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$  bismuthate which shows high  $T_c$  superconductivity for  $0.05 < x < 0.30$  is an archetypal system for the relation between the emergence of quantum coherence and lattice complexity. This system can be described as a complex solid solution made of metallic  $[\text{BaPbO}_3]$  and insulating  $[\text{BaBiO}_3]$  nano-puddles, strained by the misfit between the two different lattices. The critical temperature in high temperature superconductors has been shown to be controlled by the lattice strain [1] in cuprates [2,3], diborides [4-6] and iron-based superconductors [7,8] and by external pressure in hydrides [9,10]. While it is known that misfit strain generates a complex nanoscale phase separation in cuprates [11-13] and iron chalcogenide su-

perconductors [14] it is now emerging a percolative filamentary network mapped into a hyperbolic space [13-17] the misfit strain in  $\text{Ba}(\text{Pb}_{1-x}\text{Bi}_x)\text{O}_3$  is not known. Here we report the measurement of the local strain in the metallic  $\text{BaPbO}_3$  nanoclusters in  $\text{Ba}(\text{Pb}_{1-x}\text{Bi}_x)\text{O}_3$  due to the internal pressure at the interface lattice for the mismatch between the two components using the innovative real-space scanning micro Pb  $L_3$  edge XANES [18,19] microscopy by synchrotron radiation, recorded at the ESRF beamline ID24 (Grenoble, France). Scanning micro-XANES is a unique probe to unveil the inhomogeneity of local lattice structure in a selected nanocluster. The results show that in the superconducting phase the  $[\text{BaBiO}_3]$  cluster shows a tensile strain in the range -0.1%, -0.6 %, with maximum  $T_C$  at -0.5% strain. Therefore, we conclude that the correlated lattice disorder at -0.5% tensile strain in the  $[\text{BaBiO}_3]$  favors the nanoscale phase separation [20] giving high temperature superconductivity.

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## In-plane Anisotropy of the Pseudogap Temperature and Charge Density Wave in Underdoped Few Unit Cell $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ Thin Films



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The microscopic origin of the properties of High Tc Superconductors (HTS) remains elusive 30 years after their discovery. Various symmetry breaking electronic ordering, such as charge density waves (CDW) and nematicity, have been revealed in the underdoped region of the phase diagram, where the pseudogap dominates the normal state properties. The correlation lengths of these phenomena are in the nm-range; the study of HTS nanodevices can be instrumental for understanding the intertwining of the various orders and the superconducting state. We have developed a fabrication method to obtain nanowires from untwinned  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  films, which allows one to study transport properties as a function of hole doping and device dimensions. With this approach heavily underdoped nanowires keep the physical properties of the as-grown films [1].

Transport measurements of underdoped devices have revealed a remarkable in plane anisotropy of the pseudogap, see Fig. 1. As the thickness is reduced to 10 nm, the pseudogap features gradually disappear at  $\phi=90$  degrees (b-axis). Resonant x-ray scattering measurements of the CDW state on the same films shows the CDW is strongly suppressed along  $\phi=0$  degrees (a-axis). In the 50 nm thick films where the pseudogap is isotropic also the CDW is isotropic. These results point towards an intertwining of the two phenomena and is a first hint of a connection between the transport properties (pseudogap) and the CDW state in the cuprates.

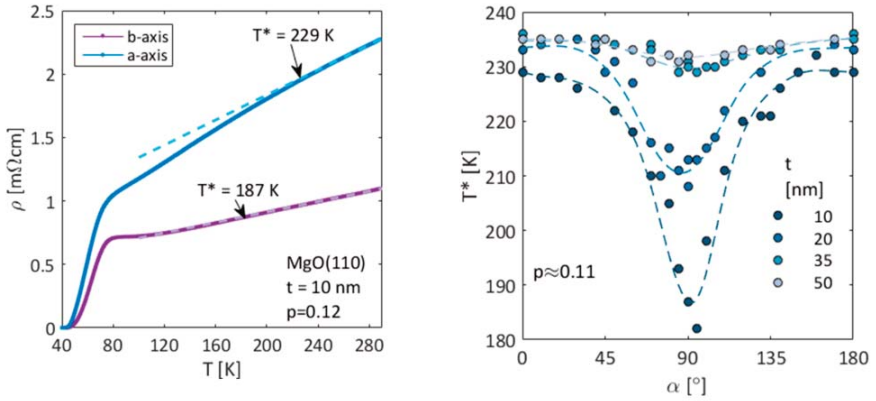


Fig. 1: Left: Resistivity vs. temperature of 10nm thick devices oriented along the a-axis( $\alpha=0$  degrees), and b-axis( $\alpha =90$  degrees). The extracted pseudogap temperature  $T^*$  is given for each device. Right: Full in-plane angular dependence of  $T^*$  for devices of different thickness ranging from 10-50 nm. Notice the suppression of  $T^*$  along the b-axis.

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## Going to nano: A comparative investigation of Sn<sub>2</sub>P<sub>2</sub>S<sub>6</sub> chalcogenide bulk and layered structures



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The Sn<sub>2</sub>P<sub>2</sub>S<sub>6</sub> (SPS) crystal is the promising ferroelectric semiconductor photosensitive in the red and near-infrared spectral range with good photorefractivity and fine photovoltaic, electrooptic and piezoelectric characteristics [1-3]. The mentioned crystal, in particular, is an interesting material for holographic recording and image processing applications [4]. Versatile physical properties of the SPS crystal were reported repeatedly and the mechanism of their appearance was explained theoretically [5]. From the observed behaviors of the SPS crystal one may see that the surface has significant influence on its physical properties.

In presented work physical properties of the SPS crystal in nanolayer form investigated theoretically using DFT method augmented by Hubbard correction are reported and the obtained results are compared to the bulk material parameters. The electronic and optical properties of the modelled material were simulated versus its thin film thickness. The significant influence of the SPS thickness on its band gap value was found. In addition, was shown the absorption edge shifts as a function of layers number giving the absorption peak at the position below a value of band gap. It may be explained by the surface electron interaction and exciton creation. Obtained results clarify the important features of interlayer interaction and the possibility of predictable corrections of the SPS electronic properties taking into account the surface effect.

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## Not only HTSCs for memristors, but also memristors for HTSCs



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The study of memristive properties or effect of resistive switchings in four classes of high-temperature superconductors (HTSCs):  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+y}$  (BSCCO),  $\text{YBa}_2\text{Cu}_3\text{O}_{7-d}$  (YBCO),  $\text{Ba}_{0.6}\text{K}_{0.4}\text{BiO}_{3-x}$  (BKBO),  $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_{4-y}$  (NCCO) is presented in order to reveal functional properties of HTSCs which become apparent in the effects under consideration. There are discussed prospects of usage of HTSC-based memristors in applications and search for new mechanisms of strongly correlated nature to realize new-generation memristors [1]. The properties are: undergoing metal-insulator transition at oxygen doping, transport anisotropy, existence of charge reservoirs through which doping of conductive copper-oxygen plays is carried out. These are the main functional properties of HTSCs which permit to use them in memristors. By the example of study of bipolar effect of resistive switching in HTSC-based heterojunctions it is shown how one can form memristor structures based on HTSCs using their functional properties.

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## Propagation of a single hole in $\text{Ca}_2\text{RuO}_4$



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**Keywords:** Ruthenates, Magnetism, Quasi 2-D, Mott Insulator

In recent years there has been a growing interest in the understanding of the correlated physics of  $\text{Ca}_2\text{RuO}_4$ , fuelled by the fundamental importance of the spin-orbit interaction in this compound on the one hand and by its close resemblance to the well-studied copper oxides on the other. In order to understand the latter, we focus here on the propagation of a single hole introduced into the Mott insulating ground state of  $\text{Ca}_2\text{RuO}_4$  and verify its quantitative as well as qualitative differences w.r.t. the cuprates. To this end we introduce an effective multiorbital t-J-like model which we then solve using the linear spin wave theory and self-consistent Born approximation. We obtain the spectral function for fermionic spinless holes whose most striking feature is its quasi-1D character.

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## First steps in graphene-TMD quasi-classical approach



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**Keywords:** Rashba, spin, transport, disorder, graphene, heterostructure

In the last decade, the attention has been focused on the condensed matter physics in heterostructures at atomic limit [1-12]. The emergence of two dimensional (2D) materials has attracted a great deal of attention due to their fascinating physical properties and potential applications [6-12]. Since the first isolation of graphene, a Dirac material, a large family of new functional 2D materials have been discovered and characterized, including insulating 2D boron nitride, semiconducting 2D transition metal dichalcogenides, black phosphorus, and superconducting 2D bismuth strontium calcium copper oxide [7,8,9], iron pnictides [10], organics [11] molybdenum disulphide [12], nickelate perovskites [13,14] and niobium selenide. It has been demonstrated that an adjacent ferromagnetic insulator layer can strongly modulate spin currents via proximity exchange field. Transition-metal dichalcogenide (TMDC) layers enable in adjacent graphene the optical injection of spin and electrical modulation of spin currents via spin absorption [6]. The experiments have measured the spin-lifetime anisotropy in graphene-TMDC heterostructures and shown the presence of proximity-induced SOC. The strong SOC of TMDC, orders of magnitude larger than the single graphene, can modulate the spin dynamics in the graphene channel, while the high quality of charge transport is preserved. At the same time, the theoretical investigation for the study of spin dynamics and relativistic transport phenomena in the last decade is going on [1-5]. Particular interest is on typical disordered two-dimensional Dirac systems with pseudospin-spin coupling, as the paradigmatic case of



graphene. This work is focused on the derivation of Eilenberger equation [1] for graphene-like heterostructures at atomic limit with, first of all the Rashba SOC, and then the Kane-Mele and disorder term. The first steps in this direction has been to find the Keldysh component of quasi-classical Green function in the extremely case of clean and stationary system using the symmetry properties of graphene in the Clifford algebra. We support the theoretical investigation on transport properties (i.e. spin hall conductivity, spin current etc.) by simulation results with Comsol software.

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## Tracking nematic fluctuations in Co-doped LaFeAsO using the Nernst effect



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We use the Nernst coefficient to track the nematic fluctuations through the Co-doped phase diagram of LaFeAsO. Similarly to our previous measurements in an 122-iron based superconductor system, we obtain a significant enhancement of the signal in the nematic fluctuation regime. The doping dependence of the Nernst coefficient exhibits a non-monotonic behavior featuring a local maximum in the vicinity of optimal doping. This peculiar doping dependence is also in agreement with our theoretical prediction and hence demonstrates the universality of the sensitivity of the Nernst effect on nematic fluctuations in iron based superconductors.

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