Book of abstracts

3rd Microscopics of Superconductivity in Perovskite Oxides: Challenges, Hurdles and Enigmas MISPOCHE Workshop

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Superconductivity of (Sr, La)Ti(^{16}O, ^{18}O)$_3$ and (Sr, Ca)(Ti, Nb)O$_3$.

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We have investigated the transport properties of (Sr, La)Ti(^{16}O, ^{18}O)$_3$ and (Sr, Ca)(Ti, Nb)O$_3$ single crystals systematically.

Because of the limited time slot, this talk will focus on the two issues below.

1) Both of the La and Nb substitutions for the electron doping exhibit the superconducting dome, but we did not observe superconductivity below around 7x10^{18} cm^{-3}.

This is contradicting to the oxygen-deficient SrTiO$_3$ which was reported in the literature to show the second superconducting dome with the peak located at around 2x10^{18} cm^{-3},

2) ^{18}O exchange and Ca substitution are considered to make the system close to the ferroelectric instability or ferroelectric metal.

Our single crystalline samples indeed showed an increase of T_c in the lower-doping side of the superconducting dome. However, the T_c enhancements were not so drastic as expected in some theoretical predictions.

Almost all of the data are yet unpublished, but we would like to take this opportunity to share them with the audience and have a meaningful discussion.

Single-gap superconductivity in Nb-doped $SrTiO_3$ revealed by mK electrodynamics

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Optical spectroscopy can reveal fundamental aspects of superconductors such as energy gap, superfluid density, and quasiparticle dynamics. Using microwave spectroscopy at mK temperatures, we have studied the full electrodynamics of Nb-doped $SrTiO_3$ for various Nb concentrations covering the maximum of the superconducting dome of $SrTiO_3$. We find that Nb-doped $SrTiO_3$ exhibits only a single superconducting gap. At the same time, our experiments confirm that Nb-doped $SrTiO_3$ is a multi-band superconductor. This combination, a multi-band single-gap superconductor, can be explained by the role of inevitable scattering, which homogenizes the gap throughout the Fermi surface.

[1] M. Thiemann, M. H. Beutel, M. Dressel, N. R. Lee-Hone, D. M. Broun, E. Fillis-Tsirakis, H. Boschker, J. Mannhart, and M. Scheffler, Phys. Rev. Lett. **120**, 237002 (2018)

Emergence of a quantum coherent state at the border of ferroelectricity

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$SrTiO_3$ exists on the border of ferroelectricity in the vicinity of a quantum critical point. It is this proximity to a quantum critical point and the fluctuations associated with it which are responsible for $SrTiO_3$'s strikingly non-classical dielectric susceptibility. The lack of itinerant electrons and the simplicity of the system make it an attractive model system for investigation of the underlying physics of quantum criticality.

I will discuss our latest results utilising ultra-high precision measurements of the temperature and pressure dependence of the dielectric susceptibility of $SrTiO_3$. These demonstrate an unconventional quantum paraelectric state exhibiting the phenomenon of 'order by disorder', namely a fluctuation-induced enhancement of electric polarization extending up to a characteristic coherence temperature T*. T* vanishes at the ferroelectric quantum critical point and the square of T* increases with a characteristic linear dependence on the applied pressure. We show that in the vicinity of T* this thermal activation phenomenon can be understood quantitatively, without the use of adjustable parameters, in terms of the hybridization of the critical electric polarization field and the volume strain field of the lattice.

We argue that this coherent optical-acoustic phonon state emerges from the ferroelectric quantum critical point and is critical to our understanding of the mechanisms behind the quantum criticality and the phenomena resulting from it in $SrTiO_3$ and more generally in quantum critical ferroelectric compounds. At still lower temperatures, well below T*, we observe a breakdown of this unconventional form of quantum paraelectricity and the emergence of a still more exotic state characterized by slowly fluctuating micro-domains of the lattice structure. We suggest that this low temperature state may be viewed as a type of instanton liquid arising from anisotropic-strain-induced long-range correlations of the electric polarization field.

Hidden fluctuations close to a quantum bicritical point

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We describe physical properties arising in the vicinity of two coupled quantum phase transitions by considering a phenomenological model based on two scalar order parameter fields locally coupled biquadratically and having a common quantum critical point as a function of a quantum tuning parameter such as pressure or magnetic field. A self-consistent treatment suggests that the uniform static susceptibilities of the two order parameter fields may have the same qualitative form at low temperature even where the forms differ sharply in the absence of the biquadratic coupling. The possible limitations of the self-consistent analysis leading to this prediction are considered.

Domain structures and superconductivity in $SrTiO_3$

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Localized superconductivity in domain walls, puddles etc may depend on the domain structure, as demonstrated in WO_3 where superconductivity is confined to twin walls in the ε-phase [1,2]. $SrTiO_3$ may offer a similar scenario with a high density of twins and twin walls below 106K. In the quantum paraelectric state twins form a “quantum domain glass” at 25 K < T < 40 K which shows intense relaxation and temperature hysteresis. Domains float collectively in a complex, smooth landscape with long relaxation times. In the “quantum domain solid” state below 25 K a temperature-dependent memory effect of the elastic response depends on the lowest temperature reached in the quantum domain solid state. The glassiness of twin boundary dynamics vanishes for temperatures approaching absolute zero and domain walls move coherently [3]. The question is asked whether such coherent domain patterns can mimic bulk superconductivity even when the condensation is constrained to domain walls.

[1] A. Aird and E.K.H. Salje, J.Phys-CM 10 L377-L380 (1998);

[2] E. Bousquet, H. Hamdi, P. Aguado-Puente, E.K.H. Salje, E. Artacho, and P. Ghosez, Phys. Rev. Research 2, 012052(R) (2020).

[3] S. Kustov, I. Liubimova and E.K.H. Salje, Phys. Rev.Lett. 124, 016801

^{16}O - ^{18}O isotope effect on thermal Hall conductivity of $SrTiO_3$

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It has been becoming increasingly clear that topology plays an essential role in bands beyond the electronic band that produces the topological insulator. However, it is a nontrivial question of how one can probe these elusive properties of states of matters in phonons and magnons' bands. Therefore, a recent discovery is most welcoming that the off-diagonal components of the Hall conductivity tensor, so-called thermal Hall effect (THE) is a useful tool for such a problem. Over the past decades or so, a dozen new report of THE has confirmed such highly unusual topological properties in a wide range of materials. One fascinating report is a large THE recently found in $SrTiO_3$ [1].

Motivated by this discovery, we measured THE in single crystals of both pristine and isotopically substituted strontium titanate using a home-made set-up with extreme precision [2]. We discovered two orders of magnitude difference in the thermal Hall conductivity between $SrTi^{16}O_3$ and ^{18}O-enriched $SrTi^{18}O_3$ samples [3]. In most temperature ranges, the magnitude of thermal Hall conductivity (k_{xy}) in $SrTi^{18}O_3$ is proportional to the magnitude of the longitudinal thermal conductivity (k_{xx}), which suggests a phonon-mediated thermal Hall effect. However, they deviate in the temperature of their maxima, and the thermal Hall angle ratio ($|k_{xy}/k_{xx}|$) shows anomalously decreasing behavior below the ferroelectric Curie temperature T_c ~25 K. This observation suggests a new underlying mechanism, as the conventional scenario cannot explain such differences within the slight change in phonon spectrum. Notably, the difference in magnitude of thermal Hall conductivity and rapidly decreasing thermal Hall angle ratio in $SrTi^{18}O_3$ is correlated with the strength of quantum critical fluctuations in this displacive ferroelectric. This relation points to a link between the quantum critical physics of strontium titanate and its thermal Hall effect, a possible clue to explain this example of an exotic phenomenon in non-magnetic insulating systems.

[1] X Li, B. Fauque, Z. Zhu, and K. Behnia, Phys. Rev. Lett. 124, 105901 (2020).

[2] Ha-Leem Kim, Matthew John Coak, J. C. Baglo, Keiron Murphy, R. W. Hill, Michael Sutherland, M. Ciomaga Hatnean, Geetha Balakrishnan, and Je-Geun Park, Rev. Sci. Instruments 90, 103904 (2019).

[3] Sangwoo Sim, Heejun Yang, Ha-Leem Kim, Matthew J Coak, Mitsuru Itoh, Yukio Noda, and Je-Geun Park, Phys. Rev. Lett. (in press): arXiv:2012.06085.

Thermal conductivity of a quantum paraelectric

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Motivated by some recent experimental results [1], we study the contribution of associated optical phonon modes to the thermal conductivity of a quantum paraelectric system. We calculate the decay rates of nearly soft optic phonons, considering its coupling with acoustic phonons and hence its contribution to thermal conductivity within Kubo formalism.

It is found that contributions from the optic phonons can increase up to an order of magnitude near the quantum critical point at low temperature [2]. Results are in qualitative agreement with the experiments and deserve further investigations.

[1] Valentina Martelli, Julio Larrea Jiménez, Mucio Continentino, Elisa Baggio-Saitovitch, and Kamran Behnia, Phys. Rev. Lett. 120, 125901 (2018)

[2] Pankaj Bhalla and Nabyendu Das: To appear soon. (2021)

What is the stability of bipolaron binding in $SrTiO_3$?

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TBA - abstract goes here

Phonons and polarons of STO studied by RIXS spectroscopy

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Politecnico di Milano – Physics Department, Italy

The electron-phonon coupling (EPC) in $SrTiO_3$ is known to be large leading to important polaronic phenomena, impacting on the conduction properties of the bulk material and at its interfaces. Resonant Inelastic X-ray Scattering (RIXS) is a new energy loss spectroscopy capable of probing electronic, magnetic and vibrational excitations at a time, and it is thus well suited to study the interplay between electrons and phonons. We measured high resolution RIXS at the Ti L_3 edge and determined how the electron-phonon interaction decreases vs the carrier density in bulk STO and at STO/LAO interfaces. Moreover, we found a clear evidence of a peak at about 130 meV of mixed phonon-electronic nature, given by an LO3+*dd* excitation, in all samples. We attribute it to the presence of large polarons in STO at all doping levels. These results were recently published in Phys Rev. Lett. 125, 126401 (2020).

Electronic consequences of intrinsic octahedral tilting in cubic $SrTiO_3$: Emergence of a direct gap component and strain-induced ferroelectricity

Zhi Wang

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Positional distortions, such as the octahedral tilting (antiferrodistortive displacement, AFD) have been known to exist in the low-symmetry tetragonal nonmagnetic $SrTiO_3$ insulator, but are unexpected in the nominal cubic phase. Indeed, when suggested by some experiments, such distortions were attributed to extrinsic factors such as strain, defect, impurities, or interfaces. However, whereas the simplest crystal models have atoms occupying precise symmetry-defined Wyckoff positions, some crystals manifest already at low temperatures deformations off Wyckoff positions (DOWP's) as part of their preferred equilibrium bonding configuration. Recognizing computationally such energy lowering symmetry breaking is contingent on abandoning the conventional single-cell monomorphous description of the XRD model and exploring DOWP's in a globally cubic N×N×N supercell description that allows for a polymorphous distribution of different local environments. Here we show that density functional total internal energy minimization calculation identifies in cubic $SrTiO_3$ supercells weak but intrinsic octahedral tilting at equilibrium lattice constant, achieving excellent agreement to experimentally measured pair distribution function (PDF). The octahedral tilting (i) leads to interesting band gap behavior: upon unfolding of the supercell band structure to the first Brillion zone, we find spectral function showing a predicted (yet unreported) distinct Γ-Γ direct band gap component as a secondary valley minimum to the well-known indirect R-Γ gap of cubic STO. (ii) The experimentally observed strongly a-symmetric ferroelectric transition temperature under positive and negative epitaxial strains, that cannot be explained with the nominal cubic single-cell model, is well-reproduced when such octahedral tilting are taken into consideration.

Electron Pairing and Superconductivity in STO-based Nanostructures

Jeremy Levy

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I will discuss the thesis that insights into the nature of superconductivity in STO can be obtained from STO-based heterostructures and nanostructures. I will focus mainly on experiments performed in my group but will also try to make connections with the broader literature.

On the character of the insulator-metal transition at polar-nonpolar perovskite interfaces

Daniel Bennett

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In 2004 it was discovered that, under the right conditions, a two-dimensional electron gas (2DEG) could appear at the interface between polar and nonpolar perovskites such as $LaAlO_3/SrTiO_3$ (LAO/STO) as a response to the polar discontinuity there. This 2DEG has been found to be associated with interesting phenomena such as superconductivity and magnetism, even coexisting. While the physical mechanism that gives rise to this 2D metal has been debated for many years, a question which has not been clearly addressed is that of the character of the insulator to metal transition, i.e. does it appear continuously or discontinuously with film thickness or applied electric field.

We discuss the character of the IM transition at polar-nonpolar perovskite interfaces, and propose a mean-field model which includes coupling of the carriers to tilting of oxygen octahedra, which both LAO and STO can exhibit. We find different scenarios, including first and second order transitions, depending on the energetics of the tilts, coupling with the polar mode and the polar discontinuity. First-principles calculations predict that the transition at the LAO/STO interface is second order, but is sensitive to the material parameters which could be tuned by chemistry or strain. A continuous transition would allow for more precise probing or control of applications such as superconductivity with an electric field applied perpendicular to the interface. Tuning to a discontinuous transition may, on the other hand, be helpful for technical applications making use of the on/off switching of the gas with an applied field.

Two-dimensional superconductivity at $KTaO_3$ (111) interfaces

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The unique electronic structure found at interfaces between materials can allow unconventional quantum states to emerge. One prominent example is the emergence of a superconducting electron gas at the interface of $LaAlO_3/SrTiO_3$. Here we observe superconductivity in electron gases formed at interfaces between (111) oriented $KTaO_3$ and insulating overlayers of either EuO or $LaAlO_3$. The superconducting transition temperature, approaching 2.2 K, is about one order of magnitude higher than that of the $LaAlO_3/SrTiO_3$ system. Strikingly, similar electron gases at (001) $KTaO_3$ interfaces remain normal down to 25 mK. The critical field and IV measurements indicate that the superconductivity is two dimensional. Low-carrier density $EuO/KTaO_3$(111) samples, with higher mobility, show spontaneous in-plane transport anisotropy at temperatures prior to the onset of global superconductivity, suggesting the emergence of a stripe phase where the superconductivity is nearly homogeneous in one direction, but modulated in the other.

Superconductivity in $SrTiO_3$: Homogeneous versus filamentary conduction mechanism

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$SrTiO_3$ is the prototype perovskite which exhibits an enormously rich phase diagram with varying ground state properties. One of those is the insulator/metal (I/M) and/or insulator/superconductor (I/S) transition upon doping which has challenged theory as well as experiment since this transition occurs at extremely low carrier density. We concentrate in this work on these transitions and demonstrate unambiguously that doped $SrTiO_3$ is an extremely inhomogeneous system where the coexistence and interplay of metallic filaments and an insulating intact matrix are the essential ingredients for these transitions to take place. This heterogeneous approach is adopted for single crystals where the surface layer contains a 3d-network of dislocations which differs in chemical composition from the matrix. The oxygen stoichiometry can preferentially be lowered in this network thereby manipulating the superconducting properties and opening up a new way of creating a filamentary superconductor with a transition temperature T_c in the mK regime and a coherence length of a few nm. Unlike common belief based on a homogeneous carrier density distribution we clarify the long standing miracle of the origin of the metal insulator transition by demonstrating that doped $SrTiO_3$ is a highly inhomogeneous system where polarity and metallicity are self-supporting and possess the essential ingredients to overcome the violation of the Mott criterion.

In collaboration with K.Szot, K.Rogacki, G.Bihlmayer, W.Speier, Ch.Rodenbücher, K.Roleder, F.Krok, H.Keller, A.Simon

Electronic consequences of intrinsic octahedral tilting in cubic $SrTiO_3$: Emergence of a direct gap component and strain-induced ferroelectricity

Zhi Wang

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Positional distortions, such as the octahedral tilting (antiferrodistortive displacement, AFD) have been known to exist in the low-symmetry tetragonal nonmagnetic $SrTiO_3$ insulator, but are unexpected in the nominal cubic Pm$\bar{3}$m phase. Indeed, when suggested by some experiments, such distortions were attributed to extrinsic factors such as strain, defect, impurities, or interfaces. However, whereas the simplest crystal models have atoms occupying precise symmetry-defined Wyckoff positions, some crystals manifest already at low temperatures deformations off Wyckoff positions (DOWP's) as part of their preferred equilibrium bonding configuration. Recognizing computationally such energy lowering symmetry breaking is contingent on abandoning the conventional single-cell monomorphous description of the Pm$\bar{3}$m XRD model and exploring DOWP's in a globally cubic N×N×N supercell description that allows for a polymorphous distribution of different local environments. Here we show that density functional total internal energy minimization calculation identifies in cubic $SrTiO_3$ supercells weak but intrinsic octahedral tilting at equilibrium lattice constant, achieving excellent agreement to experimentally measured pair distribution function (PDF). The octahedral tilting (i) leads to interesting band gap behavior: upon unfolding of the supercell band structure to the first Brillion zone, we find spectral function showing a predicted (yet unreported) distinct Γ-Γ direct band gap component as a secondary valley minimum to the well-known indirect R-Γ gap of cubic STO. (ii) The experimentally observed strongly asymmetric ferroelectric transition temperature under positive and negative epitaxial strains, that cannot be explained with the nominal cubic Pm$\bar{3}$m single-cell model, is well-reproduced when such octahedral tilting are taken into consideration.