

KFM 21: Focus Session: SrTiO₃: A Versatile Material from Bulk Quantum Paraelectric to 2D Superconductor (joint session TT/KFM/MA/O)

Strontium titanate (SrTiO₃) is a paradigmatic material that plays an important role in various fields of solid-state physics, surface science and catalysis: The pure bulk phase is a wide-band-gap semiconductor that upon cooling becomes a textbook quantum paraelectric. When slightly doped, SrTiO₃ turns into a Fermi-liquid-type metal that becomes superconducting at extremely low charge carrier density. SrTiO₃-based surfaces and interfaces host un-conventional electronic states such as quasi-two-dimensional electron liquid, magnetism and superconductivity. Despite intensive studies over the past decades, SrTiO₃ continues to reveal surprising new phenomena that challenge the established views on this material. To this end achieving light-induced nonequilibrium states and the recent preparation of a 2D oxide based on SrTiO₃ opens new playgrounds for research. This Focus Session will present exciting developments in the study of electronic states that are based on the peculiar properties of SrTiO₃.

Please note that this Focus Session comprises four parts: Posters are presented within the TT poster session TT58 (Wed 15:00-18:00, poster area E). Invited talks are compiled in the session TT62 (Thursday, 9:30 to 12:45, H0104), Contributed talks will be presented in sessions TT72 (Thursday 15:00-18:00, H0104) and TT83 (Fri 9:30-12:30, H0104).

Organizers: Rossitza Pentcheva, University of Duisburg-Essen, Marc Scheffler, University of Stuttgart

Time: Thursday 9:30–12:45

Location: H 0104

Invited Talk KFM 21.1 Thu 9:30 H 0104
Ferroelectricity and Superconductivity in SrTiO₃ — ●SUSANNE STEMMER — University of California, Santa Barbara, USA

Polar superconductors have attracted significant interest for their potential to host unconventional superconductivity. One candidate is doped strontium titanate (SrTiO₃), which can undergo successive ferroelectric and superconducting transitions. Recent experimental observations of a factor of two enhancement of the superconducting transition temperature in ferroelectric samples and the fact that both ferroelectricity and superconductivity vanish around the same carrier density, hint at common physical interactions relevant for both phenomena. We will discuss our understanding of ferroelectricity in strained SrTiO₃ films, and experiments aimed at elucidating the connection between superconductivity and ferroelectricity.

Although the ferroelectric transition of strained, undoped SrTiO₃ is usually described as a classic displacive transition, we show that it has pronounced order-disorder characteristics. Increasing the carrier concentration causes polar nanodomains to break up into smaller clusters. (Local) polar order appears to be essential to the superconducting state. For example, in strained SrTiO₃ films, suppression of superconductivity is correlated to the destruction of the (global) ferroelectric state, either by overdoping, by decreasing the film thickness or by alloying large amounts of a rare earth ion. We discuss how the length scale of polar order emerges as an important parameter in controlling the superconductivity of SrTiO₃.

Invited Talk KFM 21.2 Thu 10:00 H 0104
Dilute superconductivity in doped strontium titanate — ●KAMRAN BEHNI — LPEM-ESPCI, Paris, France

Dilute superconductivity survives in bulk strontium titanate when the Fermi temperature falls well below the Debye temperature. The onset of the superconducting dome is dopant dependent. The threshold density for superconductivity is much lower for mobile electrons introduced by removing oxygen atoms compared to those brought by substituting Ti with Nb. Our study of quantum oscillations reveals a difference in the band dispersion between the dilute metals made by these doping routes and our band calculations demonstrate that the rigid band approximation does not hold when mobile electrons are introduced by oxygen vacancies. We identify the band sculpted by these vacancies as the exclusive locus of superconducting instability in the ultradilute limit.

Invited Talk KFM 21.3 Thu 10:30 H 0104
Polarons and Excitons in quantum-paraelectric SrTiO₃ — ●CESARE FRANCHINI — University of Vienna & Bologna

SrTiO₃ stands as one of the most extensively investigated materials, captivating attention due to its distinctive electronic properties emerging from its quantum paraelectric nature. Positioned on the cusp of various collective phases, this material holds significant potential for exploitation in electronic and optical applications. In this presenta-

tion, we delve into the biphonon collective behaviors and quasiparticle properties of SrTiO₃ in both bulk and reduced dimensions, leveraging a combination of single-particle and many-body methods supported by machine learning techniques. Our exploration commences with an examination of temperature-dependent quantum and anharmonic effects employing a synergy of machine-learned potentials and the stochastic self-consistent harmonic approximation [1,2]. Shifting focus, we investigate the electron-phonon-driven formation of polarons, scrutinizing the interplay between spatially localized small polarons and dispersive large polarons in both bulk SrTiO₃ [3,4] and on the bulk-terminated SrTiO₃(001) surface [5,6]. In conclusion, our study delves into the optical and excitonic properties, with particular emphasis on the emergence of strongly bound excitonic peaks in the monolayer limit [7,8].

- [1] Adv. Quantum Technol. 6 (2023) 2200131
- [2] Phys. Rev. Mater. 7 (2023) L030801
- [3] Phys. Rev. B 91 (2015) 085204
- [4] npj Computational Materials 125 (2022)
- [5] Phys. Rev. Mater. 3, 034407 (2019); Phys. Rev. B 103 (2021) L241406
- [6] Phys. Rev. Mater. 7 (2023) 064602
- [7] Phys. Rev. Mater. 5 (2021) 074601
- [8] arXiv:2303.14830

15 min. break

Invited Talk KFM 21.4 Thu 11:15 H 0104
Controlling ferroelectrics with light — ●ANDREA CAVALLERI — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg — Department of Physics, University of Oxford

I will discuss how irradiation of ferroelectrics with intense, far and mid-infrared pulses, which are made resonant with certain phonon modes, can be used to manipulate the ferroelectric polarization. Two cases have been identified so far. On the one side, irradiation of a low temperature ferroelectric phase (e.g. in LiNbO₃) can achieve switching of the polarization. In incipient ferroelectric phases (e.g. in SrTiO₃), can lead to the formation of a long range ordered phase with stronger ferroelectricity than the paraelectric ground state. The microscopic physics of these phenomena are only in part clear, and I will discuss progress in this area.

Invited Talk KFM 21.5 Thu 11:45 H 0104
Terahertz electric field driven dynamical multiferroicity in SrTiO₃ — ●STEFANO BONETTI — Ca' Foscari University of Venice, Venice, Italy

In recent years, the ultrafast dynamical control and creation of novel ordered states of matter not accessible in thermodynamic equilibrium is receiving much attention. Among those, the theoretical concept of dynamical multiferroicity has been introduced to describe the emergence of magnetization by means of a time-dependent electric polarization in non-ferromagnetic materials. However, the experimental verifi-

cation of this effect is still lacking. Here, we provide evidence of room temperature magnetization in the archetypal paraelectric perovskite SrTiO₃ due to this mechanism. To achieve it, we resonantly drive the infrared-active soft phonon mode with intense circularly polarized terahertz electric field, and detect a large magneto-optical Kerr effect. A simple model, which includes two coupled nonlinear oscillators whose forces and couplings are derived with ab-initio calculations using self-consistent phonon theory at a finite temperature, reproduces qualitatively our experimental observations on the temporal and frequency domains. A quantitatively correct magnitude of the effect is obtained when one also considers the phonon analogue of the reciprocal of the Einstein - de Haas effect, also called the Barnett effect, where the total angular momentum from the phonon order is transferred to the electronic one. Our findings show a new path for designing ultrafast magnetic switches by means of coherent control of lattice vibrations with light.

KFM 21.6 Thu 12:15 H 0104

Emergence of a quantum coherent state at the border of ferroelectricity in SrTiO₃ — ●MATTHEW COAK^{1,2}, CHARLES HAINES², CHENG LIU², STEPHEN ROWLEY^{2,3}, GILBERT LONZARICH², and SIDDHARTH SAXENA² — ¹School of Physics and Astronomy, University of Birmingham, Birmingham, UK — ²Cavendish Laboratory, University of Cambridge, Cambridge, UK — ³Centro Brasileiro de Pesquisas Fisicas, Rio de Janeiro, Brazil

SrTiO₃ exists on the border of ferroelectricity in the vicinity of a quantum critical point (QCP). It is this proximity to a quantum critical point and the fluctuations associated with it which are responsible for SrTiO₃'s strikingly non-classical dielectric susceptibility.

I will discuss our results utilising ultra-high precision measurements of the the dielectric susceptibility to demonstrate an unconventional quantum paraelectric state exhibiting 'order by disorder' - a fluctuation-induced enhancement of electric polarization up to a coherence temperature T^* . We show that in the vicinity of T^* this phe-

nomenon can be understood quantitatively 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 QCP and is critical to our understanding of the mechanisms behind the quantum criticality and the phenomena resulting from it. At still lower temperatures, well below T^* , we observe a breakdown of this unconventional form of quantum paraelectricity and the emergence of a new instanton liquid phase.

KFM 21.7 Thu 12:30 H 0104

Dynamics of the critical phonon modes in quantum paraelectric SrTiO₃ — ●SHIYU DENG^{1,2}, CHARLES S. HAINES^{1,3}, MATTHEW J. COAK^{1,4}, ALEXANDRE IVANOV², ANDREA PIOVANO², ANDREW R. WILDES², and SIDDHARTH S. SAXENA¹ — ¹Cavendish Laboratory, University of Cambridge — ²Institut Laue-Langevin — ³University of East Anglia — ⁴University of Birmingham

The proximity of SrTiO₃ to a ferroelectric quantum critical point (FE QCP) has become a promising new branch of the study of quantum critical phenomena. New forms of quantum order have been reported in SrTiO₃ different from the quantum paraelectric state via dielectric measurements.

We report our recently performed triple-axis inelastic neutron scattering experiments on single-crystal SrTiO₃ at the temperature and pressure region of interest. These were the first direct measurements deep into the enigmatic 'quantum polar-acoustic state' in the vicinity of the FE QCP. Measurements are taken at and around $q = 0$ in multiple directions in reciprocal space to explore the transverse acoustic and soft optical phonon modes and their hybridization. In addition, we explore how pressure affects the underlying phonon modes in SrTiO₃. Our observations address directly the coupling of the soft optical mode with the acoustic phonons, and its response to external pressure. We believe this could help us understand the importance of anharmonic lattice dynamics and quantum fluctuations in SrTiO₃.