KFM 26: $SrTiO_3$: A Versatile Material from Bulk Quantum Paraelectric to 2D Superconductor II (joint session TT/KFM/MA/O)

Strontium titanate ($SrTiO_3$) 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, $SrTiO_3$ turns into a Fermi-liquid-type metal that becomes superconducting at extremely low charge carrier density. $SrTiO_3$-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, $SrTiO_3$ 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 $SrTiO_3$ 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 $SrTiO_3$.

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 15:00–18:00 Location: H 0104

KFM 26.1 Thu 15:00 H 0104

Origin of unconventional normal-state transport and superconductivity in electron-doped $SrTiO_3$ — •Stephen Rowley — Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge, CB3 0HE, United Kingdom

Quantum phase transitions may be reached in many ferroelectric systems by supressing the Curie temperature to absolute zero using a control parameter such as chemical substitution or hydrostatic pressure. In electron-doped specimens of quantum critical ferroelectrics such as $SrTiO_3$, unconventional superconductivity and unusual normal-state transport have been detected. In the latter case, a resistivity varying as temperature-squared is observed over a wide range of temperatures above the Fermi temperature. We present new experimental and model results that provide insight into the nature of the mechanisms for both superconductivity and normal-sate transport. We find in experiments and quantitative models without adjustable parameters, that both effects are connected and enhanced in samples tuned to the ferroelectric quantum critical point. Superconductivity appears to arise near the critical point due to the virtual exchange of longitudinal hybrid-polar-modes, even in the absence of a direct coupling to the transverse-optical phonon modes.

KFM 26.2 Thu 15:15 H 0104

Dilute superconductivity in the vicinity of a ferroelectric quantum critical point coupled via the "vector coupling": The case of $SrTiO_3$ — •Sudip Kumar Saha[1,2], Avraham Klein[1], Jonathan Ruhman[2], and Maria Navarro Gastiasoro[3] — [1]Ariel University, Israel — [2]Bar-Ilan University, Israel — [3]Donostia International Physics Center, Spain

Lightly doped $SrTiO_3$ (STO) is one of the most studied examples of quantum ferroelectric metal (QFEMs), where superconductivity coexists with ferroelectric order. Pristine STO is paraelectric naturally close to a ferroelectric quantum critical point (QCP). Strain or chemical substitution (for example, doping with Ba/Ca instead of Sr) drives STO through the QCP to the ferroelectric phase, which manifests itself in the softening of the transverse optical (TO) phonon mode. Doped samples are superconducting, where the T_c vs. density dome extends to very low density. To date, there is no consensus on the mechanism leading to superconductivity at such low density. Edge et al. have proposed that the ferroelectric QCP and dilute superconductivity are related [Phys. Rev. Lett. 115, 247002 (2015)]. In this work we explore the possible origin of low-density superconductivity from coupling linearly to the TO mode via a "vector coupling". We solve the critical-Eliashberg theory numerically, including fermionic and bosonic self-energy corrections, which allows us access all the way to the QCP. Notably, all our calculations are justified within standard approaches. We find the existence of a superconducting dome with magnitude and dependence on the distance from the QCP that resembles experiments.

KFM 26.3 Thu 15:30 H 0104

Dislocation-based filamentary superconductivity in reduced $SrTiO_3$ — •Christian Rodenbücher[1], Gustav Bihlmayer[2], Carsten Korte[1], and Kristof Szot[3] — [1]Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research (IEK-14), 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-1), 52425 Jülich, Germany — [3]University of Silesia, Institute of Physics, 41-500 Chorzów, Poland

Exposure of $SrTiO_3$ single crystals to reducing conditions at elevated temperatures leads to the generation of metallic filaments forming along of dislocations, which act as preferential reduction sites. This effect can be enhanced when stimulating the local deoxidation by electric fields. This results in an agglomeration of metallic filaments in nano-bundles, which are embedded in the insulating surrounding crystal matrix. Despite removing only 10^{14-15} oxygen atoms from the dislocation network, electro-reduced crystals are superconducting with a transition temperature of 0.2 K, and their residual resistance is lower than that of purely thermally-reduced crystals. As the total amount of oxygen removed during electro-reduction is much smaller than the smallest reported carrier concentration for superconducting $SrTiO_{3-x}$ so far, our findings challenge traditional explanations of superconductivity in metal oxides. Combining conductivity characterization by atomic force microscopy with theoretical analysis of the dislocation cores, we propose a model explaining the superconducting properties by the coexistence of metallic dislocation cores with polar insulating regions allowing for polaronic coupling in the bundles.

KFM 26.4 Thu 15:45 H 0104

Dislocation-Induced Photoconductivity Enhancement in Fe-Doped $SrTiO_3$: compensation of low mobility by high carrier density through the emergence of a sub-band gap level — •mehrzad soleimany[1,2], till frömling[1], jürgen rödel[1], and marin alexe[2] — [1]Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany — [2]Department of Physics, University of Warwick, Coventry, UK

Owing to the remarkable properties of $SrTiO_3$ (STO), such as quantum paraelectric state below 37 K, negative differential resistance under illumination, and significant alteration of properties by doping, STO stands out among perovskite oxides. Until recently, little attention had been paid to the tunability of its properties - especially optical properties -via the introduction of dislocations. In this study, we introduce the method of dislocation imprint, which allows us to induce high densities of dislocations ($> 1 \times 10^{14}$ m^{-2}) into a large volume of Fe-doped STO. Low-temperature I-V measurements indicated an about one order of magnitude increase in the photoconductivity of dislocation-rich samples. Photo-Hall measurements revealed that while dislocations might decrease the mobility, they could enhance the photoconductivity by increasing the number of carriers. Spectral responsivity measurements demonstrated that the higher carrier density could stem from the emergence of a sub-band gap level. Complementary C-AFM measurements conducted under illumination confirmed

the local enhancement of photoconductivity at dislocations, which fitted well to the Electron Channeling Contrast Images of dislocations.

KFM 26.5 Thu 16:00 H 0104

IR and THz studies on $(Ba_{0.45}Sr_{0.55}TiO_3)_{24}Ba_{0.45}Sr_{0.55}O$ and $(Ba_{0.45}Sr_{0.55}TiO_3)_8Ba_{0.45}Sr_{0.55}O$ thin films — Veronica Goian[1], Matthew Barone[2], Natalie Dawley[2], Christelle Kadlec[1], •Darrell Schlom[2,3], and Stanislav Kamba[1] — [1]Institute of Physics ASCR, Prague, Czech Republic — [2]Department of Materials Science and Engineering, Cornell University, Ithaca, NY, USA — [3]Kavli Institute at Cornell for Nanoscale Science, Ithaca, NY, USA

$(SrTiO_3)_nSrO$ and (n=1..6) films crystallizing in the Ruddlesdden-Popper (RP) structure are well known for low dielectric loss and large microwave permittivities which are highly tunable with electric field.[1,2] Bulk $(SrTiO_3)_nSrO$ is paraelectric, but the tensile strained thin films deposited on (110)$DyScO_3$ with n≥3, become ferroelectric at low temperatures. $(ATiO_3)_{24}AO$ and $(ATiO_3)_8AO$, A= $Ba_{0.45}Sr_{0.55}$ films deposited on (110)$DyScO_3$ exhibit no strain and yet become ferroelectric. Here we performed infrared and THz studies of phonon dynamics down to 10 K and compared it with above mentioned thin films and (Sr,Ba)TiO_3. The effect of soft mode and central mode on microwave dielectric properties and electric field tunability of permittivity will be discussed.

[1] C. H. Lee et al., Nature, 502 (2013) 532
[2] N. M. Dawley et al., Nat. Mater. 19 (2020) 176

KFM 26.6 Thu 16:15 H 0104

Polar phonon behaviour in polycrystalline Bi-doped strontium titanate thin films — •Oleksandr Tkach[1], Olena Okhay[2], Dmitry Nuzhnyy[3], Jan Petzelt[3], and Paula M. Vilarinho[1] — [1]Department of Materials and Ceramic Engineering, CICECO, University of Aveiro, Aveiro, Portugal — [2]TEMA-Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Aveiro, Portugal — [3]Institute of Physics of the Czech Academy of Sciences, Prague, Czechia

Among strontium titanate (STO) based materials, Bi-doped STO have been intensively studied as for dielectric as for resistance-switching memory and thermoelectric applications. Here, we enhance the dielectric characterisation by a lattice dynamics study of sol-gel-derived $Sr_{1-1.5x}Bi_xTiO_3$ thin films with x = 0.0053 and 0.167, deposited on Al_2O_3 substrates, using a variable-temperature far-infrared spectroscopy in a transmittance mode. Bi doping, known to induce a low-frequency dielectric relaxation in STO ceramics and films, due to off-centre dopant ion displacements generating electric dipoles, is shown to affect the polar phonon behaviour of thin films. We show that in weakly Bi-doped films, the low-frequency polar TO1 mode softens on cooling but less than in undoped STO. In heavily Bi-doped STO films, this mode displays no significant frequency variation with temperature from 300 to 10 K. The polar phonon behaviour of polycrystalline Bi-doped STO thin films is comparable with that of Bi-doped STO ceramics, which exhibit dielectric relaxations and harden soft-mode behaviour instead of the ferroelectric phase transition.

15 min. break

KFM 26.7 Thu 16:45 H 0104

Emergence of strain-Induced magnetism in plastically-deformed SrTiO3 at low temperature — •Anirban Kundu[1], Xi Wang[2], Avraham Klein[1], and Beena Kalisky[2] — [1]Department of Physics, Ariel University, Israel — [2]Institute of Nanotechnology & Advanced Materials, Bar-Ilan University, Israel

It is well established that SrTiO3 (STO) can possess ferroelectric states alongside observed superconducting states. However, so far, the phenomena of magnetism have not been established. In our collaborative work, in a plastically deformed bulk STO sample; SQUID measurements reveal strong magnetic signals which are completely absent in pristine samples. This strain-induced magnetism has two salient features. First, the magnetic moment is seen only with applied strain and increases with applied strain. Second, it also increases with temperature. Using Ginzberg Landau theory we show that these properties may be the result of coupling terms between strain, polar, and magnetic orders centered around dislocation walls induced by the plastic deformation. Our analysis implies that deformed STO is a quantum multiferroic.

KFM 26.8 Thu 17:00 H 0104

Mobility in $SrTiO_3$ Mediated by Machine Learning Predicted Anharmonic Phonons — •Luigi Ranalli[1], Carla Verdi[2], and Cesare Franchini[1] — [1]University of Vienna, Vienna, Austria — [2]University of Queensland: Brisbane, Queensland, Australia

The anharmonic corrections to ionic motion play a crucial role in influencing the electron-phonon interaction, a phenomenon typically addressed through harmonic dynamical matrices at the ground state. By combining machine learning methodologies [1] and the stochastic self-consistent harmonic approximation [2], we achieve a precise depiction of the temperature-dependent evolution of phonon frequencies and the onset of ferroelectricity in the quantum paraelectric perovskites $SrTiO_3$ [3] and $KTaO_3$ [4]. In this presentation, anharmonic dynamical matrices are incorporated into the Boltzmann transport equation calculations for $SrTiO_3$ up to 300K using the EPW code [5] and fixing the derivatives of the Kohn-Sham potential computed through density functional perturbation theory [6]. This approach yields a coherent interaction vertex, ensuring that the temperature-dependent ferroelectric soft mode explains and recovers the observed trend in experimental mobility, akin to the behavior observed in $KTaO_3$.

[1] R. Jinnouchi et al., Phys. Rev. Lett. 122 (2019) 225701
[2] L. Monacelli et al., J. Phys.: Condens. Matter 33 (2021) 363001
[3] C. Verdi et al., Phys. Rev. Materials 7 (2023) L030801
[4] L. Ranalli et al., Adv. Quantum Technol. 6 (2023) 2200131
[5] H. Lee et al., 10.1038/s41578-021-00289-w (2023)
[6] J. Zhou et al., Phys. Rev. Research 1 (2019) 033138

KFM 26.9 Thu 17:15 H 0104

Machine-learning-backed evolutionary exploration of the $SrTiO_3$(110) surface phase diagram — •Ralf Wanzenböck[1], Florian Buchner[1], Michele Riva[2], Jesús Carrete[3,1], and Georg K. H. Madsen[1] — [1]Institute of Materials Chemistry, TU Wien, A-1060 Vienna, Austria — [2]Institute of Applied Physics, TU Wien, A-1040 Vienna, Austria — [3]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, 50009 Zaragoza, Spain

We use Clinamen2, a modern functional-style Python implementation of the covariance matrix adaptation evolution strategy (CMA-ES), to gain insights into the lesser-known regions of the complex $SrTiO_3$(110) surface phase diagram. To speed up the process, we leverage the transferability of a neural-network force field (NNFF) implemented on top of the state-of-the-art JAX framework.

Starting from smaller reconstructions in well-explored phases, such as the 4×1 surface reconstruction [Wanzenböck et al., Digit Discov 1, 703-710 (2022)], the NNFF is iteratively refined using an active learning workflow that relies on uncertainty estimation techniques [Carrete et al., J. Chem. Phys 158, 204801 (2023)]. We show how this workflow and the underlying uncertainty metric lead to a flexible NNFF, highlighted by the exploration of out-of-sample $SrTiO_3$(110)-$(2 \times n)$ reconstructions.

KFM 26.10 Thu 17:30 H 0104

Quasiparticle and excitonic properties of monolayer $SrTiO_3$ — •Lorenzo Varrassi[1], Peitao Liu[2], and Cesare Franchini[1,3] — [1]Dipartimento di Fisica e Astronomia, Università di Bologna, Bologna — [2]Shenyang National Laboratory for Materials Science, Institute of Metal Research — [3]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna.

Recently, a breakthrough has been achieved with the synthesis of free-standing $SrTiO_3$ ultrathin films down to the monolayer limit[1]; its optical and excitonic properties remain however largely unexplored. This talk will provide insights on the quasiparticle and excitonic properties of monolayer $SrTiO_3$, employing many-body perturbation theory.

Our analysis[2] emphasizes the need to go beyond the diagonal GW approximation and include off-diagonal self-energy elements in order to obtain correct description of the orbital hybridizations. A fully satisfying description is achieved by treating non-locality in both exchange and correlation.

The optical properties are studied through the solution of the Bethe-Salpeter equation. We observe a significant enhancement of the excitonic effects with respect to the bulk phase, with a binding energy at the optical gap about four times greater. Furthermore, the two-dimensional polarizability at the long wavelength limit is dominated by two strongly bound excitonic peaks; their character is determined through the analysis of the excitonic wavefunctions.

[1] D. Ji et al., Nature 570 (2019) 87

[2] L. Varrassi et al., arxive:2303.14830 (2023)

KFM 26.11 Thu 17:45 H 0104

$SrTiO_3$: Thoroughly investigated but still good for surprises — •Annette Bussmann-Holder[1], Reinhard K. Kremer[1], Krystian Roleder[2], and Ekhard K. H. Salje[3] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Institute of Physics, University of Silesia, ul. 75 Pułku Piechoty 1, 41-500 Chorzów, Poland — [3]Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, United Kingdom

For decades $SrTiO_3$ is in the focus of research with seemingly never-ending new insights regarding its ground state properties, its application potentials, its surface and interface properties, the superconducting state, the twin boundaries and domain functionalities, etc. Here, we focus on the already well-investigated lattice dynamics of STO and show that four different temperature regimes can be identified which dominate the elastic properties, the thermal conductivity and the birefringence. These regimes are the low-temperature quantum fluctuation dominated one, followed by an intermediate regime, the region of the structural phase transition at 105 K and its vicinity, and at high temperatures a regime characterized by precursor and saturation effects. They can all be elucidated by lattice dynamical aspects. The relevant temperature dependencies of the soft modes are discussed and their relationship to lattice polarizability is emphasized.