Berlin 2024 – KFM Friday

## KFM 30: SrTiO<sub>3</sub>: A Versatile Material from Bulk Quantum Paraelectric to 2D Superconductor III (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: Friday 9:30–12:30 Location: H 0104

 $KFM\ 30.1 \quad Fri\ 9:30 \quad H\ 0104$ 

High-mobility two-dimensional electron gases based on strain engineered ferroelectric SrTiO<sub>3</sub> thin films — •Ruchi Tomar<sup>1</sup>, Tatiana Kuznetsova<sup>2</sup>, Srijani Mallik<sup>1</sup>, Luis M. Vicente-Arche<sup>1</sup>, Fernando Gallego<sup>1</sup>, Maximilien Cazayous<sup>3</sup>, Roman Engel-Herbert<sup>2,4</sup>, and Manuel Bibes<sup>1</sup> — <sup>1</sup>Unité Mixte de Physique, CNRS, Thales, Université Paris-Saclay, 91767 Palaiseau, France. — <sup>2</sup>Pennsyvlania State University, University Park, PA 16802, USA. — <sup>3</sup>Laboratoire Matériaux et Phénomènes Quantiques (UMR 7162 CNRS), Université de Paris, 75205 Paris Cedex 13, France. — <sup>4</sup>Paul Drude Institute for Solid State Electronics, Leibniz Institute within Forschungsverbund Berlin eV, Hausvogteiplatz 5-7, 10117, Berlin, Germany.

Two-dimensional electron gases (2DEGs) based on the quantum paraelectric  $\rm SrTiO_3$  display fascinating properties such as large electron mobilities, superconductivity, and efficient spin-charge interconversion owing to their Rashba spin-orbit coupling. Here, we use oxide molecular beam epitaxy to grow high-quality strain-engineered  $\rm SrTiO_3$  films that are ferroelectric up to 170 K. We then generate a 2DEG by sputtering a thin Al layer and demonstrate an increase in mobilities compared to earlier literature. Furthermore, through Raman spectroscopy and magneto-transport measurements, we show that the ferroelectric character is retained after 2DEG formation. These results thus qualify our samples as ferroelectric 2DEGs up to temperatures well above previous results based on Ca-SrTiO\_3 substrates, opening the way towards ferroelectric 2DEGs operating at room temperature.

KFM 30.2 Fri 9:45 H 0104

Two-dimensional electron liquids at truly bulk-terminated  $\operatorname{SrTiO}_3$ —•Igor Sokolović<sup>1,2</sup>, Eduardo B. Guedes³, Thomas van Waas⁴, Samuel Poncé⁴,⁵, Craig M. Polley⁶, Michael Schmid², Ulrike Diebold², Milan Radović³, Martin Setvín²,², and J. Hugo Dil³,8—¹Institute of Microelectronics, TU Wien, Vienna, Austria—²Institute of Applied Physics, TU Wien, Vienna, Austria—³Photon Science Division, PSI, Villagen, Switzerland—⁴ETSF, Institute of Condensed Matter and Nanosciences, UCLouvain, Louvain-la-Neuve, Belgium—⁵WEL Research Institute, Wavre, Belgium—6MAX IV laboratory, Lund University, Lund, Sweden—7Faculty of Mathematics and Physics, Charles University, Prague , Czech Republic—8Institut de Physique, ÉPFL, Lausanne, Switzerland

A truly bulk-terminated SrTiO<sub>3</sub>(001) surface prepared by cleaving in situ was investigated with angle-resolved photoemission spectroscopy (ARPES) and noncontact atomic force microscopy (ncAFM). The (1×1) SrTiO<sub>3</sub>(001) surfaces were achieved through our cleaving procedure that exploits the strain-induced ferroelectric transition in SrTiO<sub>3</sub>, and provides both possible surface terminations, TiO<sub>2</sub> and SrO. Each hosts a specific two-dimensional electron liquid (2DEL): the first with split and the other with degenerate bands. The origin of the 2DELs and the band-splitting mechanisms are elucidated by correlating the

observed reciprocal- and real-space electronic and atomic structure.

KFM 30.3 Fri 10:00 H 0104

Low-energy excitations at SrTiO<sub>3</sub>(001) surfaces in absence and presence of a two-dimensional electron gas — ●HANNES HERRMANN, ANNE OELSCHLÄGER, and WOLF WIDDRA — Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

The low-energy excitations of  $SrTiO_3$ , a large-bandgap oxide perovskite, are dominated by phonons and phonon polaritons. At the surface they couple to dipole-active surface phonon polaritons that are bound to the  $SrTiO_3$ -vacuum interface. These excitations can be addressed by surface vibrational spectroscopy techniques as, e.g., high-resolution electron energy loss spectroscopy (HREELS).

Here we will present HREELS studies that identify all  $SrTiO_3(001)$  dipole-active excitations, including their specific line shapes and will discuss the electron-phonon coupling to a two-dimensional electron gas. The latter are prepared with variable charge-carrier concentrations either by annealing under ultrahigh-vacuum condition or by growth of an ultrathin layers of EuO on top. With formation of the 2DEGs, the discrete surface phonon polaritons couple to the electron-hole pair continuum as is witnessed by a substantial line broadening and asymmetric Fano-like line shapes. A quantitative description that accounts for all details of the line shape paves the way for an in-situ analysis of the 2DEG charge carrier dynamics.

KFM 30.4 Fri 10:15 H 0104

Confined ionic-electronic systems based on SrTiO<sub>3</sub> — •Felix Gunkel, Marcus Wohlgemuth, Moritz L. Weber, and Regina Dittmann — Peter Gruenberg Institute, Forschungszentrum Juelich

SrTiO<sub>3</sub> reflects a a prototype ionic-electronic oxide, in which the physical properties are significantly affected by the ionic defect structure. [Gunkel et al., APL 2020] At the same time, spatial confinement of electronic charge carries led to unexpected electronic and magnetic phenomena, including 2DEG formation, magnetoresistance and localization phenomena. Here we will discuss, how spatial confinement also affects the ion-dynamics and defect-equilibria of SrTiO3, yielding interfacial defect structures and ion-dynamics that significantly differ from the bulk. [Rose et al., Adv. Mater. (2023); Weber et al., Nature Mater., to be published (Jan 2 2024)]. New opportunities to tailor such confined ionic-electronic systems arise from synthesis advances in generating transferable, free-standing SrTiO<sub>3</sub> sheets. These reflect ideally-confined nanosheets of  $\mathrm{SrTiO_3}$  and can serve as model system for ionic-electronic confinement phenomena as well as template for the synthesis of functional bilayer structures. We discuss the state-of-theart of controlled bilayer synthesis and derive the required finite-size corrections in the thermodynamic description of the defect chemistry of SrTiO<sub>3</sub>, indicating that the average reduction enthalpy of SrTiO<sub>3</sub> can be effectively reduced via confinement.

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Origin of spin-polarized 2DEG at the EuTiO<sub>3</sub>(001) surface and LaAlO<sub>3</sub>/EuTiO<sub>3</sub>/SrTiO<sub>3</sub>(001) interface — ●MANISH VERMA and ROSSITZA PENTCHEVA — Department of Physics, Universität Duisburg-Essen

Since the discovery of a two-dimensional electron gas (2DEG) at the interface between the LaAlO<sub>3</sub> and SrTiO<sub>3</sub> band insulators, studies on oxide surfaces and interfaces uncovered an intriguing and rich physics, such as possible magnetism in 2DEG. Using density functional theory with an on-site Coulomb repulsion term U, we find a spin-polarized 2DEG at the EuTiO<sub>3</sub>(001) surface arising from the interplay of ferromagnetic (FM) order of Eu-4f magnetic moments and the localization of electrons released from oxygen divacancies at the surface Ti sites, in agreement with in situ high-resolution angle-resolved photoemission [1]. The 2DEG at the LaAlO<sub>3</sub>/EuTiO<sub>3</sub>/SrTiO<sub>3</sub>(001) interface is formed due to the polar discontinuity. The spin-polarization is due to the FM exchange interaction between Eu 4f and Ti 3d states and steers the occupation of  $d_{xz}/d_{yz}$  orbitals [2].

R. Di Capua et al., Phys. Rev. Research 3 (2021) L042038
R. Di Capua et al., npj Quantum Mater. 7 (2022) 41

KFM 30.6 Fri 10:45 H 0104

A multiferroic STO-based 2D-electron gas — •Marco Salluzzo¹, Yu Chen¹, Martando Rath¹, Daniela Stornaiuolo², Julien Brehin³, Manuel Bibes³, Julien Varignon⁴, and Cinthia Piamonteze⁵ — ¹Cnr-Spin Complesso Monte S. Angelo via Cinthia 80126, Napoli, Italy — ²Università "Federico II" di Napoli, Dipartimento di Fisica "Ettore Pancini", Complesso Monte S. Angelo via Cinthia 80126, Napoli, Italy — ³Unité Mixte de Physique, CNRS, Thales, Université Paris Saclay, Palaiseau, France — ⁴Crismat, CNRS, Ensicaen, Normandie Université, Caen, France — ⁵Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland.

The fabrication of artificial materials combining different functional properties is a powerful method to create novel quantum states. Here we demonstrate the realization of a 2D electron gas exhibiting a coexistence of ferroelectric and ferromagnetic order parameters, by heteroepitaxy.

The novel 2DEG is realized by inserting few unit cells of the antiferromagnetic insulator EuTiO<sub>3</sub> between a LaAlO<sub>3</sub> band insulating thin film (10 unit cells) and a Ca-doped SrTiO<sub>3</sub> single crystal.

By using Ti-L<sub>2,3</sub> and Eu M<sub>4,5</sub> edges x-ray linear dichroism and x-ray magnetic circular dichroism, we provide evidences of a switchable polarization, non-volatile tuning of Ti3d orbital splitting, and of a modulation of Eu-4f magnetic moment of the 2DEG by the FE-polarization[1]. The result is of interest for quantum spin-orbitronic applications.

[1] J. Bréhin et al., Nat. Phys. 19 (2023) 823

KFM 30.7 Fri 11:00 H 0104 Magnetotransport properties of a spin polarized STO-based 2D electron system tuned by visible light — MARIA D'ANTUONO<sup>1,2</sup>, YU CHEN<sup>2</sup>, ROBERTA CARUSO<sup>1,2,3</sup>, BENOIT JOUAULT<sup>4</sup>, MARCO SALLUZZO<sup>2</sup>, and •DANIELA STORNAIUOLO<sup>1,2</sup> — <sup>1</sup>Department of Physics, University of Naples Federico II, Italy. — <sup>2</sup>CNR-SPIN, Naples, Italy. — <sup>3</sup>Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory, NY, USA. — <sup>4</sup>Laboratoire Charles Coulomb, CNRS, Université de Montpellier, France

Two-dimensional electron systems (2DES) developing in STO-based heterostructures possess a wide range of properties which are largely tunable thanks to the systems band structure and carrier density. In LaAlO<sub>3</sub>/EuTiO<sub>3</sub>/SrTiO<sub>3</sub> (LAO/ETO/STO) heterostructure, for instance, the charge carriers, above a critical value, start to fill Ti-3d bands with  $\mathrm{d}_{xz,yz}$  character, leading to the stabilization of a ferromagnetic order of Ti and Eu magnetic moments, and to a spin polarization of the 2DES. In this work we show that such mechanism can be achieved not only using electric field effect, but also using visible light irradiation. Furthermore, the analysis of the Anomalous Hall effect and of magnetocodnuctance curves demonstrate that visible light irradiation leads to enhanced stabilization of ferromagnetic correlations in the 2DES. Our results establishs the combined use of visible light and gate voltage as a straightforward way to access unexplored regions of the LAO/ETO/STO 2DES phase diagram.

15 min. break

 $KFM\ 30.8 \quad Fri\ 11:30 \quad H\ 0104$ 

All-electrical measurement of the spin-charge conversion effect in nanodevices based on  $\operatorname{SrTiO_3}$  two-dimensional electron gases —  $\bullet \operatorname{Fernando}$  Gallego¹, Felix Trier¹,², Srijani Mallik¹, Julien Brehin¹, Sara Varotto¹, Luis Moreno¹, Tanay Gosavy³, Chia-Ching Lin³, Jean-René Coudevylle⁴, Lucía Iglesias¹, Fèlix Casanova⁵,⁶, Ian Young³, Laurent Vila³, Jean-Philippe Attané², and Manuel Bibes¹ — ¹Unité Mixte de Phys, CNRS-Thales, Univ. Paris-Saclay, 91767 Palaiseau, France. — ²Dept of Energy Conservation and Storage, Univ. of Denmark, 2800 Kgs. Lyngby, Denmark. — ³Comp. Res. Intel Corp., Hillsb., OR 97124, USA. — ⁴Centre de Nanosciences et de Nanotech., CNRS, Université Paris-Saclay, France. — ⁵CIC nanoGUNE BRTA, 20018 Donostia, Spain. — ⁴IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain. —  $^7$ Univ. Grenoble Alpes, CNRS, CEA, SPINTEC, Grenoble, France.

We report all-electrical spin-injection and spin-charge conversion experiments in nanoscale devices harnessing the inverse Edelstein effect of  $\rm SrTiO_3$  2DEGs. We have designed, patterned and fabricated nanodevices in which a spin current injected from a cobalt layer into a  $\rm LaAlO_3/SrTiO_3$  2DEG is converted into a charge current. We optimized the spin-charge conversion signal by back-gating. We further disentangled the inverse Edelstein contribution from spurious effects. The combination of non-volatility and high energy efficiency of these devices could potentially lead to new technology paradigms for beyond-CMOS computing architectures.

KFM 30.9 Fri 11:45 H 0104

Effect of confinement and coulomb interactions on the electronic structure of the (111) LaAlO<sub>3</sub>/SrTiO<sub>3</sub> interface — •Mattia Trama<sup>1,2,3</sup>, Vittorio Cataudella<sup>4,5</sup>, Carmine Antonio Perroni<sup>4,5</sup>, Francesco Romeo<sup>1</sup>, and Roberta Citro<sup>1,2</sup> — <sup>1</sup>Universitá degli Studi di Salerno, Fisciano, Italy — <sup>2</sup>INFN Sezione di Napoli, Naples, Italy — <sup>3</sup>Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany — <sup>4</sup>Universitá degli Studi di Napoli Federico II, Naples, Italy — <sup>5</sup>CNR-SPIN Napoli Unit, Naples, Italy

A tight-binding supercell approach is used for the calculation of the electronic structure of the (111) LaAlO<sub>3</sub>/SrTiO<sub>3</sub> interface. The confinement potential at the interface is evaluated solving a discrete Poisson equation by means of an iterative method. In addition to the effect of the confinement, local Hubbard electron-electron terms are included at the mean-field level within a fully self-consistent procedure. The calculation carefully describes how the two dimensional electron gas arises from the quantum confinement of electrons near the interface due to the band bending potential. The resulting electronic sub-bands and Fermi surfaces show full agreement with the electronic structure determined by angle-resolved photoelectron spectroscopy experiments. In particular, we analyse how the effect of local Hubbard interactions change the density distribution over the layers from the interface to the bulk. Interestingly, the two-dimensional electron gas at the interface is not depleted by local Hubbard interactions which indeed induce an enhancement of the electron density between the first layers and the

KFM 30.10 Fri 12:00 H 0104

Enhanced Non-linear Response by Manipulating the Dirac Point in the (111) LaTiO<sub>3</sub>/SrTiO<sub>3</sub> Interface — •YORAM DAGAN, GAL TUVIA, AMIR BURSHTEIN, ITAI SILBER, AMNON AHARONY, ORA ENTIN-WOHLMAN, and MOSHE GOLDSTEIN — School of Physics and Astronomy, Tel Aviv University

Tunable spin-orbit interaction (SOI) is an important feature for future spin-based devices. In the presence of a magnetic field, SOI induces an asymmetry in the energy bands, which can produce non-linear transport effects  $(V \sim I^2)$ . Here, we focus on such effects to study the role of SOI in the (111) LaTiO<sub>3</sub>/SrTiO<sub>3</sub> interface. This system is a convenient platform for understanding the role of SOI since it exhibits a single-band Hall-response through the entire gate-voltage range studied. We report a pronounced rise in the non-linear longitudinal resistance at a critical in-plane field  $H_{cr}$ . This rise disappears when a small out-of-plane field component is present. We explain these results by considering the location of the Dirac point formed at the crossing of the spin-split energy bands. An in-plane magnetic field pushes this point outside of the Fermi contour, and consequently changes the symmetry of the Fermi contours and intensifies the non-linear transport. An out-of-plane magnetic field opens a gap at the Dirac point, thereby significantly diminishing the non-linear effects. We propose that magnetoresistance effects previously reported in SrTiO<sub>3</sub>-based interfaces could be comprehended within our suggested scenario.

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KFM 30.11 Fri 12:15 H 0104

Tunable 2D Electron- and 2D Hole States Observed at Fe/SrTiO $_3$  Interfaces — •PIA MARIA DÜRING $^1$ , PAUL ROSENBERGER $^{1,2}$ , LUTZ BAUMGARTEN $^3$ , FATIMA ALARAB $^4$ , FRANK LECHERMANN $^5$ , VLADIMIR N. STROCOV $^4$ , and MARTINA MÜLLER $^1$ —  $^1$ FB Physik, Universität Konstanz, 78457 Konstanz —  $^2$ TU Dortmund, 44221 Dortmund —  $^3$ FZ Jülich, PGI-6, 52425 Jülich —  $^4$ PSI, SLS, CH-5232 Villingen —  $^5$ TP III, RU Bochum, 44780 Bochum

Oxide electronics provide the key concepts and materials for enhancing silicon-based semiconductor technologies with novel functionalities. However, a crucial property of semiconductor devices remains undisclosed in their oxide counterparts: the ability to set or even switch be-

tween negatively (n) charged electrons or positively (p) charged holes. Using resonant angle-resolved photoelectron spectroscopy, we provide direct evidence for individually emerging n- or p-type 2D band dispersions in SrTiO<sub>3</sub> (STO)-based heterostructures [1]. The key to setting the carrier character is the oxidation state of a Fe-based interface layer: For Fe and FeO, hole bands emerge in the empty band gap region of STO, while for Fe<sub>3</sub>O<sub>4</sub> overlayers, an 2D electron system (2DES) is formed. Unexpected oxygen vacancy characteristics arise for the hole-type interfaces, which as of yet had been exclusively assigned to the emergence of 2DESs. In general, this study unveils the potential to seamlessly alter the conductivity type at STO interfaces by manipulating the oxidation state of a redox overlayer.

[1] P. M. Düring et al., Adv. Mater. (accepted)