# TT 17: Low-Dimensional Systems: Oxide Hetero-Interfaces

Time: Monday 15:00-17:15

Location: H22

correlations comes in two flavors. Either the compound is metallic with usually well-defined quasiparticles at low energy, or it is in a Mott-(or charge-transfer-)insulating state with robust Hubbard bands at high energy seperated by a sizable charge gap. Doped Mott insulators are more difficult to characterize, since e.g. introduced itinerancy often has to cope with preexisting ordered states of magnetic kind. Furthemore, bulk doping of Mott insulators is plagued by disorder effects, which are hard to capture theoretically by simple means.

Novel oxide heterostructures provide an alternative way of doping Mott-insulating materials by introducing well-defined doping layers in given host materials. Recent experimental work on  $\delta$ -doped titanates has shown the possibility for new emerging physics [1]. In this talk an advanced DFT+DMFT study of the  $\delta$ -doped  $3d^1$  titanate SmTiO<sub>3</sub> is presented. Layer- and temperature-dependent multi-orbital Mott transitions as well as spin and orbital polarizations are discussed. The intricate transport behavior in the conducting layers of the established itinerant interface state will be elucidated.

[1] C. A. Jackson, J. Y. Zhang, C. R. Freeze and S. Stemmer,

Nat. Commun. 5, 4258 (2014).

## 15 min. break

TT 17.5 Mon 16:15 H22 Magnetism, spin texture and in-gap states: Atomic specialization at the surface of oxygen-deficient  $SrTiO_3 - \bullet$ HARALD O. JESCHKE<sup>1</sup>, MICHAELA ALTMEYER<sup>1</sup>, MARCELO ROZENBERG<sup>2</sup>, MARC GABAY<sup>2</sup>, and ROSER VALENTI<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany — <sup>2</sup>Laboratoire de Physique des Solides, Bat 510, Université Paris-Sud, 91405 Orsay, France

We investigate the electronic structure and spin texture at the (001) surface of SrTiO<sub>3</sub> in the presence of oxygen vacancies by means of *ab initio* density functional theory (DFT) calculations of slabs. Relativistic non-magnetic DFT calculations exhibit Rashba-like spin winding with a characteristic energy scale ~ 10 meV. However, when surface magnetism on the Ti ions is included, bands become spin-split with an energy difference ~ 100 meV at the  $\Gamma$  point. This energy scale is comparable to the observations in SARPES experiments performed on the two-dimensional electronic states confined near the (001) surface of SrTiO<sub>3</sub>. We find the spin polarized state to be the ground state of the system, and while magnetism tends to suppress the effects of the relativistic Rashba interaction, signatures of it are still clearly visible in terms of complex spin textures.

TT 17.6 Mon 16:30 H22 **Pressure effects on the 2D electron system in LaAlO**<sub>3</sub>/**SrTiO**<sub>3</sub>. — •VLADISLAV BORISOV<sup>1</sup>, JONE ZABALETA<sup>2</sup>, HARALD O. JESCHKE<sup>1</sup>, THILO KOPP<sup>3</sup>, and ROSER VALENTI<sup>1</sup> — <sup>1</sup>Institute of Theoretical Physics, Goethe University, D-60438 Frankfurt am Main, Germany — <sup>2</sup>Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — <sup>3</sup>Center for Electronic Correlations and Magnetism, Experimental Physics VI, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany

We present a theoretical study of pressure effects on the electronic properties of the  $LaAlO_3/SrTiO_3$  (001) interface. Lattice relaxation plays a crucial role for the formation of the 2D electron system (2DES), in agreement with previous reports. We observe that the carrier density of the 2DES at zero pressure is much lower than the "polar catastrophe" estimate of  $0.5 \ e^-$  per two-dimensional unit cell, which agrees with most experimental works. Under hydrostatic pressure, structural distortions in LaAlO<sub>3</sub> (LAO) are largely suppressed, whereas they increase in SrTiO<sub>3</sub> (STO), and the carrier density of the 2DES is enhanced by almost 45% using a moderate pressure of 4.1 GPa. The origin of this behavior as well as the explanation for the low carrier density at the interface at ambient pressure are discussed in terms of the lattice polarization and electronic Berry phase in the LAO oxide. Reduction of the calculated static dielectric constants of LAO and STO under pressure might account for the recent experimental findings [1] regarding the carrier mobility.

[1] J. Zabaleta et al. (in preparation).

 $TT \ 17.7 \quad Mon \ 16:45 \quad H22$ 

TT 17.1 Mon 15:00 H22 Universal Fabrication of Two-Dimensional Electron Systems in Functional Oxides — •TOBIAS C. RÖDEL<sup>1,2</sup>, FRANK FORTUNA<sup>1</sup>, SHAMASHIS SENGUPTA<sup>3</sup>, EMMANOUIL FRANTZESKAKIS<sup>1</sup>, PATRICK LE FÉVRE<sup>2</sup>, FRANÇOIS BERTRAN<sup>2</sup>, BERNARD MERCY<sup>4</sup>, SYLVIA MATZEN<sup>5</sup>, GUILLAUME AGNUS<sup>5</sup>, THOMAS MAROUTIAN<sup>5</sup>, PHILIPPE LECOEUR<sup>5</sup>, and ANDRÉS FELIPE SANTANDER-SYRO<sup>1</sup> — <sup>1</sup>CSNSM, Univ. Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, 91405 Orsay, France — <sup>2</sup>Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin-BP48, 91192 Gif-sur-Yvette, France — <sup>3</sup>Laboratoire de Physique des Solides, Univ. Paris-Sud, CNRS, Université Paris-Saclay, 91405 Orsay, France — <sup>4</sup>CRISMAT, ENSICAEN-CNRS UMR6508, 6 bd. Maréchal Juin, 14050 Caen, France — <sup>5</sup>Institut d'Electronique Fondamentale, Univ. Paris-Sud, CNRS, Université Paris-Saclay, 91405 Orsay, France

Two-dimensional electron systems (2DESs) in transition metal oxides are currently a field of intense research in the quest of novel functionalities in materials showing competing ground states. The 2DESs in SrTiO<sub>3</sub>-based interfaces have been the cornerstone of such research. To go beyond, it is essential to create new types of oxide 2DESs in a technically easy way. Here we show, using (angle-resolved) photoemission spectroscopy in UHV that the deposition of atomically-thin layers of an elementary reducing agent results in the creation of 2DESs at the interface of several functional oxides, such as the ferroelectric BaTiO<sub>3</sub>. This technique can be adapted for transport studies and opens the possibility to study 2DESs in strongly-correlated insulating oxides.

## TT 17.2 Mon 15:15 H22

Gating effect in a lateral LaAlO<sub>3</sub>/SrTiO<sub>3</sub> 2DEG - SrTiO<sub>3</sub> heterostructure — •ALEXANDER MÜLLER<sup>1</sup>, MOHSIN MINHAS<sup>1</sup>, HANS-HELMUTH BLASCHECK<sup>1</sup>, BODO FUHRMANN<sup>2</sup>, and GEORG SCHMIDT<sup>1,2</sup> — <sup>1</sup>Fachbereich Physik, Martin-Luther Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — <sup>2</sup>Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

We have successfully patterned the two dimensional electron gas which forms at the interface between LaAlO<sub>3</sub> (LAO) and SrTiO<sub>3</sub>(STO) [1] using electron beam lithography and reactive Ion Etching (RIE). With this process small gaps between electrodes were created which at low temperature show the characteristics of the channel of a tunneling field effect transistor. An additional side gate can be used to modulate the I/V characteristics and thus create a true three terminal device. At low temperatures the transistor exhibits a transconductance of 32  $\mu$ A/V for a channel width of 4  $\mu$ m and a sub threshold swing of 9 mV/dec. [1] A. Ohtomo, H.Y. Hwang, Nature **427**, 6973 (2004)

#### TT 17.3 Mon 15:30 H22

Anisotropic transport in the two dimensional electron gas at oxide hetero-interfaces — •ROLAND SCHÄFER<sup>1</sup>, DIRK FUCHS<sup>1</sup>, KARSTEN WOLFF<sup>1,2</sup>, AHMED SLEEM<sup>1,2</sup>, RICHARD THELEN<sup>3</sup>, RUDOLF SCHNEIDER<sup>1</sup>, and HILBERT V. LÖHNEYSEN<sup>1,2</sup> — <sup>1</sup>Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe — <sup>2</sup>Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe — <sup>3</sup>Karlsruher Institut für Technologie, Institut für Mikrostrukturtechnik, 76021 Karlsruhe

We observe a resistive transition to superconductivity in the two dimensional electron gas which forms at the interface of strontium titanate and lanthanum aluminate or amorphous aluminium oxide. Resistivity is measured on quadratic samples in van der Pauw geometry; the voltage drop resulting from current injected at two contacts on one side of the sample is probed at the opposite side by two further contacts. The two possible, orthogonal arrangements show distinct different behavior indicating strong anisotropy in the transport properties of the electron gas. The results will be discussed with respect to a reduced dimensionality of the superconducting condensate.

TT 17.4 Mon 15:45 H22 Non-Fermi-liquid behavior in  $\delta$ -doped SmTiO<sub>3</sub> from first principles —  $\bullet$ FRANK LECHERMANN — I. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg — Institut für Keramische Hochleistungswerkstoffe, Technische Universität Hamburg-Harburg, 21073 Hamburg

Most stoichiometric condensed matter underlying stronger electronic

Interplay of oxygen vacancies and electronic correlations in SrVO<sub>3</sub> — •STEFFEN BACKES<sup>1</sup>, AARAM J. KIM<sup>1</sup>, FRANK LECHERMANN<sup>2</sup>, HARALD O. JESCHKE<sup>1</sup>, MARCELO J. ROZENBERG<sup>3</sup>, ANDRES F. SANTANDER SYRO<sup>4</sup>, and ROSER VALENTI<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str.1, 60438 Frankfurt am Main, Germany — <sup>2</sup>Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany — <sup>3</sup>Laboratoire de Physique des Solides, Université Paris-Sud, Bâtiment 510, 91405 Orsay, France — <sup>4</sup>CSNSM, Université Paris-Sud and CNRS/IN2P3, Bâtiments 104 et 108, 91405 Orsay cedex, France

We investigate the role of oxygen vacancies in SrVO<sub>3</sub> within LDA+DMFT (density functional theory combined with dynamical mean-field theory). We show that, in addition to the usual  $t_{2g}$  lower Hubbard band, oxygen vacancies are responsible for an additional peak around -1 eV of V  $3d_{z^2}$  orbital character, which is not present in the bulk system without vacancies. We discuss our results in the light of recent angle-resolved photoemission (ARPES) experiments.

#### TT 17.8 Mon 17:00 H22 Engineering the work function of oxide heterostructures — •ZHICHENG ZHONG and PHILIPP HANSMANN — Max-Planck Institute for Solid State Research

The design of novel materials for new functionality that push the frontiers of technology is one of the most important challenges in electronic structure calculations. One specific technology, still in its infancy, presents an alternative to thermoelectric conversion of heat to electrical energy and was coined as the thermoelectronic approach. The key components of a thermoelectronic device are an electron emitter and an electron collector separated by a vacuum. The creation of an electron current in the vacuum and the efficiency of the device crucially depends on the absolute value and the ratio of the work functions of emitter and collector material. In our study we investigate work functions of various transition metal oxide surfaces and how we can tune the work function by manipulating the surface by heterostructuring.