TT 94: Low-Dimensional Systems: Oxide Hetero-Interfaces

Time: Thursday 15:00–17:45 Location: HSZ 204

TT 94.1 Thu 15:00 HSZ 204

Surface / interface interaction in $LaAlO_3/SrTiO_3$ heterostructures: an *in-situ* transport and photoemission study — •Philipp Scheiderer[1], Florian Pfaff[1], Judith Gabel[1], Mihaela Gorgoi[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems, Universität Würzburg, Germany — [2]Helmholtz Zentrum Berlin, Germany

Oxide heterostructures display many interesting phenomena, one example being the formation of a two-dimensional electron system (2DES) at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface beyond a critical thickness of 4 monolayers (ML) of the polar LAO [1, 2]. An explanation for this behavior is the so-called electronic reconstruction. In this context it has recently been shown that polar adsorbates can enhance the conductivity of the 2DES [3]. Besides their electrostatic influence it was discussed that surface defects/adsorbates can also act as a charge reservoir [4]. To examine the impact of surface adsorbates on the 2DES we performed *in-situ* conductivity measurements and *in-situ* photoelectron spectroscopy (PES) on 6ML thick LAO/STO heterostructures exposed to a defined amount of water vapor. PES experiments indicate that water adsorbates induce additional charge carriers at titanium sites which are located at the interface. We correlate these spectroscopic findings with *in-situ* conductivity measurements.

[1] Ohtomo et al., Nature **427** (2004) 423
[2] Thiel et al., Science **313** (2006) 1942
[3] Xie et al., Nature Comm. **2** (2011) 494
[4] Bristowe et al., Phys. Rev. B **83** (2011) 205405

TT 94.2 Thu 15:15 HSZ 204

Direct k-space mapping of interface states in oxide-oxide heterostructures — •Florian Pfaff[1], Hidenori Fujiwara[2], Judith Gabel[1], Götz Berner[1], Atsushi Yamasaki[3], Akira Sekiyama[2], Yunzhong Chen[4], Nini Pryds[4], Shigemasa Suga[5,6], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg — [2]Graduate School of Engineering Science, Osaka University — [3]Department of Physics, Konan University — [4]Department of Energy Conversion and Storage, Technical University of Denmark, — [5]Institute of Scientific & Industrial Research, Osaka University — [6]Max-Planck-Institute for Microstructure Physics, Halle

The most prominent example of unexpected quantum phases that can form at oxide heterointerfaces is the 2D electron system (2DES) in $LaAlO_3/SrTiO_3$ (LAO/STO). Its origin has been related to electronic reconstruction due to the polar character of the LAO. The novel γ-Al_2O_3 (GAO)/STO also exhibits a 2DES with even higher mobility although GAO is regarded to be non-polar. Here, it is assumed that O vacancies at the STO side of the interface induce the 2DES. We have mapped the momentum-resolved electronic structure of the interface Ti 3d states by resonant soft x-ray photoemission for both types of heterostructures. While one can observe in both systems a dichotomy of mobile and trapped interface charges they also show remarkable differences regarding the proportion of mobile and trapped carriers as well as the electron dispersions and Fermi surfaces.

TT 94.3 Thu 15:30 HSZ 204

Correlated electron states in realistic oxide heterostructures — •Frank Lechermann[1], Lewin Boehnke[1], Christoph Piefke[1], and Daniel Grieger[2] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]SISSA, Via Bonomea 265, I-34136 Trieste

The interface physics that arises from merging different metal oxides is currently one of the most intensive condensed matter research areas. For instance, bringing bulk band- and/or Mott-insulating materials together most often leads to the formation of an intricate two-dimensional electron gas (2DEG) at the interface. This 2DEG may be susceptible to various orderings, e.g. ferromagnetism or superconductivity. Using the charge self-consistent combination of density functional theory (DFT) and dynamical mean-field theory (DMFT) with a continuous-time quantum Monte Carlo impurity solution to DMFT, the relevance of electron correlation in many of these novel designed materials will be elucidated. The methodology allows to treat many-body effects beyond static mean field on the realistic structural/chemical level of such challenging systems like $LaTiO_3/SrTiO_3$ superlattices [1].

[1] F. Lechermann, L. Boehnke, and D. Grieger, Phys. Rev. B 87, 241101(R) (2013)

TT 94.4 Thu 15:45 HSZ 204

Emerging magnetism and electronic phase separation at titanate interfaces — •Natalia Pavlenko[1], Thilo Kopp[1], and Jochen Mannhart[2] — [1]EKM und Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

The emergence of magnetism in otherwise nonmagnetic compounds and its underlying mechanisms have become the subject of intense research. Here we demonstrate that the nonmagnetic oxygen vacancies are responsible for an unconventional magnetic state common for titanate interfaces and surfaces. Using an effective multiorbital modelling, we find that the presence of localized vacancies leads to an interplay of ferromagnetic order in the itinerant t_{2g} band and complex magnetic oscillations in the orbitally-reconstructed e_g-band, which can be tuned by gate fields at oxide interfaces. The magnetic phase diagram includes highly fragmented regions of stable and phase-separated magnetic states forming beyond nonzero critical defect concentrations.

TT 94.5 Thu 16:00 HSZ 204

Interaction induced instabilities in $LaAlO_3/SrTiO_3$ interfaces — •Mathias Scheurer and Jörg Schmalian — Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

At the interface between insulating oxides, novel phases with peculiar electronic properties arise. In this talk, we focus on one specific example, the heterostructure formed by the perovskite oxides $LaAlO_3$ and $SrTiO_3$. Using the renormalization group approach, the effect of electron-electron interactions is studied. We consider all interaction terms consistent with the symmetries of the system and analyze the stability of the electron fluid towards the formation of symmetry broken phases.

15 min. break.

TT 94.6 Thu 16:30 HSZ 204

The Rashba spin-orbit coupling for superconductivity in oxide interfaces — •Stefan Beyl, Peter P. Orth, and Jörg Schmalian — Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

We investigate the role of the Rashba spin-orbit coupling on the superconducting order parameter and the phase stiffness at the interface of $LaAlO_3$ and $SrTiO_3$. In particular, we analyze the gate controlled crossover between BCS superconductivity and Bose-Einstein condensation of Cooper pairs, amplified by the Rashba coupling and the possibility of a phase fluctuation induced quantum critical point.

TT 94.7 Thu 16:45 HSZ 204

Spin-orbit coupling in 2DEGs at a polar/non-polar oxide interface — •Kourosh Rahmanizadeh, Gustav Bihlmayer, Daniel Wortmann, and Stefan Blügel — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The investigation of a two-dimensional electron gas (2DEG) at the polar / non-polar oxide interface (e.g. the discovery of highly mobile electrons at the $LaAlO_3$ / $SrTiO_3$ interface) is attractive for spintronic applications. Similar to the 2DEGs formed in semiconductor heterostructures, Rashba spin-orbit coupling (SOC) can have a big impact for the magnetotransport properties at these oxide interfaces [1]. Moreover, the combination of Rashba SOC and magnetic (or exchange) fields offer unique properties sought for in the hunt for Majorana fermions [2]. The $BiAlO_3$ (BAO) exhibits the same polar layers as $LaAlO_3$. The ferroelectricity of the material further allows to manipulate the carrier density at the interface. Using density functional theory, we investigated the 2DEG in $BAO/SrTiO_3$, $BAO/EuTiO_3$ and BAO/Sr_2NiWO_6 heterostructures. In the latter two structures, the proximity to ferroelectric insulators breaks the time-reversal symmetry in the 2DEG and leads, in combination with Rashba SOC to a single Fermi surface, analogous to the situation in topological insulators.

Financial support of the EU grant NMP3-LA-2010-246102 (IFOX) is gratefully acknowledged.
[1] A. D. Caviglia et al., Phys. Rev. Lett. **104**, 126803 (2010).
[2] J. D. Sau et al., Phys. Rev. Lett. **104**, 040502 (2010).

TT 94.8 Thu 17:00 HSZ 204

Confinement-driven electronic phases in $(LaAlO_3)_M/(LaNiO_3)_N(111)$ superlattices — •David Doennig and Rossitza Pentcheva — Ludwig-Maximilians University Munich

Complex oxide heterostructures exhibit a broad variability of functional properties and electronic states, not available in the bulk. Beyond the much studied (001)-oriented systems, here we highlight theoretical results on (111) perovskite superlattices (SLs) containing the correlated metal $LaNiO_3$ (LNO) and the band insulator $LaAlO_3$ (LAO). Density functional theory calculations with an on-site Coulomb repulsion term reveal a rich spectrum of electronic phases in $(LAO)_M/(LNO)_N(111)$ SLs as a function of the LNO and LAO thickness N and M in the superlattice. In the double perovskite 1/1 system, a Jahn-Teller distortion with d_{z^2} orbital polarization leads to a ferromagnetic Mott insulating phase, so far unanticipated for nickelates. For the LNO bilayer (N=2) with graphene topology, a Dirac-point Fermi surface is obtained, while symmetry breaking leads to band gap opening with two inequivalent interfaces. For $N \geq 3$ the confined LNO slab undergoes a metal-to-insulator transition to a half-semimetallic phase with conduction originating from the interfaces. Antiferromagnetic arrangements allow combining motifs of the bilayer and single trigonal layer band structures in engineered artificial mixed phases. We acknowledge funding by the DFG, SFB/TR80.

TT 94.9 Thu 17:15 HSZ 204

Enhanced ferromagnetism in $BiFeO_3/NgGaO_3$ thin film — •Chang-Yang Kuo[1], Zhiwei Hu[1], Jan-Chi Yang[2], Ying-Hao Chu[2], Stefano Agrestini[1], Tunwen Pi[3], Eric Pellegrin[4], and Liu Hao Tjeng[1] — [1]Max Planck Institut CPfS, Dresden, Germany — [2]National Chiao Tung University, Hsinchu, Taiwan — [3]National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan — [4]CELLS-ALBA, Barcelona, Spain

Multiferroic material $BiFeO_3$ has attracted a tremendous interest from the fundamental research as well as application points of view because of its high ferroelectric Curie temperature of 820 ^{o}C and high Neel temperature of 370 ^{o}C. Recently, strain engineering has emerged as a powerful means for tuning the various properties of $BiFeO_3$ thin film remarkably, such as by modifying ferroelectric domain walls or direction in $BiFeO_3$, enhancing ferroelectricity. Also a weak ferromagnetic component, induced by spin canting, has been observed in strained thin films. Here we report a x-ray absorption magnetic circular dichroism (XMCD) and x-ray absorption magnetic linear dichroism (XMLD) study showing a strong enhancement of the ferromagnetic component and tetragonal distortion for $BiFeO_3$ thin film grown on $NdGaO_3$ substrate.

TT 94.10 Thu 17:30 HSZ 204

DFT+DMFT study of epitaxially strained $LaVO_3$ — •Gabriele Sclauzero, Krzysztof Dymkowski, and Claude Ederer — Materials Theory, ETH Zurich, Switzerland

$LaVO_3$ is a t_{2g} perovskite showing a rich phase diagram as a function of temperature, with a paramagnetic Mott-Hubbard insulating state at room temperature. Recently, it has become possible to produce and characterize strained lattices of $LaVO_3$ in thin films and superlattices of high structural quality. In such heterostructures both interface effects and epitaxial strain play an important role in the electronic reconstruction of the material, and it is often difficult to distinguish between these two effects in experiments. Moreover, the epitaxial strain can induce at least two different important modifications of the atomic geometry, namely: (i) a change in the amplitudes of the VO_6 octahedral rotations; (ii) a stretching or compression of V–O bonds.

In this work, we perform density functional theory plus dynamical mean field theory (DFT+DMFT) simulations to study how the correlated Mott-Hubbard phase of $LaVO_3$ is affected by epitaxial strain. We separate the effect of bond-length changes from that of octahedral rotations by comparing an idealized structure without rotations and a realistic one derived from the bulk orthorhombic phase. We interpret our findings through the strain-induced changes in the energies of the crystal-field t_{2g} levels of the local DFT Hamiltonian and in the occupation matrix obtained from DMFT. A comparison with the t_{2g} perovskite $LaTiO_3$, which shows an insulator-to-metal transition upon compressive strain, will also be presented.