TT 8: Low-Dimensional Systems: Oxide Hetero-Interfaces

Time: Monday 9:30–12:30 Location: H 3010

TT 8.1 Mon 9:30 H 3010

Transport properties of $LaAlO_3/SrTiO_3$ nanostructures — •Alexander Müller[1], Mohsin Minhas[1], Hans-Helmuth Blaschek[1], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale) , Germany

Deposition of thin layers of $LaAlO_3$ (LAO) on top of a TiO_2 terminated $SrTiO_3$ (STO) substrate with Pulsed Laser Deposition results in a two dimensional electron gas at the interface [1]. Using PMMA as resist and etch mask this electron gas can be patterned by a standard electron-beam lithography step and subsequent Reactive Ion Etching to remove the LAO.

With this process transport structures with minimum dimensions in the sub-micron regime have been fabricated. The structures include gaps of approx. 100 nm width. Transport through the gap is characterized by taking I/V characteristics in a standard four point geometry from room temperature down to 1.5 K.

Between 1.5 and 30 K up to a threshold voltage of tens of mV no current is observed. Beyond that threshold voltage the current increases dramatically. Within a few tens of mV the current can increase by up to eight orders of magnitude. The threshold voltage is temperature dependent in a non-monotonic fashion and all I/V curves are free of any hysteresis.

[1] A. Ohtomo, H.Y. Hwang, Nature **427**, 6973 (2004)

TT 8.2 Mon 9:45 H 3010

An industry compatible low-damage nano-patterning process for LAO/STO heterostructures — •Mohsin Zamir Minhas[1], Hans-Helmuth Blaschek[1], Frank Heyroth[2], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle (Saale) , Germany

The discovery of an electron gas at the interface between the two band insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO)[1] has initiated a huge effort to study this interface in detail. Later on other interesting properties such as induced ferromagnetism[2] and superconductivity[3] have been reported which make the LAO/STO interface a model system to study the fundamental physics of strongly correlated electronic system and also a candidate for future multifunctional oxide electronics. A reproducible nano-patterning technique is required to develop this unique interface into useful technologies. Here we present a reliable technique to physically pattern the quasi-two-dimensional electron gas (q2DEG) down to lateral dimensions as small as 100nm while maintaining its conducting properties. The fully industry compatible process uses electron beam lithography in combination with reactive ion etching. Temperature dependent transport properties of patterned Hall bars of various widths show a small size dependence of conductivity. The deviation can be explained by a narrow lateral depletion region.

[1] Ohtomo, A. et al. Nature 427 (2004) 423.
[2] Brinkman, A. et al. Nat. Mater. 6 (2007) 493.
[3] Reyren, N. et al. Science 317 (2007) 1196.

TT 8.3 Mon 10:00 H 3010

Valence Band Electronic Structure and Band Alignment of $LaAlO_3/SrTiO_3$(111) Heterointerfaces — •J. Gabel[1], P. Scheiderer[1], M. Zapf[1], P. Schütz[1], C. Schlüter[2], T.-L. Lee[2], M. Sing[1], and R. Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg — [2]Diamond Light Source, Didcot

As in the famous $LaAlO_3$(LAO)/$SrTiO_3$(STO) (001) a two-dimensional electron system (2DES) also forms at the interface between LAO and STO in (111) orientation. A distinct feature of the (111) interface is its peculiar real space topology. Each bilayer represents a buckled honeycomb lattice similar to graphene which is known theoretically to host various topologically non-trivial states. Bilayer STO in proximity to the interface can be regarded as a three-orbital generalization of graphene with enhanced electron correlations making it a promising candidate for the realization of strongly correlated topological phases. We have investigated the electronic structure of the LAO/STO (111) heterostructure in relation to the oxygen vacancy concentration which we can control by synchrotron light irradiation and oxygen dosing. With hard X-ray photoemission we study the core levels, whereas resonant soft X-ray photoemission is used to probe the interfacial valence band (VB) states. Two VB features are found: a peak at the Fermi level associated with the 2DES and in-gap states at higher binding energies attributed to oxygen vacancies. By varying the oxygen vacancy contribution we can tune the emergence of the VB states and engineer the interfacial band alignment.

TT 8.4 Mon 10:15 H 3010

Oxygen Dosing the Surface of $SrTiO_3$ — •L. Dudy[1], P. Scheiderer[1], J.D. Denlinger[2], P. Schütz[1], J. Gabel[1], M. Buchwald[1], C. Schlueter[3], T.-L. Lee[3], M. Sing[1], and R. Claessen[1] — [1]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, 94270, USA — [3]Diamond Light Source Ltd., Didcot, Oxfordshire OX11 0DE, United Kingdom

The highly mobile two-dimensional electron system (2DES) on the surface of the insulating $SrTiO_3$(STO) offers exciting perspectives for advanced material design. This 2DES resides in a depletion layer caused by oxygen deficiency of the surface. With photoemission spectroscopy, we monitor the appearance of quasi-particle weight (QP) at the Fermi energy and oxygen vacancy induced states in the band gap (IG). Both, QP and IG weight, increase and decrease respectively upon exposure to extreme ultraviolet (XUV) light and in-situ oxygen dosing. By a proper adjustment of oxygen dosing, any intermediate state can be stabilized providing full control over the charge carrier density. From a comparison of the charge carrier concentrations obtained from an analysis of core-level spectra and the Fermi-surface volume, we conclude on a spatially inhomogeneous surface electronic structure with at least two different phases.

TT 8.5 Mon 10:30 H 3010

***Ab initio* determination of the spin texture in $SrTiO_3$ surfaces** — •Michaela Altmeyer[1], Klaus Koepernik[2], Harald O. Jeschke[1], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]IFW, 01171 Dresden, Germany

The appearance of oxygen vacancies in a surface of strontium titanate has been recently identified to be a likely reason for the formation of a two-dimensional electron gas close to the surface. Lately the first SARPES measurements [1] on these surfaces unveiled an interesting spin texture which shows besides the expected Rashba effect a huge spin splitting that can not be attributed to spin-orbit interaction. Employing density functional theory we therefore examined oxygen deficient slabs and found that indeed magnetism is capable of explaining the measured spin splittings. Moreover we obtain a very rich spin texture where we find not only rotating spins due to the Rashba interaction, but a very complex spin structure most likely caused by an interplay of orbital and spin degrees of freedom.

[1] A.F. Santander-Syro *et al.*, Nature Materials **13**, 1085 (2014).

TT 8.6 Mon 10:45 H 3010

Effect of band filling and symmetry breaking on the electronic ground state in $(LaXO_3)_2/(LaAlO_3)_4$(111) (X = 3d) superlattices — •David Doennig[1], Warren E. Pickett[2], and Rossitza Pentcheva[3,1] — [1]Forschungs-Neutronenquelle (FRMII), TU München — [2]University of California Davis, U.S.A. — [3]Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Structural patterns, e.g. a buckled honeycomb lattice, realized in (111)-oriented perovskite bilayers may lead to exotic electronic ground states such as a Dirac-point Fermi surface [1-3]. Based on density functional theory calculations including a Hubbard U term, we explore systematically the effect of band filling in [111]-oriented $(LaXO_3)_2/(LaAlO_3)_4$ superlattices with X spanning the series of open shell 3d ions. The interplay of charge, spin, orbital, and lattice degrees of freedom reveals some regularities over the series, but also several unexpected symmetry lowering reconstructions that can guide the design of artificial materials with desired spin-charge-orbital order in conjunction with size of the energy gap and the possibility for emergent topological character. We acknowledge funding by the DFG (SFB/TR80, project G3).

[1] D. Xiao *et al.*, Nat. Commun. **2**, 596 (2011).
[2] D. Doennig, W. E. Pickett, and R. Pentcheva, Phys. Rev. Lett. **111**, 126804 (2013).
[3] D. Doennig, W. E. Pickett, and R. Pentcheva, Phys. Rev. B **89**, 121110(R) (2014).

15 min. break.

TT 8.7 Mon 11:15 H 3010

Towards Mott design by δ-doping of strongly correlated titanates — •Frank Lechermann and Michael Obermeyer — I. Institut für Theoretische Physik, Universität Hamburg

Oxide heterostructures are promising systems for exploring novel composite materials beyond nature's original conception. Already the doping of distorted-perovskite Mott-insulating titanates such as $LaTiO_3$ and $GdTiO_3$ with a single SrO layer gives rise to a rich correlated electronic structure [1]. A realistic superlattice study by means of the charge self-consistent combination of density functional theory (DFT) with dynamical mean-field theory (DMFT) reveals layer- and temperature-dependent multi-orbital metal-insulator transitions. Doped along the [001] direction, an orbital-selective metallic layer at the interface dissolves via an orbital-polarized doped-Mott state into an orbital-ordered insulating regime beyond the two conducting TiO_2 layers. Breaking the spin symmetry in δ-doped $GdTiO_3$ results in blocks of ferromagnetic itinerant and ferromagnetic Mott-insulating layers which are coupled antiferromagnetically.

[1] F. Lechermann and M. Obermeyer, arXiv:1411.1637 (2014)

TT 8.8 Mon 11:30 H 3010

DFT+DMFT study of strain and interface effects in $LaTiO_3$ and $LaVO_3$ — Krzysztof Dymkowski, Gabriele Sclauzero, and •Claude Ederer — Materials Theory, ETH Zurich, Switzerland

Metal-insulator transitions in thin films of early transition metal correlated oxides are linked to both epitaxial strain and electronic reconstruction at the film/substrate interface. We separately address these two key factors for $LaTiO_3$ and $LaVO_3$ through density functional theory plus dynamical mean-field theory (DFT+DMFT). We find that mere epitaxial strain suffices to induce an insulator-to-metal transition in $LaTiO_3$ [1], but not in $LaVO_3$, in agreement with recent experiments [2]. We show that this difference can be explained by the combined effect of strain-induced changes in the crystal field splitting of t_{2g} orbitals and different orbital filling in these two materials. The role of the interface is investigated through DFT+DMFT simulations of $LaVO_3/SrTiO_3$ heterostructures with varying superlattice periodicities and substrate terminations. Our aim is to assess whether the metallicity observed at the LaVO3/SrTiO3 interface could be driven by pure electronic reconstruction effects, rather than structural or stoichiometric reasons (such as, e.g., O-related defects).

[1] Dymkowski/Ederer, Phys. Rev. B 89, 161109 (2014).
[2] He et al., Phys. Rev. B 86, 081401 (2012).

TT 8.9 Mon 11:45 H 3010

$LaAlO_3$–$LaNiO_3$ (111) interfaces: a DFT+DMFT study — •Oleg Janson and Karsten Held — Institut für Festkörperphysik, Technische Universität Wien, Österreich

As a peculiarity of (111) perovskite interfaces, the e_g electrons can retain their degeneracy and facilitate the emergence of topological phases. From the materials perspective, $LaAlO_3$–$LaNiO_3$ (111) interfaces based on Ni^{3+} are among the most promising candidates. A recent DFT+U study predicted a sizable orbital polarization for 1/1 (double perovskite) interfaces and a multiferroic behavior for Ni-bilayers [2]. Here, we further explore the properties of $LaAlO_3$-$LaNiO_3$ (111) interfaces by considering purely local as well as cooperative Jahn-Teller distortions and taking dynamical electronic correlations into account. Possible terminations and orbital reconstructions of these highly polar surfaces will be discussed. This work has been supported in part by European Research Council under the European Union's Seventh Framework Programme (FP/2007-2013)/ERC through grant agreement n. 306447.

[1] A. Rüegg and G. A. Fiete, Phys. Rev. B **84**, 201103 (2011).
[2] D. Doennig, W. E. Pickett and R. Pentcheva, Phys. Rev. B **89**, 121110 (2014).

TT 8.10 Mon 12:00 H 3010

Spin-orbit controlled capacitance of a polar heterostructure — •Kevin Steffen[1], Florian Loder[2], and Thilo Kopp[1] — [1]Center for Electronic Correlations and Magnetism, EP VI, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Center for Electronic Correlations and Magnetism, EP VI and TP III, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Oxide heterostructures with polar films display special electronic properties, such as the electronic reconstruction at their internal interfaces with the formation of two-dimensional metallic states. Moreover, the electrical field from the polar layers is inversion-symmetry breaking and may generate a strong Rashba spin-orbit coupling (RSOC) in the interfacial electronic system. We investigate the capacitance of a heterostructure in which a strong RSOC at a metallic interface is controlled by the electric field of a surface electrode. Such a structure is for example given by a $LaAlO_3$ film on a $SrTiO_3$ substrate which is gated by a top electrode. We find that due to a strong RSOC the capacitance can be larger than the classical geometric value.

TT 8.11 Mon 12:15 H 3010

Magnetism and Charge Transfer in $PrNiO_3$-$La_{0.7}Ca_{0.3}MnO_3$ Heterostructures — •Martin Bluschke[1,2], Alex Frano[1,2], Enrico Schierle[2], Matthias Hepting[1], Matteo Minola[1], Georg Christiani[1], Gennady Logvenov[1], Eugen Weschke[2], Eva Benckiser[1], and Bernhard Keimer[1] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Helmholz-Zentrum Berlin, Germany

Heterostructures of the bulk antiferromagnet $PrNiO_3$ (PNO) and the bulk ferromagnetic metal $La_{0.7}Ca_{0.3}MnO_3$ (LCMO) are grown by pulsed laser deposition on $LaSrAlO_4$ substrates for a systematic series of superlattice geometries. A characterization of the structural, magnetization, and transport properties is combined with the results of soft x-ray absorption and resonant scattering measurements to understand how the bulk properties of the individual components are modified via epitaxial strain and heterostructuring. In particular the PNO-LCMO interface is studied. A net transfer of electrons from Mn to Ni sites is observed near the interface. In addition the saturation magnetization and Curie temperature of the ferromagnetic response are found to be reduced compared to bulk LCMO. The antiferromagnetic order characteristic of bulk PNO is observed in superlattices containing 8 unit cells of PNO per bilayer, but suppressed below the detection limit for thinner 4 unit cell layers. Finally a transition between metallic and insulating behaviour in PNO is observed as the layer thickness is reduced from 12 to 4 unit cells, whereas the LCMO layers studied (4-18 unit cells) were insulating in all cases.