TT 80: Low-Dimensional Systems: Oxide Hetero-Interfaces

Time: Friday 9:30–11:00 Location: HSZ 103

TT 80.1 Fri 9:30 HSZ 103

Metal-Insulator Transition in $CaVO_3$ Thin Films from DFT+DMFT — •Sophie Beck, Gabriele Sclauzero, and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

The wide variety of interesting phenomena and functionalities of complex oxide thin films and heterostructures is generally determined by a number of different factors, such as substrate-induced epitaxial strain, dimensional confinement, interface-related effects, or defects. Here, we investigate the effects of epitaxial strain, dimensional confinement, as well as interface and surface effects on the electronic properties of the correlated metal $CaVO_3$ using a combination of density functional theory (DFT) and dynamical mean-field theory (DMFT). We show that tensile epitaxial strain can induce a metal-insulator transition in $CaVO_3$, and we demonstrate that this strain effect cooperates with a similar tendency originating from the finite thickness of the thin film. The latter effect, however, is quantitatively only relevant in the ultra-thin limit. Furthermore, we also address the influence of the substrate-film interface in $CaVO_3/LaAlO_3$ heterostructures.

TT 80.2 Fri 9:45 HSZ 103

Electronic and orbital reconstruction in $La_2CuO_4/LaNiO_3$ superlattices — •Benjamin Geisler[1], Friederike Wrobel[2], Eva Benckiser[2], Bernhard Keimer[2], and Rossitza Pentcheva[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany — [2]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

Artificial transition metal oxide heterostructures can display exotic characteristics notably different from their bulk components. In a combined experimental and theoretical study we report on superlattices formed by the parent compound of cuprate superconductors La_2CuO_4 (d^9) and the correlated metal $LaNiO_3$ (formal d^7). TEM reveals high quality $(La_2CuO_4)_N/(LaNiO_3)_M(001)$ structures ($N = 2, 3$; $M = 4$). Density functional calculations with on-site correlation show that the electrostatic doping due to an extra LaO layer at the interface is exclusively accommodated in the $LaNiO_3$ region, while the electronic and magnetic properties of the La_2CuO_4 part remain bulk-like. This is consistent with our Ni L-edge XAS measurements which provide evidence for Ni^{2+} in addition to the expected Ni^{3+}. In addition, a charge disproportionation arises at the Ni sites that drives a metal-to-insulator transition in the interface layers and is reflected also by the magnetic moments and the octahedral volumes. The simulations show a preference for a layerwise AFM order of the Ni moments but with a net total moment, which agrees with our XMCD measurements. A Ni orbital polarization of $\sim 6\%$ in favor of $3d_{z^2}$ arises near the interfaces.

Funding by the DFG within TRR 80 (G1, G3, G8) is acknowledged.

TT 80.3 Fri 10:00 HSZ 103

Anisotropic electrical transport at the Al_2O_3-$SrTiO_3$ interface — •Karsten Wolff[1], Roland Schäfer[1], Hilbert von Löhneysen[1,2], Matthieu le Tacon[1], and Dirk Fuchs[1] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe

At the interface of TiO_2-terminated $SrTiO_3$ and amorphous Al_2O_3, we observe anisotropic electrical transport behavior of the two dimensional electron system (2DES). Temperature and magnetic field dependence of the sheet resistance R_s is measured for various current directions with respect to the [100] direction of $SrTiO_3$. Below 30 K, R_s shows a distinct anisotropic behavior which can be attributed to anisotropic defect scattering. In addition, application of magnetic field parallel to the 2DES results in a non-crystalline anisotropy which we will discuss in terms of spin-orbit coupling.

TT 80.4 Fri 10:15 HSZ 103

2DEGs in binary oxides studied by ARPES: *s* vs. *d* orbitals and electron-phonon coupling — •Tobias C. Rödel[1,2,3], Franck Fortuna[1], François Bertran[2], Patrick Le Fèvre[2], and Andrés Felipe Santander-Syro[1] — [1]CSNSM, Univ. Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, 91405 Orsay, France — [2]Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin-BP48, 91192 Gif-sur-Yvette, France — [3]LPV, Physics and Material Science, University of Luxembourg, L-4422 Belvaux, Luxembourg

Two-dimensional electron gases (2DEGs) in $SrTiO_3$ attracted a lot of interest after the initially discovery at the $LaAlO_3/SrTiO_3$ interface due to its controversial origin and various different ground states (*e.g.* superconductivity, magnetism) which are tunable by a gate-voltage. We demonstrated that 2DEGs can be created in various other perovskite oxides using a simple Al-capping. This technique works also for non-perovskite systems and we studied the 2DEGs in the binary oxides TiO_2 and ZnO by angle-resolved photoelectron spectroscopy. One major difference between the two systems is that the orbital character of the 2DEG is either *s*-type (ZnO) or *d*-type (TiO_2) and the resulting differences in the measured electronic structure of the 2DEG will be discussed. Recently, electron-phonon coupling in the 2DEG in $SrTiO_3$ was the focus of various studies. Similar to $SrTiO_3$, the transition from a polaron gas to a Fermi liquid can be observed in the two binary oxides depending on the charge carrier density. We will focus on the characterization of electron-phonon coupling for high charge densities.

TT 80.5 Fri 10:30 HSZ 103

Tunable redox-created 2DES at the $EuO/SrTiO_3$ interface — •Patrick Lömker[1], Tobias Rödel[2], Timm Gerber[1], Patrick LeFevre[3], Francois Bertran[3], Emmanouil Frantzeskakis[2], Andrés Santander-Syro[2], and Martina Müller[1,4] — [1]Forschungszentrum Jülich GmbH, PGI-6, Jülich, Germany — [2]CSNSM, CNRS/IN2P3 and Université Paris-Sud, Orsay, France — [3]Synchrotron SOLEIL, Saint-Aubin, France — [4]Universität Duisburg-Essen, Duisburg, Germany

Two-dimensional electron systems (2DES) of transition metal oxides are of interest in the research for novel properties of oxidic systems. Well known systems, such as $LaAlO_3/SrTiO_3$, are challenging to fabricate in a consistent way for varying deposition techniques. A recent study enabled the fabrication of 2DES in a experimentally simple way by utilizing a non-magnetic reducing agent. [1]

In our study, we use Eu metal as the reducing agent in order to redox-create EuO. EuO belongs to the rare material class of magnetic insulators. This property combination makes EuO interesting for fundamental spintronics studies, e.g. decoupling spin from charge currents or electrical sensing of magnetic properties.

The $EuO/SrTiO_3$ interface is studied using *in-situ* ARPES. *Ex-situ* magnetometry is utilized to analyze the ferromagnetic properties of 1-2ML EuO films and element-selective XPS depth-profiling probes the thickness of the 2DES region. We find a 2DES in which electrical and ferromagnetic properties can be controlled simultaneously.

[1] Rödel, Advanced Materials 28, 1976-1980 (2016).

TT 80.6 Fri 10:45 HSZ 103

Band alignment and charge transfer in complex oxide interfaces — •Zhicheng Zhong and Philipp Hansmann — Max Planck Insitute Solid State Research , Stuttgart

Synthesis of transition metal heterostructures presents one of the most vivid fields in the design of novel functional materials. We propose a simple scheme to predict band alignment and charge transfer in complex oxide interfaces. For semiconductor heterostructures band alignment rules like the well known Anderson or Schottky-Mott rule are based on comparison of the work function of the bulk components. This scheme breaks down for oxides due to the invalidity of a single workfunction as it was recently shown. We propose a new scheme which is built on a continuity condition of valence states originating in the compounds' shared network of oxygen. It allows for the prediction of sign and relative amplitude of the intrinsic charge transfer, taking as input only information about the bulk properties of the components. We support our claims by numerical density functional theory simulations as well as (where available) experimental evidence. Specific applications include i) controlled doping of $SrTiO_3$ layers with the use of $4d$ and $5d$ transition metal oxides and ii) the control of magnetic ordering in manganites through tuned charge transfer.