TT 22: Correlated Electrons: Low-dimensional Systems - Materials 1

Time: Wednesday 9:30–13:00 Location: H 0104

TT 22.1 Wed 9:30 H 0104

Magnetic properties of ultra-thin layer of LCMO in oxides heterostructures — •Soltan Soltan[1,2], Joachim Albrecht[3], Eberhard Goering[4], Georg Christiani[1], Gennady Logvenov[1], and Hanns-Ulrich Habermeier[1] — [1]Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Physics Department, Faculty of Science, Helwan University,11792-Cairo, Egypt — [3]Hochschule Aalen, Beethovenstr. 1, 73430 Aalen, Germany — [4]Max-Planck-Institut fue Intelligent System, Heisenbergstr. 3, D-70569 Stuttgart, Germany

We investigate the variety of high quality magnetic heterostructures of different nonmagnetic oxides (YBCO and LNO) with magnetic LCMO layers grown by PLD on single crystal substrate $SrTiO_3$ with <100> and <110> orientations. We have used the X-ray diffraction to characterize the quality of these heterostructures including crystal structure and interface roughness. We have measured magnetization of these heterostructures at different temperatures and magnetic fields by using SQUID magnetometer. It has been found that a single LCMO layer with thickness of 2-3 unit cells shows ferromagnetism with a Curie temperature close to the bulk value. We present detailed discussion of the magnetic properties of the ultrathin LCMO layers in these heterostructures.

TT 22.2 Wed 9:45 H 0104

Negative compressibility at $LaAlO_3/SrTiO_3$ interfaces explored with scanning force microscopy — •Veronika Tinkl[1], Martin Breitschaft[1], Christoph Richter[1,2], German Hammerl[1], Thilo Kopp[1], and Jochen Mannhart[1,2] — [1]Experimentalphysik VI, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg, Augsburg — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart

The interface between the band insulators $LaAlO_3$ and $SrTiO_3$ is currently one of the most actively investigated structures in the field of oxide interfaces. If the $LaAlO_3$-film thickness exceeds three unit cells on a TiO_2-terminated $SrTiO_3$ substrate a conducting layer is formed at the interface. This conducting layer can be driven insulating by electric fields. In this presentation we will demonstrate that the interface exhibits negative compressibility as the carrier density is reduced.

We investigated interfaces consisting of four unit cells $LaAlO_3$ with a low temperature ultra-high vacuum scanning probe microscope. Contact potential difference measurements were performed at various carrier densities of the interface electron system. The difference in the work functions of interface and tip depends on the applied electric field. We will show that the chemical potential at the interface increases with decreasing carrier density. This effect is caused by electron-electron interactions and corresponds to a negative compressibility. The negative compressibility gives rise to applications by, for example, making use of the resulting large enhancement of the capacitance.

[1] Lu Li *et al.*, Science **332**, 825 (2011).

TT 22.3 Wed 10:00 H 0104

Magnetism and superconductivity at LAO/STO-interfaces: the role of Ti 3d interface electrons — •Natalia Pavlenko[1], Thilo Kopp[1], Evgeny Tsymbal[2], George Sawatzky[3], and Jochen Mahhnart[4] — [1]EKM and Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — [2]Department of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588-0299, USA — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada V6T1Z1 — [4]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Ferromagnetism and superconductivity are in most cases adverse. However, recent experiments reveal that they coexist at interfaces of $LaAlO_3$ and $SrTiO_3$. We analyze the ferromagnetic state within density functional theory and provide evidence that it is also generated by Ti 3*d* interface electrons, as is the two-dimensional electron liquid at the interface which gives rise to superconductivity. We demonstrate that oxygen vacancies in the TiO_2 interface layer enhance the tendency for ferromagetism considerably. This allows for the notion that areas with increased density of oxygen vacancies produce ferromagnetic puddles and account for the previous observation of a superparamagnetic behavior in the superconducting state.

TT 22.4 Wed 10:15 H 0104

Electrostatic doping of a Mott insulator in an oxide heterostructure: the case of $LaVO_3/SrTiO_3$ — •Andreas Müller[1], Hans Boschker[2], Florian Pfaff[1], Martin Kamp[2], Gertjan Koster[2], Guus Rijnders[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Insititut and Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany — [2]Faculty of Science and Technology and MESA$^+$ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

The discovery of a quasi-two-dimensional electron system at the interface between the two band insulators $LaAlO_3$ and $SrTiO_3$ has triggered intense investigations of oxide heterostructures with other material combinations. The hope is that by combining a polar overlayer with a non-polar substrate electronic reconstruction will lead to highly mobile interface charge carriers with special properties. The formation of a conducting interface layer in epitaxial $LaVO_3/SrTiO_3$, where $LaVO_3$ is a Mott insulator, is studied by transport measurements and hard x-ray photoelectron spectroscopy. We identify an insulator-to-metal transition above a critical $LaVO_3$ thickness with transport properties similar to those recently reported for $LaAlO_3/SrTiO_3$ interfaces. Interestingly, our photoemission measurements give evidence that electronic charge is transferred exclusively to the $LaVO_3$-side of the interface caused by an electronic reconstruction within the film itself. This opens the opportunity to study a band-filling controlled Mott transition induced by a purely electrostatic mechanism.

TT 22.5 Wed 10:30 H 0104

Confinement induced metal-to-insulator transition in strained $LaNiO_3/LaAlO_3$ superlattices — •Arianda Blanca-Romero and Rossitza Pentcheva — Ludwig Maximilians University, Munich, Germany.

Using density functional theory calculations including a Hubbard U term we explore the effect of strain and confinement on the electronic ground state of superlattices containing the band insulator $LaAlO_3$ and the correlated metal $LaNiO_3$. Besides a suppression of holes at the apical oxygen, a central feature is the asymmetric response to strain in single unit cell superlattices: For tensile strain a band gap opens due to charge disproportionation at the Ni sites with two distinct magnetic moments of $1.45\mu_B$ and $0.71\mu_B$. Under compressive stain, charge disproportionation is nearly quenched and the band gap collapses due to overlap of $d_{3z^2-r^2}$ bands through a semimetallic state. This asymmetry in the electronic behavior is associated with the difference in octahedral distortions and rotations under tensile and compressive strain. The ligand hole density and the metallic state are quickly restored with increasing thickness of the $(LaAlO_3)_n/(LaNiO_3)_n$ superlattice from $n = 1$ to $n = 3$.

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TT 22.6 Wed 10:45 H 0104

Soft-X-Ray ARPES: From Three-Dimensional Materials to Multilayer Heterostructures — •Vladimir N. Strocov[1], Masaki Kobayashi[1,2], Ming Shi[1], Thorsten Schmitt[1], and Luc Patthey[1] — [1]Swiss Light Source, Paul Scherrer Institute, 5232 Villigen-PSI, Switzerland — [2]Department of Applied Chemistry, University of Tokyo, Tokyo 113-8656, Japan

Soft-X-ray ARPES benefits from free-electron final states, simplified matrix elements and increasing photoelectron escape depth. The latter, apart from allowing bulk sensitivity and access to deep layers in heterostructures, improves intrinsic resolution in surface-perpendicular momentum k_z crucial for three-dimensional (3D) systems.

The ADRESS beamline (J. Synchrotron Rad. **17** (2010) 631) delivers soft X-rays with photon energies from hv = 300 to 1600 eV. The flux tops up 10^{13} photons/s/0.01%BW which allows breakthrough of the notorious valence band cross-section problem. The acquisition time is typically only a few minutes with energy resolution of 110 meV, increasing to a few tens of with 60 meV.

Apart from technical details, we give an overview of recent soft-X-ray ARPES results, including 3D Fermi surface (FS) of VSe_2, with its warping giving rise to 3D charge density waves, alternating FS shapes in 3D pnictides, topological surface state in 3D valence band of $PbBi_4Te_7$, FS of buried layers in $LaAlO_3/LaNiO_3$ and

$LaAlO_3/SrTiO_3$ hererostructures, etc. These results demonstrate an immense potential of soft-X-ray ARPES for electronic structure of 3D materials and multilayer heterostructures.

TT 22.7 Wed 11:00 H 0104

Geometric frustration and competing phases of the Sn/Si(111) surface system — •Gang Li[1], Philipp Höpfner[2], Jörg Schäfer[2], Ralph Claessen[2], and Werner Hanke[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany

One third of a monolayer of Sn adatoms on the (111) surface of Si presents a quasi-two dimensional realization of a Mott-Hubbard system on an effective triangluar lattice, displaying an intricate interplay between lattice reconstructions, inherent (magnetical) frustration and emerging and competing low-T phases. We study the Sn/Si(111)-$(\sqrt{3} \times \sqrt{3})$ adatom system with material specific many-body calculations and with angle-resolved photoelectron spectroscopy (ARPES). In a first step, we investigate the electronic correlation effects by combining the ab-initio density-functional approach with sophisticated many-body methods, i.e. DMFT, DCA, Dual Fermion and Variational Cluster methods. A metal-insulator transition with first (second) order at finite (zero) temperature is predicted, and the system is proven to be short-range correlated. The interplay of the electron-electron interaction and geometrical frustration favors a row-wise antiferromagnetic (RW-AFM) order. Comparing to ARPES, we find a good overall agreement between theory and experiment for the spectral function and its temperature dependence. In particular, the additional 3×3 symmetry observed in ARPES is explained as a spectral-weight redistribution corresponding to the RW-AFM.

15 min. break.

TT 22.8 Wed 11:30 H 0104

Charge density wave formation in $ErTe_3$ — •Hans-Martin Eiter[1], Michela Lavagnini[1], Rudi Hackl[1], E. A. Nowadnick[2,3], A. F. Kemper[2,3], Thomas P. Devereaux[2,3], J.-H. Chu[2,3], J. G. Analytis[2,3], Ian R. Fisher[2,3], and Leonardo Degiorgi[4] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA — [3]Geballe Laboratory for Advanced Materials & Dept. of Applied Physics, Stanford University, CA 94305, USA — [4]Laboratorium für Festkörperphysik, ETH - Zürich, CH-8093 Zürich, Switzerland

Rare-earth tritellurides are model systems to study low dimensional interacting electron gases. $ErTe_3$ undergoes two charge density wave (CDW) phase transitions at 265 K and 155 K at ambient pressure. External pressure can suppress both CDW transitions completely. Using Raman scattering, it is possible to detect the signature of both CDW energy gaps as well as the corresponding collective amplitude mode excitations. This allows us to map out the high pressure phase diagram. We also provide calculations on the basis of the electronic band structure which allow us to understand the selection rules as well as the spectra in a semi-quantitatively fashion.
This work is supported by the DFG under Grant No. Ha2071/5.

TT 22.9 Wed 11:45 H 0104

Pressure-induced superconducting phase in rare-earth tritellurides ($R\mathbf{Te_3}$, R = Gd, Tb, Dy) — •Diego A. Zocco[1], James J. Hamlin[1], M. Brian Maple[1], Jiun-Haw Chu[2], and Ian R. Fisher[2] — [1]Department of Physics, University of California, San Diego — [2]Department of Applied Physics, Geballe Laboratory for Advanced Materials, Stanford University

It has recently been reported that the low-dimensional rare-earth tritellurides $R\mathrm{Te}_3$ (R = La-Nd, Sm, Gd-Tm) enter an unidirectional, incommensurate charge-density-wave (CDW) state when cooled below a temperature $T_{CDW1} \sim$ 450 - 250 K, which decreases with increasing rare earth atomic number, due to the effect of chemical pressure. For the heavier R (*i.e.*, Dy-Tm), a second CDW appears at $T_{CDW2} < T_{CDW1}$, orthogonal to the first one. We have recently found that the application of external pressure induces a superconducting (SC) state in $GdTe_3$, $TbTe_3$ and $DyTe_3$ at low temperatures, coexisting or competing with the two CDWs and the local moment rare-earth magnetism. In this talk, we present the results of experiments we have performed on these materials at high pressure and low temperature, to help develop an understanding of the origin of the superconducting state.

TT 22.10 Wed 12:00 H 0104

High-pressure studies of electronic order and lattice dynamics in 1T-TaS_2 — •Tobias Ritschel[1], Jan Trinckauf[1], Jorge Enrique Hamann Borrero[1], Gaston Garbarino[2], Alexei Bossak[2], Helmuth Berger[3], Martin von Zimmermann[4], Bernd Büchner[1], and Jochen Geck[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden (IFW Dresden), Germany — [2]ESRF, Grenoble, France — [3]Ecole polytechnique Federale de Lausanne, Switzerland — [4]HASYLAB, Hamburg, Germany

The layered compound 1T-TaS_2 shows a very complex pressure-temperature phase diagram, including a commensurate (C), a nearly commensurate (NC) and an incommensurate (IC) charge density wave (CDW) phase. In addition, the material exhibits a pressure-induced superconducting phase with $T_c \approx 5\,K$.

We studied the static CDW-order performed by means of elastic X-ray diffraction as a function of temperature and external pressure. The intensity of the CDW-superlattice reflections within each phase was found to decrease with pressure, while the peak width and the position in reciprocal space was found to remain constant.

Furthermore, we investigated the pressure dependency of the lattice dynamics in the NC and IC phase at room temperature, using inelastic X-ray scattering. The Phonon dispersion around the IC wave vector is strongly pressure dependent and a Kohn anomaly was observed well above the NC to IC phase transition temperature. We will present the experimental data along with model calculations and discuss the results in relation to the pressure-induced superconductivity.

TT 22.11 Wed 12:15 H 0104

Phonon Instability in the CDW Systems $2H$-$NbSe_2$ and $TiSe_2$ — •Roland Hott[1], Rolf Heid[1], Klaus-Peter Bohnen[1], Frank Weber[1,2], Stephan Rosenkranz[2], John-Paul Castellan[2], Raymond Osborn[2], Goran Karapetrov[2], Takeshi Egami[3], Ayman Said[4], and Dmitry Reznik[1,5] — [1]Karlsruhe Institute of Technology, Institute of Solid State Physics, P. O. Box. 3640, D-76021 Karlsruhe, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, Illinois, 60439, USA — [3]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee, 37996, USA — [4]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois, 60439, USA — [5]Department of Physics, University of Colorado at Boulder, Boulder, Colorado, 80309, USA

Further investigations on the soft-mode behaviour of phonons in the Charge Density Wave (CDW) systems $2H$-$NbSe_2$ and $TiSe_2$ have been performed both theoretically in Density Functional Theory (DFT) based on ab-initio phonon calculations as well as experimentally by means of high resolution Inelastic X-ray Scattering (IXS). For both materials, the theoretical predictions for the phonon softening coincide with the experimentally observed CDW instability behaviour. For $2H$-$NbSe_2$ the wave vector dependence of the electron-phonon coupling drives the CDW formation and determines its periodicity [1]. For $TiSe_2$, electron-phonon-coupling is strong enough to stabilize the structural phase transition at finite temperatures [2].
[1] F. Weber et al., Phys. Rev. Lett. 107, 107403 (2011).
[2] F. Weber et al., Phys. Rev. Lett. 107, 266401 (2011).

TT 22.12 Wed 12:30 H 0104

Realignment of the charge density wave in $TiSe_2$ by variation of the conduction band population — •Matthias M. May[1,2], Christoph Janowitz[1], and Recardo Manzke[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, D-12489 Berlin — [2]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin

Recent experimental [1] and theoretical [2] studies of the charge density wave phase of $TiSe_2$ have pronounced the strong excitonic contributions to this phase transition. The effect of increasing the conduction band population by water adsorption [1] was studied with ARPES. Our results suggest a change of the energetically most favourable direction of the electronic superstructure in k-space above a certain population threshold: The 2x2 in plane part of the 2x2x2 superstructure is observable by ARPES for low H_2O-coverage, whereas the perpendicular x2 signature appears only for higher coverage, after the 2x2 has been reduced.
[1] May et al., *Phys. Rev. Lett.* **107**, 176405 (2011)
[2] van Wezel et al., *Phys. Rev. B* **81**, 165109 (2010)

TT 22.13 Wed 12:45 H 0104

Effect of Charge Order on the Plasmon Dispersion in Transition-Metal Dichalcogenides investigated by Electron Energy-Loss Spectroscopy — •Andreas König[1], Jasper van Wezel[2], Roman Schuster[1], Martin Knupfer[1], Helmuth Berger[3], Jeroen van den Brink[1], and Bernd Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, P. O. Box 270116, D-01171 Dresden, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA — [3]Institut de Physique de la Matière Condensée, EPFL, CH-1015 Lausanne, Switzerland

$2H$-$TaSe_2$ is one of the various polytypes of the transition-metal dichalchogenides (TMDC) that show a phase transition to a charge-density wave (CDW) and to a superconducting state. It is already proven for $2H$-$TaSe_2$ [1] and a few other TMDCs that they show a negative dispersion of the bulk plasmon energy in the normal state and an even larger bandwidth of this negative dispersion in the CDW state, which is altogether not a behavior of a common metal.

We discuss the connection of the susceptibility to a CDW phase and of the negative plasmon dispersion by applying Electron Energy-Loss Spectroscopy (EELS) measurements in transmission on thin films of $2H$-$TaSe_2$ as well as a semiclassical Ginzburg-Landau model [2]. The connection is further emphasized by intercalation experiments with potassium that show a suppression of the CDW as well as a change of slope of the plasmon dispersion.

[1] Schuster et al., Phys. Rev. B **79**, 045134 (2009)
[2] van Wezel et al., Phys. Rev. Lett. **107**, 176404 (2011)