

O 79: Electronic structure II

Time: Thursday 15:00–17:00

Location: WIL C107

O 79.1 Thu 15:00 WIL C107

Towards a molecular understanding of cation-anion interactions in ionic liquids — •TILL CREMER¹, CLAUDIA KOLBECK¹, FLORIAN MAIER¹, NATALIA PAAPE², PETER SCHULZ², RENÉ WÖLFEL², PETER WASSERSCHIED², KEVIN LOVELOCK³, JENS THAR⁴, HENRY WEBER⁴, BARBARA KIRCHNER⁴, and HANS-PETER STEINRÜCK¹ — ¹Physikalische Chemie II, FAU Erlangen, D — ²Chemische Reaktionstechnik, FAU Erlangen, D — ³School of Chemistry, University of Nottingham, UK — ⁴Ostwald Institut, University of Leipzig, D

Ionic liquids (ILs), organic salts with melting points below 100°C, are a new class of materials labelled "designer solvents" for the exciting prospect of tailoring their physical properties by combining an appropriate choice of cation and anion. Regarding the enormous number of possible ion combinations, reliable prediction concepts based on the chemical nature of the IL compounds are needed. In order to estimate the deviation from a simplified superposition of individual anion- and cation-related properties, one has to understand the complex nature of interactions between IL ions, namely coulombic, hydrogen-bond-type and dispersive forces. In this combined XPS, NMR and DFT study¹, interionic interactions in ten different imidazolium-based ILs are examined. In particular, first direct experimental and theoretical evidence for anion-cation charge transfer phenomena in ionic liquids is found. This work was supported by the DFG through SPP1191 "Ionic Liquids" and the Cluster of Excellence "Engineering of Advanced Materials".

¹ T. Cremer et al., Chem. Eur. J. 2010, 16, 9018

O 79.2 Thu 15:15 WIL C107

Lattice-strain induced changes in the electronic structure of SrRuO₃ investigated by angle-resolved photoelectron spectroscopy — •ERIK KRÖGER¹, MATTHIAS KALLÄNE¹, ARNDT QUER¹, ADRIAN PETRARU², ROHIT SONI², HERMANN KOHLSTEDT², LUTZ KIPP¹, and KAI ROSSNAGEL¹ — ¹Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany — ²Department of Nanoelectronics, Technical Faculty, University of Kiel, 24143 Kiel, Germany

Changes of magnetic and electrical properties associated with atomic rearrangements, such as magnetostriction and piezoelectricity, have attracted much attention in basic research due to the possibility of novel applications. Especially transition metal oxides with perovskite crystal structure exhibit multiple electronic correlations that are linked to the crystal lattice. Ferromagnetic SrRuO₃, for example, shows lattice-strain induced changes in the magnetic moment. In order to investigate the origin of this behavior we studied the electronic structure of SrRuO₃ in different strain states by angle-resolved photoelectron spectroscopy. The SrRuO₃ samples were grown by pulsed laser deposition and were measured in different strain-states of the order of -1% to +1%. Experiments were performed at BL7 of the Advanced Light Source (Berkeley). This work was supported by the DFG through SFB 855 "Magnetoelectric Composite Materials — Biomagnetic Interfaces of the Future".

O 79.3 Thu 15:30 WIL C107

Fermi Surface Mapping and Heavy Fermion Behaviour in ARPES on CePt₅ and CeAg₅ Surface Alloys — •HOLGER SCHWAB¹, MARKUS KLEIN¹, ANDREAS NUBER¹, JOHANNES ZIROFF¹, H. HAYASHI², JIAN JIANG², KENYA SHIMADA³, MATTIA MULAZZI¹, F.F. ASSAAD⁴, and FRIEDRICH REINERT¹ — ¹Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany — ²Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan — ³Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan — ⁴Universität Würzburg, Institut für Theoretische Physik und Astrophysik, Am Hubland, D-97074 Würzburg, Germany

Using high-resolution angle-resolved photoemission we studied ordered Cerium surface alloys on Pt(111) and Ag(111) surfaces. We present light polarization dependent bandstructure and Fermi surfaces for several photon energies including Ce 4d-4f resonant photoemission. In the CePt₅ surface alloy, we show the temperature dependence of the Cerium 4f electron spectral weight near the Fermi level. There we observed the opening of a hybridisation gap between the flat 4f Cerium band and one strongly dispersing Pt conduction band that has a strong

temperature dependence. The comparison to LDA+DMFT calculations based on an NCA solver shows the on-set of the coherent heavy fermion state at low temperature below the Kondo temperature of the material.

O 79.4 Thu 15:45 WIL C107

Electronic structure of RScO₃ from x-ray spectroscopies and first-principles calculations — •CHRISTINE DERKS¹, KARSTEN KUEPPER², ANDREE POSTNIKOV³, REINHARD UECKER⁴, and MANFRED NEUMANN¹ — ¹Department of Physics, University of Osnabrück, D-49069 Osnabrück — ²Department of Solidstate Physics, University of Ulm, D-89069 Ulm — ³Laboratoire de Physique des Milieux Denses, Université Paul Verlaine, F-57078 Metz — ⁴Institute for Crystal Growth, D-12489 Berlin

Perovskites of the type RScO₃, where R represents a trivalent rare-earth metal, are *high k* materials and belong to the best available thin film substrates for the epitaxial growth of high quality thin films. This allows a so called strain tailoring of ferroelectric, ferromagnetic, or multiferroic perovskite thin films by choosing different RScO₃.

With respect to these interesting properties there is up to now only rare knowledge available about the electronic structure of RScO₃. In a previous work we have already published a work on the electronic structure of SmScO₃, GdScO₃, and DyScO₃ [1]. As far as we know, it is the only work combining XPS, XES and XAS with ab initio electronic structure calculations. We are extending these successful investigations to single crystalline PrScO₃, NdScO₃, EuScO₃ and TbScO₃. A complete electronic structure was obtained and the band gaps could be deduced for all these rare-earth scandates. All the results were found to be in good agreement with LDA+U calculations.

[1] M. Raekers et al., Phys. Rev. B79 125114 (2009)

O 79.5 Thu 16:00 WIL C107

localized vs. delocalized character of charge carriers in LaAlO₃/SrTiO₃ heterostructure — •KEJIN ZHOU¹, MILAN RADOVIC^{2,1}, JUSTINE SCHLAPPA¹, VLADIMIR STROCOV¹, RUGGERO FRISON¹, JOEL MESOT^{1,2}, LUC PATTHEY¹, and THORSTEN SCHMITT¹ — ¹Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — ²Laboratory for synchrotron and neutron spectroscopy, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland

Oxide heterostructures have been attracting great attention due to extraordinary phenomena occurring at the interface and their potential application for device design. A particularly fascinating system is the two-dimensional conductive interface between the band insulators LaAlO₃ (LAO) and SrTiO₃ (STO), which can be even driven to magnetic and superconducting phases at low temperatures. Resonant inelastic x-ray scattering at Ti L-edges is particularly suitable to address the electronic structure of its interface since the Ti³⁺ states clearly display strong dd excitations while Ti⁴⁺ states exhibit only elastic emission in the low energy loss regime. Our studies on LAO/STO superlattices prepared by pulsed laser deposition unambiguously reveal the presence of both localized and delocalized Ti 3d carriers generated during the building of the LAO/STO interfaces. Systematic studies on samples before and after annealing under O₂ atmosphere and high temperature show that the dual character carriers can be either induced by electron transfer due to the polar-discontinuity or by oxygen vacancies defects. Oxygen vacancies and electronic reconstruction are equivalent in balancing the built-up electric potential.

O 79.6 Thu 16:15 WIL C107

Band Structure of ZrS_xSe_{2-x} by ARPES — •MOHAMED MOUSTAFA, ALEXANDER PAULHEIM, CHRISTOPH JANOWITZ, and RICCARDO MANZKE — Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

The valence band structure of mixed samples of ZrS_xSe_{2-x} single crystals, where x varies from 0 to 2, has been studied by means of high-resolution angle-resolved photoelectron spectroscopy (ARPES) using synchrotron radiation. The crystals were found to be extrinsic n-type semiconductors with indirect bandgap. The composition dependence of the band structure is presented and discussed. A characteristic splitting of the chalcogen p-derived valence bands at the symmetric point A is observed. The size of the splitting shows to increase almost linearly as progressing from ZrS₂ to ZrSe₂ reaching 320 meV. Further,

the energy gap values are estimated from the valence band maximum to the observed emission close to the conduction band minimum. The gaps are found to vary from 1.78 eV to 1.16 eV for ZrS_2 to ZrSe_2 , respectively, and are compared to our previously reported optical values [1].

[1] M. Moustafa, Th. Zandt, C. Janowitz, and R. Manzke, *Phys. Rev. B* 80, 035206 (2009).

O 79.7 Thu 16:30 WIL C107

Energetics and dynamics of hot electrons at GaP and InP surfaces — ●PHILIPP SIPPEL, ROBERT SCHÜTZ, KLAUS SCHWARZBURG, THOMAS HANNAPPEL, and RAINER EICHBERGER — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The surface electronic structure and dynamics of hot electrons was investigated for InP(100) and GaP(100) samples with time-resolved 2PPE (TR-2PPE). The In- and Ga-rich grown surfaces were prepared via metal organic chemical vapour deposition, exhibiting (2x4) reconstruction checked by in-situ reflectance anisotropy spectroscopy. The samples were transferred to the experimental setup with a contamination-free UHV commuting system. TR-2PPE spectroscopy was used, applying laser pulses of 40fs duration. The technique allowed for detection of surface states for this GaP(100) reconstruction and a comparison with the similar surface electronic structure of InP(100) was made. For InP, the dynamics of unoccupied surface states was studied, varying excitation energies. Using 4.66eV pump-photons, we excited hot electron bulk states and observed subsequent filling of surface states by scattering of electrons. Furthermore, we excited elec-

trons from the valence band to bulk levels that were isoenergetic with the well known C2 surface state. This energy also corresponds to a potential excitation scheme, involving a direct optical transition from an occupied surface state (V1) to C2. Since we could not observe a noticeable magnification of the surface state peak in the photoelectron spectra, we assume that this resonant transition is not allowed.

O 79.8 Thu 16:45 WIL C107

Unveiling a two-dimensional electron gas with universal subbands at the surface of SrTiO_3 — ●OLIVIER COPIE^{1,2}, ANDRÉS FELIPE SANTANDER-SYRO³, TAKESHI KONDO⁴, MARCELO ROZENBERG⁵, and AGNÈS BARTHÉLÉMY² — ¹Universität Würzburg, Experimentelle Physik VII, 97074 Würzburg, Germany — ²Unité Mixte de Physique CNRS/Thales, 1 Av. A. Fresnel 91767 Palaiseau, France. — ³CSNSM, Université Paris-Sud and CNRS/IN2P3 Bâtiments 104 et 108, 91405 Orsay, France. — ⁴Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, IA 50011. — ⁵Laboratoire de Physique des Solides, Université Paris-Sud, Bâtiments 510, 91405 Orsay, France.

We present our angle-resolved photoemission spectroscopy (ARPES) results showing that there is a highly metallic universal two-dimensional electron gas (2DEG) at the vacuum-cleaved surface of SrTiO_3 , independent of bulk carrier densities. Our data unveil a remarkable electronic structure consisting on multiple subbands of heavy and light electrons. The similarity of this 2DEG with those reported in SrTiO_3 -based heterostructures suggests that different forms of electron confinement at the surface of SrTiO_3 lead to essentially the same 2DEG.