

O 67: Electronic structure of surfaces: Spectroscopy, surface states III

Time: Wednesday 15:00–18:00

Location: MA 042

Invited Talk

O 67.1 Wed 15:00 MA 042

Ultrafast dynamics of two-dimensional electron systems probed by time- and angle-resolved two-photon photo-emission — ●JENS GÜDDE — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, 35032 Marburg

Two-dimensional (2D) electron systems have attracted interest for more than 40 years due to unique properties that have no counterpart in 3D. In this talk I will first report on a 2D electron gas with close to ideal properties for fundamental studies. Ultrathin He films on single-crystal metal surfaces allow for an isolation of the electron system from the bulk and at the same time achieve a relatively large binding energy due to a strong image-force interaction with the metal. Our results for a monolayer (ML) of He/Cu(111) let us extrapolate lifetimes of nanoseconds for only a few ML of He on substrates such as Cu(100) with binding energies that are still large enough to support electron densities up to the quantum regime without instabilities [1].

Topologically protected states at the surfaces of 3D topological insulators represent a model for relativistic 2D electron systems with a characteristic Dirac-like energy dispersion. Optical excitation with near-infrared light pulses offers the possibility to induce and control spin-polarized electrical surface currents without exciting the bulk electron system [2]. Our experiments reveal unusually long elastic decay times of these currents due to spin-momentum locking of the Dirac electrons.

[1] N. Armbrust *et al.* Phys. Rev. Lett. **116**, 256801 (2016).

[2] K. Kuroda *et al.*, Phys. Rev. Lett. **116**, 076801 (2016).

O 67.2 Wed 15:30 MA 042

Light-molecule interactions in plasmonic environments — ●EMILIANO CORTES — Physics Department, Imperial College London, UK

Unravelling the interaction of single molecules with plasmonic interfaces sets the basis for plasmonic chemistry. Enhanced electric fields, energetic (hot) electron-hole pairs and abrupt thermal gradients, build up a complex scenario for molecules sitting next to a metal nanoparticle illuminated at visible wavelengths. However, at the same time, this combination offers all the necessary ingredients to manipulate photochemical reactions and ultimately revolutionize the electromagnetic-into-chemical energy conversion processes. In this context, single molecule and/or single nanoparticle approaches, even being methodologically challenging, should reduce the complexity of the problem allowing to explore, rationalize and optimize energy transfer pathways in these systems. Here, I will show a range of examples where the energy confinement achieved by plasmonic nanoparticles has been further employed to in-situ monitor, guide or induce charge-transfer processes at the single molecule and/or the single nanoparticle level. Using light to study, enhance and drive chemical reactions, beyond the traditional photochemistry or photocatalysis fields, is now possible thanks to plasmonic chemistry.

O 67.3 Wed 15:45 MA 042

Electronic structure of LAO/STO thin films: artificial control of the quantum well states or enhanced polaronic tail?

— ●MARCO CAPUTO¹, ALESSIO FILIPPETTI², MARGHERITA BOSELLI³, ALLA CHIKINA¹, HUGO DIL⁴, CLAUDIA CANCELLIERI⁵, STEFANO GARIGLIO³, JEAN-MARC TRISCONE³, and VLADIMIR N. STROCOV¹ — ¹Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen-PSI, Switzerland — ²CNR-IOM, Istituto Officina dei Materiali, Cittadella Universitaria, Cagliari, Monserrato 09042-I, Italy. 7 — ³DPMC, University of Geneva, 24 Quai Ernest Ansermet, 1211 Geneva, Switzerland — ⁴Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — ⁵EMPA, Swiss Federal Laboratories for Materials Science & Technology, Ueberlandstrasse 129, CH-8600 Dübendorf, Switzerland

Transition Metal Oxides (TMO) represent an ideal platform to exploit exotic phenomena in solid state physics. Conductivity and superconductivity in the 2D Electron System (2DES) at the LAO₃/STO₃ (LAO/STO) interface is one of them.

The 2DES sits on the STO part of the interface, in a potential well created by band bending. Reducing the thickness of the hosting STO material can provide a platform for new exotic phenomena, like quantum well states.

In this work we analyze the electronic structure of a LAO/STO interface, where the STO side was a thin layer of few unit cells grown on a LAO layer deposited on a STO substrate.

O 67.4 Wed 16:00 MA 042

Optical anisotropy of SrTiO₃(110) for different surface terminations — ●KARSTEN FLEISCHER, BRIAN WALLS, KUANYSH ZHUSUPBEKOV, and IGOR V. SHVETS — School of Physics, Trinity College Dublin, The University of Dublin, Dublin 2, Ireland

In this work we investigate the SrTiO₃(110) surface by reflectance anisotropy spectroscopy (RAS) at varying preparation steps including ex-situ wet etching, high temperature oxygen annealing, as well as in-situ vacuum annealing. Different surface terminations show distinctly different RAS spectra which are correlated to an altered surface stoichiometry measured by X-ray photoelectron spectroscopy (XPS) and an altered valence band structure measured by UV-photoelectron spectroscopy (UPS) in cases of conductive samples. We link the changes in the observed RAS spectra to various surface reconstructions, with particular focus of the signature of (3×1) and (1×4) reconstructed surfaces, and a metallic surface state observed in vacuum annealed SrTiO₃.

O 67.5 Wed 16:15 MA 042

Revealing the Wave Nature of Hot Electrons with a Molecular Nanoprobe — ●MARKUS LEISEGANG¹, JENS KÜGEL¹, LUCAS KLEIN¹, and MATTHIAS BODE^{1,2} — ¹Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — ²Wilhelm Conrad Röntgen Center of Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg

Electron transport in materials is usually determined by conductance measurements performed in between two contacts which are typically separated by a minimal distance of hundreds of nanometers. Future nanoscale applications like single-molecule logic gate structures [1], however, will require characterization of transport properties on much shorter length scales. Here we show how STM-induced molecular nanoprobe (MONA) can be used for the characterization of quasiparticle transport on a length scale well below 10 nanometer [2]. We present results obtained on dehydrogenated H₂Pc molecules. Isomerization was triggered by hot electrons injected from a STM tip into the Ag(111) substrate close to the molecule. By utilizing various atom-by-atom-engineered Ag nano structures we are able to determine how quasiparticles propagate and under which conditions interference of coherent quantum-mechanical wave functions are observed. We will show how these findings can be utilized to create an energy-selective filter for single-molecule switches.

[1] C. Li *et al.*, Nature Nano. **12**, 1071-1076 (2017)

[2] J. Kügel *et al.*, Nano Lett. **17**, 5106-5112 (2017)

15 min. break

O 67.6 Wed 16:45 MA 042

First-principles modeling of secondary electron emission from slow ion bombardment — ●MARNIK BERCX, BART PARTOENS, and DIRK LAMOEN — EMAT & CMT groups, Department of Physics, University of Antwerp

Secondary electron emission (SEE) is an important phenomenon where electrons of a target material are emitted through the impact of energetic (primary) particles. Such processes lie at the foundation of several techniques for characterizing materials and play an important role in applications such as plasma sputtering deposition or plasma display panels. In our work, we start from the pioneering work of Hagstrum [1] to construct a quantitative model that allows for the determination of the SEE yield from slow ions incident on a surface. We provide a fully ab initio approach by calculating the required input from first-principles Density Functional Theory calculations, as well as making some major conceptual improvements to the model. We further expand the model to include plasmon excitations, which are believed to have a significant effect on the yield spectrum for materials with low plasmon frequencies [2]. The calculated yield spectra, i.e. the kinetic energy distribution of the emitted electrons, are in excellent agreement with experimental results for several semiconductors (Ge,

Si) and metals (Al, Mg, Be).

O 67.7 Wed 17:00 MA 042

First-principles study on the bulk and surface Rashba states of GeTe — ●JAE MO LIHM and CHEOL-HWAN PARK — Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea

GeTe displays giant bulk and surface Rashba-type spin splitting as a result of its ferroelectric polarization and strong spin-orbit coupling [1,2]. The energy and spin polarization of the bulk and surface Rashba states of GeTe has been closely studied both theoretically and experimentally, due to its potential in the external control of electron spin [3]. In this presentation, we report the results of our first-principles study on the electronic structure of bulk and surface Rashba split bands using density-functional-theory calculations. We find the different roles of broken inversion symmetry and the spin-orbit coupling in the Rashba effect of GeTe. The bulk-surface resonance effect brings about complexity in the electronic structure of the surface Rashba states. The effects of potassium adsorption on the surface Rashba states are also investigated.

- [1] D. Di Sante et al., Adv. Mater. 25, 509-513 (2013)
- [2] M. Liebmann et al., Adv. Mater. 28, 560-565 (2016)
- [3] J. Krempaský et al., arXiv:1707.08431 (2017)

O 67.8 Wed 17:15 MA 042

Giant Rashba Splitting in Cu₂Te and Ag₂Te Surface Alloys — ●MAXIMILIAN ÜNZELMANN¹, HENDRIK BENTMANN¹, DEAN NESTOROV¹, PHILIPP ECK², DOMENICO DI SANTE², GIORGIO SANGIOVANNI², PHILIPP ROSENZWEIG³, SEBASTIAN OTTO³, THOMAS FAUSTER³, and FRIEDRICH REINERT¹ — ¹Experimentelle Physik 7, Universität Würzburg — ²Theoretische Physik 1, Universität Würzburg — ³Lst. f. Festkörperphysik, Universität Erlangen-Nürnberg

By deposition of a 1/3 ML of Tellurium on M(111) surfaces (M=Cu,Ag) a ($\sqrt{3} \times \sqrt{3}$)-R30° superstructure in M₂Te stoichiometry is formed whereby every third M-atom is replaced by a Te-atom. This type of substitutional surface alloys is very well known as a model system for large Rashba-type spin-orbit splittings.

We investigated the surface band structure of M₂Te/M(111) by means of one- and two-photon photoelectron spectroscopy and compare our photoemission data to density functional theory (DFT) band structure calculations. For both substrates two fully occupied hole-like bands are found. We assign these to Te induced *sp_z*- and *p_xp_y*-states. Our ARPES data shows strong indications for a Rashba-type spin splitting with a Rashba parameter of about 2 eVÅ for the Ag₂Te *sp_z*-state. Interestingly this value is much larger than that for Sb which has a similar atomic SOC. This manifests the influence of the atomic struc-

ture on the Rashba spin splitting. Besides a series of image-potential-resonances 2PPE shows Te-induced unoccupied states in good agreement with DFT calculations.

O 67.9 Wed 17:30 MA 042

First-principles calculations on the surface states of KHgSb: hourglass fermions — ●JI HOON RYOO and CHEOL-HWAN PARK — Department of Physics & Astronomy, Seoul National University 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Korea

It has been recently proposed [1] and experimentally confirmed [2] that exotic surface states reside in the surface of KHgSb, so-called hourglass fermions named after their peculiar energy band structure. In this contribution, we present the results of our comprehensive first-principles study on the electronic structure of KHgSb surface and bulk. Especially, we highlight the role of spin-orbit coupling and symmetry on the spin texture of these hourglass fermions.

- [1] Z. Wang, A. Alexandradinata, R. J. Cava, B. A. Bernevig, Nature 532, 189 (2016).
- [2] J. Ma et al., Science Advances 3, e1602415 (2017).

O 67.10 Wed 17:45 MA 042

Density-Functional Theory based calculation of core-level spectroscopies: Transition and Rare Earth Metals — ●GEORG S. MICHELITSCH and KARSTEN REUTER — Technische Universität München

Core-level spectroscopies are among the most established methods of characterization in modern material science, providing information about chemical interactions and the environment of an atomic species in a composite material matrix. A reliable interpretation of experimental signatures often requires support by computational spectroscopy. Parametrized, effective models are in most cases sufficient to explain main features or isolated resonances based on general assumptions of ligand field theory. Overlapping resonances and strong chemical shifts due to interatomic bonding instead demand an explicit calculation of the intricate electronic structure from first principles. For extended systems, the latter generally translates to density-functional theory (DFT), relying on an approximate treatment of core-hole screening via occupational constraints. While established and highly successful for light elements, this approach is challenged by transition and rare earth metals with their partially filled *d*- and *f*-states, where relativistic effects and strong local Coulomb repulsion need to be appropriately described. We assess this situation through DFT calculations for hybrid organometallic materials incorporating transition and rare earth metals with an emphasis on the impact of the chemical environment on the X-ray signatures. We find good agreement with experiment already at the level of perturbative spin-orbit coupling.