O 49: Poster Session IV: Electronic structure of surfaces: Spectroscopy, surface states II

Time: Tuesday 13:30–15:30 Location: P

O 49.1 Tue 13:30 P

Intrinsic excess charge on polar surfaces: charge density waves, polarons and bipolarons. — •Michele Reticcioli[1], Zhichang Wang[2,3], Michael Schmid[2], Ulrike Diebold[2], Martin Setvin[2,4], and Cesare Franchini[1,5] — [1]University of Vienna (Austria) — [2]Technische Universitaet Wien, Vienna (Austria) — [3]Xiamen University (China) — [4]Charles University, Prague (Czech Republic) — [5]University of Bologna (Italy)

Surfaces of oxide materials hosting excess charge show electronic and chemical properties completely different than the corresponding bulk crystal. Due to uncompensated broken bonds, bulk-terminated polar surfaces are known to intrinsically host excess charge, conventionally assumed to form a metallic two-dimensional electron gas. Here, by investigating the $KTaO_3(001)$ polar surface by density functional theory calculations and surface sensitive experiments, we show that excess charge is accommodated more effectively by in-homogeneous distributions, with different degree of charge localization. Our data provide evidence for the coexistence of standing density waves with long periodicity, eventually combined with minor structural distortions, and strongly localized charge in form of small electron polarons and bipolarons (quasi particles originating from the electron-phonon coupling, associated to sharp in-gap states and local distortions). These novel solutions emerging spontaneously on polar surfaces, dominate the electronic and chemical properties of the material, with large impact on the device functionalities (*e.g.*, the effects of bipolarons on the CO adsorption are discussed in a separate session by M. Setvin).

O 49.2 Tue 13:30 P

Efficient orbital imaging using ToF momentum microscopy with a femtosecond HHG light source — •Wiebke Bennecke[1], G. S. Matthijs Jansen[1], David Schmitt[1], Marius Keunecke[1], Christina Möller[1], Daniel Steil[1], Russell Luke[2], Sabine Steil[1], and Stefan Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Institut für Numerische und Angewandte Mathematik, Georg-August-Universität Göttingen

Orbital imaging (OI) is a powerful method to visualize molecular orbitals in molecule-metal interfaces using angle-resolved photoemission spectroscopy (ARPES) data and phase retrieval algorithms. Here, we will report on our advances in both of these aspects.

So far, successful orbital imaging has been based on the support constraint, for which the shape of the orbital must be known and which can be difficult to estimate. We have developed a sparsity-driven approach to phase retrieval, which uses only the number of non-zero pixels in the orbital and is independent of the actual orbital shape. This algorithm has been applied successfully to both simulated and experimental static ARPES data of different organic molecules.

Our photoemission setup consists of a femtosecond high harmonic generation beamline and a time-of-flight momentum microscope which yields the full momentum- and energy-resolved photoelectron spectrum in a single measurement. This enables us to image multiple molecular orbitals simultaneously. Combined with the sparsity-driven phase retrieval, this setup provides the ideal platform for orbital imaging with great potential to move towards time-resolved measurements.

O 49.3 Tue 13:30 P

Exploring polaron stability and defect structures in $Li_4Ti_5O_{12}$ (LTO) surface: A combined theoretical and experimental approach — •Yu-Te Chan[1], Matthias Kick[2], Cristina Grosu[2,3], Christoph Scheurer[1], and Harald Oberhofer[2] — [1]Fritz Haber Institute — [2]TU München — [3]IEK-9, FZ Jülich

Spinel $Li_4Ti_5O_{12}$ (LTO) is a promising anode material for next-generation all-solid-state Li-ion batteries (ASSB) by its "zero strain" charge/discharge behavior. Pristine, white LTO possesses poor ionic and electronic conductivity. The latter can be increased by tailoring the sintering protocol to produce oxygen vacancies, resulting in a performant, blue LTO material. Polarons induced by oxygen vacancies have been proposed as one of the origins of the high conductivity. Detailed knowledge about polaron stability, distribution, and dynamics in LTO bulk and surface has been lacking, though. By performing *Hubbard corrected density functional theory* (DFT+U) calculations we are able to show that in fact polaron formation and a possible polaron hopping mechanism can play a significant role in the experimentally observed improved conductivities. Moreover we are able to gauge polaronic charge mobility by explicitly calculating polaron hopping barriers.[1,2] In combination with positron lifetime spectroscopy (PALS) data and theoretical positron lifetimes we arrive at a rather complete picture of the bulk vs. surface defect chemistry in LTO particles and their resulting mixed ionic electronic conductivity. [1] M. Kick et al., J. Phys. Chem. Lett. 11 (2020), 2535 [2] M. Kick et al., J. Chem. Phys. 153 (2020), 144701

O 49.4 Tue 13:30 P

Switching current distribution in a STM Josephson junction on a Pb(111) surface with Mn adatoms — •Martina Trahms[1], David Wander[2], J. Rika Simon[1], Nils Bogdanoff[1], Olof Peters[1], Katharina Biel[1], Gaël Reecht[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Univ. Grenoble Alpes, Institut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

Magnetic impurities on superconducting surfaces are expected to locally disturb the superconducting ground state. The critical current of a Josephson junction is a measure of the superconducting order parameter. We employ current-biased Josephson spectroscopy in a scanning tunneling microscope (STM) to measure the junction's switching current which is directly related to the critical current and marks the transition from Cooper-pair tunneling to quasi-particle tunneling. To investigate the activation processes of the switching events, we statistically analyse the switching of a Josephson junction formed between a Pb tip and a Pb adatom on a Pb(111) surface. By adding Mn adatoms to the Pb surface, we show a local reduction of the switching current and thereby a disturbance of the local order parameter due to the magnetic interaction. Additionally, we probe the switching current distribution in close proximity to the Mn atoms.

O 49.5 Tue 13:30 P

Electronic structure and charge density wave properties of $NdTe_3$ — •Henriette E. Lund[1], Alla Chikina[1], Marco Bianchi[1], Davide Curcio[1], Kirstine J. Dalgaard[2], Shiming Lei[3], Martin Bremholm[2], Leslie M. Schoop[3], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNano), Aarhus University, 8000 Aarhus C, Denmark — [2]Department of Chemistry and Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark — [3]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

Rare-earth tritellurides (RTe_3) are a group of materials exhibiting high charge carrier mobility and, depending on the rare-earth element R, the materials host either one or two incommensurate charge density waves (CDWs). The electronic properties of RTe_3 have previously been investigated by quantum oscillations and angle-resolved photoemission spectroscopy (ARPES), but reconciling the Fermi surface elements observed by both techniques remains an unresolved issue which is complicated by the presence of the CDW and possible additional electronic phase transitions caused by strong magnetic fields.

The goal of the present study is to investigate whether the quantum oscillations reported for $NdTe_3$ can be reconciled with ARPES results. To this end, we refine a tight-binding model to include all relevant interactions and to describe the Fermi surface elements identified by both approaches.

O 49.6 Tue 13:30 P

Metallic Antiferromagnetic Spintronics: Mn2Au a case study — •Sunil Wilfred DSouza[1], Hans-Joachim Elmers[2], Satya Prakash Bommanaboyena[2], Vladimir N Strocov[3], Martin Jourdan[2], and Jan Minár[1] — [1]New Technologies Research Centre, University of West Bohemia, Univerzitní 8, CZ-306 14 Pilsen, Czech Republic — [2]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, D-55099 Mainz, Germany — [3]Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen-PSI, Switzerland

The band structure of Mn2Au has been investigated by first-principles density-functional theory calculations based on the Green's function technique. The total density of state reveals contributions mainly from the Au5d and Mn3d states with rigid local moments on the Mn sites. The existence of significant out-of-plane magnetic anisotropy combined with the large strength of short range antiferromagnetic exchange in-

teractions between Mn atoms located at two different Wyckoff positions results in the stabilization of the antiferromagnetic ground state. Two dimensional plots of constant energy surfaces in the Γ-X-Σ plane of the Brillouin zone exibits a 4-fold to 2-fold symmetry breaking as a function of the binding energy at 0.00 eV and 0.25 eV below the Fermi surface. We find that such a symmetry breaking in Mn2Au is arising due to the degeneration of the electronic bands in the presence of external magnetic field indicating a strong spin-orbit coupling interaction. Our results describes the tuning of the magnetic and electronic properties of Mn2Au for spintronic applications.