O 82: Electronic Structure of Surfaces 2

Time: Friday 10:30–12:15 Location: S053

O 82.1 Fri 10:30 S053

Electron- and Hole-Like Transport in Shockley Type Surface States Detected by MONA — •Andreas Christ, Markus Leisegang, Patrick Härtl, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

In recent years, we have established the STM-based molecular nanoprobe (MONA) technique to detect the transport of hot charge carriers over distances of a few nanometers [1,2]. In short, MONA uses a charge carrier-driven molecular switching events, such as a tautomerization or rotation, to detect currents injected a few nanometers away. Earlier experiments performed on Ag(111) showed that the surface state characteristic for fcc(111) surfaces facilitates effective charge transport between the charge injection point at the tip position and a single phthalocyanine (HPc) detector molecule [3]. Since, however, the energy threshold for tautomerization of HPc exceeds the energy onset of the Ag(111) surface state ($E = -63\,\mathrm{meV}$), hole transport remained inaccessible. In order to investigate the influence of the band structure on the propagation of hot charge carriers we compare results of MONA experiments performed on Ag(111) with the isoelectronic Cu(111) surface. Our results reveal that due to the lower surface state onset in Cu(111) at $E = -440\,\mathrm{meV}$ hole-like charge transport can also be detected.

[1] M. Leisegang *et al.*, Nano Lett. **18**, 2165-2171 (2018)
[2] M. Leisegang *et al.*, Phys. Rev. Lett. **126**, 146601 (2021)
[3] J. Kügel *et al.*, Nano Lett. **17**, 5106 (2017)

O 82.2 Fri 10:45 S053

Exploring polaron stability and defect structures at the $Li_4Ti_5O_{12}$ (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-Institut — [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) due to its "zero strain" charge/discharge behavior. Pristine, white LTO possesses poor ionic and electronic conductivity. Through tailoring the sintering protocol, one can 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 higher electronic conductivity. However, detailed knowledge about polaron stability, distribution, and dynamics in LTO bulk and surface has been lacking. 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 not only play a significant role in enhancing electronic conductivity but boost Li^+ diffusion nearby through lowering the hopping barrier, in line with the experimentally observed improved conductivities.[1,2] In combination with positron lifetime spectroscopy data and theoretical positron lifetimes, we arrive at a rather complete picture of the bulk vs. surface defect chemistry in LTO particles and the resulting mixed ionic electronic conductivity.

[1] M. Kick et al.,J. Phys. Chem. Lett. 11 (2020), 2535
[2] M. Kick et al., ACS Appl. Energy Mater 4 (2021), 8583

O 82.3 Fri 11:00 S053

Spin-polarized VLEED from Au(111): Surface sensitivity of the scattering process — •Christoph Angrick[1], Jürgen Braun[2], and Markus Donath[1] — [1]Westfälische Wilhelms-Universität Münster — [2]Ludwig-Maximilians Universität München

Low-energy electron diffraction from Au(111) shows the well-known threefold symmetry of the diffracted electron beams despite the sixfold symmetry of the surface layer. This is due to the influence of the second and deeper layers and the probing depth of the electrons. In this work, we investigated Au(111) with spin-polarized very-low-energy electron diffraction (VLEED) [1,2] experimentally and theoretically. We monitor the reflected specular beam at a fixed polar angle of incidence of $\Theta = 45°$ while the azimuthal orientation of the crystal is varied. This puts the surface sensitivity of the VLEED scattering process to a test.

Our results show that the electron reflection and the spin-orbit-induced reflection asymmetry along $\overline{\Gamma}\,\overline{\mathrm{M}}$ and $\overline{\Gamma}\,\overline{\mathrm{M}}'$ are equivalent. The observed sixfold symmetry suggests a sensitivity to one atomic layer only. At azimuth angles deviating from the high-symmetry directions $\overline{\Gamma}\,\overline{\mathrm{M}}$ and $\overline{\Gamma}\,\overline{\mathrm{M}}'$, however, the VLEED signal from Au(111) shows a threefold symmetry. To reveal the origin of this effect, we varied the parameters in the calculation. The results indicate a non-negligible influence of the second atomic layer in the VLEED scattering process.

[1] Burgbacher *et al.*, Phys. Rev. B **87**, 195411 (2013)
[2] Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020)

O 82.4 Fri 11:15 S053

The quantum corral: Pertubation by adatoms and bonding description by LCAO — •Andreas Bereczuk[1], Martin Steinau[1], Fabian Stilp[2], Franz Josef Giessbil[2], and Klaus Richter[1] — [1]Institut of Theoretical Physics, University of Regensburg, Germany — [2]Institute of Experimental and Applied Physics, University of Regensburg, Germany

The quantum corral, first investigated in 1993 [1] consists of a circle of 48 iron atoms placed on a copper surface and gives rise to a standing wave pattern of the local charge density (LDOS). Afterwards a plurality of different confinement shapes have been investigated [2,3]. We revisited this structure in [4] using atomic force microscope (AFM) and scanning tunneling microscopy (STM). A tight-binding model [5] provides a LDOS in consistency with STM measurements for the original and the perturbed quantum corral. We further consider weak bonds between the AFM tip and the artifical atom, indicated by a widely spread LDOS, by using linear combinations of atomic orbitals (LCAO).

[1] M. F. Crommie et al., Science 262, 218 (1993)
[2] M. Crommie et al., Physica D: Nonlinear Phenomena 83, 98 (1995)
[3] E. Heller et al., Nature 369, 464 (1994)
[4] F. Stilp et al., Science 372, 1196 (2021)
[5] C. W. Groth et al., New J. Phys. 16, 063065 (2014)

O 82.5 Fri 11:30 S053

Single-Molecule Ultrafast Fluorescence-Detected Pump–Probe Microscopy — •Daniel Fersch[1], Pavel Malý[1,2], Jessica Rühe[3], Victor Lisinetskii[1], Matthias Hensen[1], Frank Würthner[3,4], and Tobias Brixner[1,4] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16 Prague, Czech Republic — [3]Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [4]Center for Nanosystems Chemistry (CNC), Universität Würzburg, Theodor-Boveri-Weg, 97074 Würzburg, Germany

The spectroscopic signatures of bulk samples can differ vastly from those of the respective single molecules. In particular, access to the femtosecond dynamics of single molecules remains a large experimental challenge. Here, we present a novel setup consisting of a spectrally tunable femtosecond laser source and a scanning confocal fluorescence microscope with fully reflective excitation geometry and single-molecule sensitivity. Using a phase-stable interferometer we create a pulse pair with variable time delay to measure the molecular fluorescence excitation spectrum by means of Fourier-transform spectroscopy. By exciting the molecule with an additional prior pump pulse, we gain access to the dynamics of the excited state as a function of the pump–probe delay, resulting in a fluorescence-detected pump–probe spectrum. We have obtained first results on single terrylene bisimide molecules and compare them to a spincoated thin film.

O 82.6 Fri 11:45 S053

Anomalies at the Dirac point in doped graphene (B, N, BN) — •Sangeeta Thakur[1,2], Arindam Pramanik[3], Bahadur Singh[3], Philip Willke[4], Martin Wenderoth[4], Hans Hofsäss[5], Giovanni Di Santo[1], Luca Petaccia[1], and Kalobaran Maiti[3] — [1]Elettra Sincrotrone Trieste, Strada Statale 14 km 163.5, 34149 Trieste, Italy — [2]Freie Universität Berlin, Institut für Experimentalphysik Arnimallee 14, 14195 Berlin, Germany — [3]Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research,Homi Bhabha Road, Colaba, Mumbai 400005, India — [4]IV. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [5]II. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

The changes in the electronic properties of graphene on SiC, induced by different atomic species, B, N and BN, substituted, via low energy (25eV) ion bombardment were investigated via angle-resolved photoemission spectroscopy. The anomalies at the Dirac point for B, N, and BN doped graphene are attributed to the spectral width arising from the lifetime and momentum broadening in the experiments. An energy gap at the Dirac point of graphene is not observed even after 5 % of B and N substitution [1]. These results will provide new insight to tune the carrier properties of graphene while keeping the Dirac fermionic properties protected, which is important for exploring its technological applications.

[1] A. Pramanik, Sangeeta Thakur et.al. PRL 128, 166401 (2022).

O 82.7 Fri 12:00 S053

Interplay of intrinsic and extrinsic states in pinning and passivation of m-plane facets of GaN n-p-n junctions — •Lars Freter[1,2], Yuhan Wang[1,2], Michael Schnedler[1], Jean-François Carlin[3], Raphaël Butté[3], Nicolas Grandjean[3], Holger Eisele[4], Rafal Edward Dunin-Borkowski[1,5], and Philipp Ebert[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Lehrstuhl für Experimentalphysik IV E, RWTH Aachen University, 52056 Aachen, Germany — [3]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland — [4]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [5]Ernst Ruska-Centrum, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Intrinsic and extrinsic pinning and passivation of *m*-plane cleavage facets of GaN *n*-*p*-*n* junctions were investigated by cross-sectional scanning tunneling microscopy and spectroscopy. On freshly cleaved and clean *p*-type GaN($10\bar{1}0$) surfaces, the Fermi level is found to be extrinsically pinned by defect states, whereas *n*-type surfaces are intrinsically pinned by the empty surface state. For both types of doping, air exposure reduces the density of pinning states and shifts the pinning levels toward the band edges. These effects are assigned to water adsorption and dissociation, passivating intrinsic and extrinsic gap states. The revealed delicate interplay of intrinsic and extrinsic surface states at GaN($10\bar{1}0$) surfaces is a critical factor for realizing flatband conditions at sidewall facets of nanowires exhibiting complex doping structures.