O 34: Poster: Surface Dynamics & Electron-Driven Processes

Time: Tuesday 18:00–20:00 Location: Poster C

O 34.1 Tue 18:00 Poster C

Targeted growth of metastable interface polymorphs — •Simon B. Hollweger, Anna Werkovits, and Oliver T. Hofmann — Institute of Solid State Physics, TU Graz, Austria

Growing a specific interface polymorph of organic molecules on inorganic substrates is far from trivial. The target structure is usually not the one that is thermodynamically most favorable, but rather an energetically higher-lying, metastable structure. It is primarily unclear how the growth conditions need to be tuned to maximize the yield of a higher-energy polymorph. These conditions are usually explored experimentally by a tedious trial-and-error routine. To avoid this obstacle we theoretically investigate the growth behavior of such systems. We discuss a class of systems where we can start from a lower-energy polymorph and through systematic changes of pressure and temperature induce a structural change to the desired target structure. For that two requirements need to be fulfilled, (a) the metastable target structure has a similar packing density as the initial structure and (b) an 'elevator' polymorph exists that has a higher packing density and is thermodynamically accessible at lower temperatures. To explore in which range of substrate-molecule and molecule-molecule interactions the necessary conditions are fulfilled we employ a combination of kinetic Monte Carlo simulations and ab-initio thermodynamics. This allows us to formulate structure-to-property relationships. For actually determining 'growth recipes' for a specific target structure we utilize Deep Reinforcement Learning combined with kinetic Monte Carlo simulations to obtain optimal temperature and pressure curves.

O 34.2 Tue 18:00 Poster C

Exploring the Commensurate Charge Density Wave in Tantalum Disulfide: Insights from Scanning Tunneling Microscopy and Spectroscopy — •Georg A. Traeger[1], Jan-Niclas Schmidt[1], Kai Rossnagel[3,4], Murat Sivis[1,2], Claus Ropers[1,2], and Martin Wenderoth[1] — [1]University of Göttingen, IV. Physik, Fredrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany — [3]Institute for Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany — [4]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

In recent years, transition-metal dichalcogenides have attracted great interest, owing to a wide range of correlated and tunable physical phenomena. 1T-tantalum disulfide is a widely-studied model system, which exhibits a series of charge-density wave states and a strong influence of stacking on its electronic properties. Here, we present a study of the low-temperature commensurate charge density wave and its metastable states by means of Scanning Tunneling Microscopy (STM) and Spectroscopy (STS). We investigate the defect- and laser-induced creation and manipulation of metastable states, emphasizing the roles of translational phase boundaries and heterochirality.

O 34.3 Tue 18:00 Poster C

Invariant embedding approach to secondary electron emission from surfaces — •Franz Xaver Bronold and Felix Willert — Institut für Physik, Universität Greifswald, 17489 Greifswald, Germany

Secondary electron emission from the walls confining a gas discharge is an important surface process in low-temperature plasma physics. It affects, for instance, the operation modii of barrier discharges, Hall thrusters, and divertor plasmas in fusion devices. Little is however known quantitatively about the process because it typically occurs at energies below 50 eV which are hard to access experimentally. In this contribution, we present a theoretical scheme for calculating the secondary electron emission yield in this energy range. It is based on applying the invariant embedding principle, originally developed for calculating the albedo of planetary atmospheres, to the electron surface scattering kernel characterizing the interaction of a primary electron with a surface [1]. To illustrate the approach we apply it to polycrystalline silicon and germanium surfaces using a semiempirical randium-jellium model containing the Schottky barrier, impact ionization across the band gap as well as scattering on phonons, defects, and ion cores. The emission yields we obtain by solving the full nonlinear embedding equation numerically without an approximate decoupling of angle and energy variables are in satisfactory agreement with measured data to also support the use of the scattering kernel in the boundary condition of the electron Boltzmann equation of a plasma simulation.
[1] F. X. Bronold and F. Willert, arXiv:2309.00534.

O 34.4 Tue 18:00 Poster C

Power discontinuity and shift of the energy onset of a molecular de-bromination reaction induced by hot-electron tunneling — Ana Barragan[1], Roberto Robles[2], Nicolas Lorente[2,4], and •Lucia Vitali[1,2,3,4] — [1]Advanced Polymers and Materials: Physics, Chemistry and Technology, Chemistry Faculty (UPV/EHU) — [2]Centro de Física de Materiales CFM/MPC(CSIC-UPV/EHU), — [3]Ikerbasque Research Foundation for Science, Bilbao 48009, Spain; — [4]Donostia International Physics Center (DIPC), 20018 San Sebastián,

Understanding the mechanism of molecular dissociation under applied bias is a fundamental requirement to progress in (electro)- catalysis as well as in (opto)-electronics. The working conditions of a molecular-based device and the stability of chemical bonds can be addressed in metal-organic junctions by injecting electrons in tunneling conditions. Here, we have correlated the energy of debromination of an aryl group with its density of states in a self-assembled dimeric structure of 4'-bromo-4-mercaptobiphenyl adsorbed on a Au(111) surface. We have observed that the electron-energy range where the molecule is chemically stable can be extended, shifting the bias threshold for the rupture of the -C-Br bond continuously from about 2.4 to 4.4 V by changing the electron current. Correspondingly, the power needed for the dissociation drops sharply at 3.6 V, identifying different reaction regimes and the contribution of different molecular resonance states.

O 34.5 Tue 18:00 Poster C

Investigation of Ballistic Transport on Black Phosphorus with MONA — •Manuel Seitz, Andreas Christ, Emilian Eisermann, Patrick Härtl, Markus Leisegang, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Due to the ever-increasing miniaturization of electronic components, we are approaching a frontier where 2D-materials are promising for nanoscale electronic devices. One auspicious material is the semiconductor black phosphorus (BP) [1]. BP exhibits an anisotropic surface structure and shows a band gap that is influenced by the number of layers [1, 2]. The strong anisotropy as well as the possibility to tune the band gap are properties which may strongly impact the charge transport.
In this project, we aim to investigate surface transport in the ballistic regime of BP using the molecular nanoprobe (MONA) technique[4]. We thoroughly evaluated various cleaving techniques and investigated the resulting surfaces. Furthermore, single adatoms with bistable binding configurations are characterized [5]. In a proof-of-principle experiment we show that these bistable atoms can be used as detectors for MONA measurements.
[1] X. Ling *et al.*, Proc. Natl. Acad. Sci. **112**, 4523 (2015)
[2] J. Kim *et al.*, Science **349**, 723 (2015)
[3] Y. Du *et al.*, J. Appl. Phys. **107**, 093718 (2010)
[4] M. Leisegang *et al.*, Nano Lett. **18**, 2165 (2018)
[5] B. Kiraly *et al.*, Nat. Commun. **9**, 3904 (2018)