O 31: Metal & Semiconductor substrates: Adsorption and reaction of small molecules – Poster

Time: Monday 18:00–20:00 Location: P2

O 31.1 Mon 18:00 P2

Investigating the native oxide layer of CoCrFeNi(100) by co-adsorption of O_2 and H_2: an XPS study — •Peter Richter, Kavya Harsha Kumar, Susanne Wolff, and Thomas Seyller — Technische Universität Chemnitz, Chemnitz, Deutschland

High-entropy alloys (HEAs) are a relatively new class of materials with potential applications under ambient conditions. Hence, understanding the formation and the properties of their native oxides is essential. In this study, we use X-ray photoelectron spectroscopy to investigate the native oxide layer present on CoCrFeNi(100) as well as on the clean surface subjected to controlled exposures of O_2 and H_2.

To evaluate the stability of the native oxide layer, samples were annealed in ultra-high vacuum at temperatures in the range of 350 to 1100 °C. Oxide reduction increased significantly at 700 °C and was complete at 1100 °C. The exposure of clean CoCrFeNi(100) surfaces to 1 to 1000 L of O_2 leads to controlled oxidation, with Cr contributing most to oxide formation, followed by Co and Fe. The subsequent introduction of H_2 at sample temperatures of up to 500 °C leads to systematic changes in the surface chemistry.

Experimentally, the information of the bonding configuration is best observed in the 2p core levels of Co, Cr, Fe and Ni. However, when using the Al K_α line, several Auger peaks overlap with the Co2p and Fe2p core levels. In addition, multiplet splitting and satellite features further complicate the evaluation of the XPS data. To improve this, we performed reference measurements and developed fitting models for the Auger lines using pure metal foils.

O 31.2 Mon 18:00 P2

Molecular bottom up: Site-selective adsorption of cyclooctyne on partially passivated Si(001) — Jannick A. Peters[1], •Sophie Göbel[1], Dominik Scharf[2], Ulrich Koert[2], and Michael Dürr[1] — [1]Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany — [2]Fachbereich Chemie, Philipps-Universität Marburg, Germany

Organic molecular structures on the technologically most important Si(001) surface are of great potential for future applications in terms of "more than Moore". The synthesis of organic structures on semiconductor surfaces requires several aspects to be considered, such as precise choice of adsorbates and their functional groups, as well as a well-prepared surface where the reaction sites can be controlled. For a lateral ordering of the organic layer, pre-patterned substrates are seen as promising starting point; e.g., alternating passivated and non-passivated surface areas are generated by means of STM in hydrogen desorption lithography. A self-organized approach might be based on ethylene on Si(001) which is known to show a well-ordered adsorbate structure on Si(001) in the submonolayer regime due to nearest-neighbor interactions. The reaction of cyclooctyne and its derivatives on the Si(001) surface pre-passivated with ethylene was studied by means of XPS and STM. Whereas C_2H_4 shows strongly reduced reactivity at the remaining, unreacted silicon dimers, cyclooctyne with its direct reaction channel on clean Si(001) shows high reactivity also at these strongly hindered sites. Furthermore, the reaction of bifunctional cyclooctynes was observed to be more selective than on clean Si(001).

O 31.3 Mon 18:00 P2

Quantitative imaging of surface potential of PTCDA molecules on Ag(111) and Pb(111) — •Sandhya Anchamkudy[1], Janine Lorenz[1,2], Amin Karimi[1], Christian Wagner[1,2], Ruslan Temirov[1,3], Henry Thake[4], Reinhard Maurer[4], Stefan Tautz[1,2], and Felix Lüpke[1,3] — [1]Peter Grünberg Institut (PGI 3), Forschungszentrum Jülich, Germany — [2]Institut für Experimentalphysik IV A, RWTH Aachen, Germany — [3]Institute of Physics II, Universität zu Köln, Germany — [4]Department of Chemistry, University of Warwick, United Kingdom

Scanning Quantum Dot Microscopy (SQDM) enables quantitative imaging of surface dipoles with unprecedented energy and spatial resolution. In the past, SQDM has been applied to molecular adsorbates, adatoms, defects, and atomic assemblies on silver [Phys. Rev. Lett. 115, 026101 (2015), Nat. Mater. 18, 853 (2019)] - and provided valuable benchmarks for theory where metal-organic hybrid systems are particularly challenging. Here, we investigate the adsorption geometry dependent effects of isolated perylene tetracarboxylic dianhydride (PTCDA) molecules on Ag(111). We identified two preferred orientations of PTCDA molecules: along the <1-10> and <11-2> directions of the Ag(111) surface. In SQDM measurements, the two orientations yield distinct dipole moments of -0.51 D and -0.65 D, respectively. In addition, we carried out SQDM of a single PTCDA molecule on superconducting Pb(111) and found that the dipole is seven times larger compared to PTCDA on Ag(111). This difference can be attributed to a significantly higher charge transfer and adsorption height on Pb(111).

O 31.4 Mon 18:00 P2

Redox Molecules on Gold Surfaces: Insights into Triboelectric Behavior through Simulations — •Zohreh Izadi[1,2], Michael Moseler[1,2,3], Michael Walter[1,2,3], and Leonhard Mayrhofer[3] — [1]Cluster of Excellence livMatS @Freiburg Center for Interactive Materials and Bioinspired Technologies(FIT), University of Freiburg, Freiburg, Germany — [2]Institute of Physics, University of Freiburg, Freiburg, Germany — [3]Fraunhofer IWM, MikroTribologie Centrum μTC, Freiburg, Germany

Triboelectricity, the electrostatic charge generated during the contact and separation of materials, remains poorly understood at the microscopic level. Redox-active molecules on metal surfaces provide a controlled platform to probe these charge-transfer processes. We studied donor and acceptor molecules adsorbed on Au(111) and evaluated their adsorption geometries and binding energies, as well as the electronic signatures associated with interfacial charge transfer. We also considered different environments and found that humidity was a key factor facilitating charge transfer between the molecules and the surface. Our results are in very good agreement with the experimental findings from our joint study, offering insight into how redox-driven charge transfer at metal-molecule interfaces contributes to triboelectric behavior.

Reference: N. Ranjan, Z. Izadi et al., Contact Electrification via Redox-Active Molecules, Angewandte Chemie International Edition, 2025, e10031. DOI: 10.1002/anie.202510031.

O 31.5 Mon 18:00 P2

TPD Studies of Metal-Substrate Interactions in LOHCs and Polyfluorinated Compounds — Kassandra Zoltner, •Evelyn Versok, Leonard Neuhaus, Stefan R. Kachel, and J. Michael Gottfried — Fachbereich Chemie und mar.quest, Philipps-Universität Marburg, Germany.

Metal-substrate interactions critically govern catalytic reaction pathways and degradation mechanisms. Here, we investigate two chemically contrasting classes of adsorbates - hydrogen-rich liquid organic hydrogen carriers (LOHCs) and fluorocarbons - to clarify their stability and reactivity on metal surfaces. LOHCs such as decalin and tetralin are attractive hydrogen-storage materials but are prone to side reactions and catalyst-induced decomposition. In contrast, fluorocarbons including all-cis-hexafluorocyclohexane and perfluoromethylcyclohexane exhibit exceptional thermal and chemical stability, which is technologically valuable yet contributes to unwanted environmental persistence. Understanding molecule-metal interactions is therefore important for both hydrogen-storage chemistry and fluorocarbon degradation strategies. We employ temperature-programmed desorption (TPD) to determine adsorption energies, reaction kinetics, and product distributions. Systematic analysis of the selected LOHCs and fluorinated compounds on Au(111), complemented by comparison with partially dehydrogenated and defluorinated analogues, reveals detailed metal-induced transformation pathways. These insights advance the mechanistic understanding of hydrocarbon and fluorocarbon degradation on metal surfaces and support catalyst development.

O 31.6 Mon 18:00 P2

Orientation-dependent Adsorption and Manipulation of a Boron-doped Polycyclic Aromatic Hydrocarbon — •Elishka Vaz[1], Matthias Schnitzlein[2], Frank Würthner[2], Matthias Bode[1], and Jing Qi[1] — [1]Physikalisches Institut, Experimentelle Physik 2, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institut für Organische Chemie, Organische Chemie II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The incorporation of boron atoms into polycyclic aromatic hydrocarbons (PAHs) alters their electronic properties since the boron centres act as π-acceptors [1]. In this contribution, we present a novel boroncentered PAH with terminal bromine-substituents. Upon adsorption on the Cu(111) surface, the B-PAHs adopt twelve distinct azimuthal orientations: six aligned with the crystallographic directions of the (111) surface, and six rotated by 30°. Differential-conductance spectroscopy and apparent-height analyses reveal a pronounced influence of the substrate on both the topographic appearance and electronic structure. Atomic-resolution imaging enables assignment of adsorption sites via interpolation of the surface atomic rows. Moreover, lateral tip-induced manipulation demonstrates controlled stacking along the molecular short axis. Finally, we identify a double-chain arrangement, likely composed of intact molecules, which exhibits a notable spectral shift in the differential-conductance signature relative to isolated adsorbates.

[1] M. Schnitzlein *et al.*, ChemistryEurope **3**, e202500135 (2025)