O 5: Poster Session I: Metal substrates I

Time: Monday 10:30–12:30 Location: P

O 5.1 Mon 10:30 P

Multi-method study of trans-DBPen on coinage metal (111)-surfaces — •Felix Otto, Maximilian Schaal, Tobias Huempfner, Falko Sojka, Marco Gruenewald, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Several polycyclic aromatic hydrocarbons (PAHs) become superconducting after the intercalation of alkali metal atoms. The number of promising candidates has increased in the last few years. Among them, $K_{3.45}$1,2:8,9-dibenzopentacene (trans-DBPen, $C_{30}H_{18}$) is the one with the highest critical temperature reported so far. Nevertheless, the microscopic mechanisms of superconductivity in K-doped PAHs are still under debate. One open question is, for example, the effect of structural order in bulk materials as well as two-dimensional layers.

Our work deals with the growth of trans-DBPen on Ag(111), Au(111), and Cu(111) in the monolayer (ML) regime. The self-assembled thin films were prepared using organic molecular beam epitaxy. The structure was characterized by means of low energy electron diffraction (LEED). In the sub-ML range, we observe a 2D gas-like behavior, whereas the first MLs on the different substrates are characterized by highly ordered structures. Photoelectron spectroscopy (PES) including photoelectron momentum maps (PMMs) was used to study the interaction of the molecules with the substrate as well as the influence of the second ML on the electronic structure. The investigated systems exhibit notable differences according to the different interaction strengths with the substrate.

O 5.2 Mon 10:30 P

Scanning tunneling microscopy study of submonolayer growth of Mn_xAu_{1-x} on Cu(001) — •Ismet Gelen[1], Tauqir Shinwari[1], Yasser A. Shokr[1,2], Evangelos Golias[1], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Faculty of Science, Department of Physics, Helwan University, 17119 Cairo, Egypt

Mn_xAu_{1-x} exhibits many antiferromagnetic (AFM) phases. Mn_2Au is one of them that has a high Néel temperature ($\approx$ 1600 K) and, due to its noncentrosymmetric spin structure and metallic nature, is an interesting AFM material for spintronic applications. Here, we study the growth of Mn_xAu_{1-x} in the submonolayer (sub-ML) regime on Cu(001) by medium- and low-energy electron diffraction (MEED, LEED), Auger electron spectroscopy (AES), and scanning tunneling microscopy (STM). Different Mn concentrations ($x \approx 0.7-0.9$) and different thicknesses ($\approx 0.2-1.1$ ML) were studied, as monitored by AES. Mn and Au were coevaporated by electron bombardment on Cu(001) at room temperature (RT). The growth of thicker films showed MEED intensity oscillations up to around 9 ML. The LEED images display substrate patterns for thicknesses < 0.5 ML, while they display a $c(2 \times 2)$ structure for thicker sub-ML films. We observe Mn_xAu_{1-x} islands on Cu(001) for all sub-ML films with island sizes between $\approx 5 \times 5$ and 30×30 nm^2.

O 5.3 Mon 10:30 P

Submonolayer growth of Te on Cu(111) — •Tilman Kisslinger, Andreas Raabgrund, Maximilian Ammon, M. Alexander Schneider, and Lutz Hammer — Lehrstuhl für Festkörperphysik, Universität Erlangen–Nürnberg, D–91058 Erlangen, Germany

Tellurium (Te) based alloys play an important role in metallurgy, thermoelectricity and photovoltaics [1]. Thus, an accurate knowledge of the crystallographic surface structure and elemental composition of such systems is the first step to any understanding of their diverse physical properties. We studied the adsorption of Te on Cu(111) for submonolayer coverages with quantitative low-energy-electron diffraction (LEED), scanning tunneling microscopy (STM) and density-functional theory (DFT).
Below Θ =1/12 ML we find Te atoms to form a disordered structure. Above this threshold a $(2\sqrt{3} \times \sqrt{3})R30°$ structure evolves that is fully developed at a coverage of 1/3 ML. STM shows a well-ordered surface phase that is solved by our LEED-analysis (Δ E = 8.9 keV, R = 0.099) to consist of Te_2Cu_2 chains in hcp-sites of the first substrate layer in perfect agreement with the structure calculated by DFT [2].

[1]: Ibers J., Nat. Chem. **1**, 508 (2009)
[2]: Kisslinger T., Phys. Rev. B. **102**, 155422 (2020)

O 5.4 Mon 10:30 P

Inducing and Probing the Rotational Motion of a Single Carbon Monoxide Molecule — •Nicolas Néel and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

The control and observation of reactants forming a chemical bond at the single-molecule level is a longstanding challenge in quantum physics and chemistry. Using a single CO molecule adsorbed at the apex of an atomic force microscope tip and a Cu(111) surface at bonding distances, the molecular rotational motion is induced by torques due to van der Waals attraction and Pauli repulsion. As a result, the vertical force exhibits a characteristic dip-hump evolution with the molecule-surface separation, which depends sensitively on the initial tilt angle the CO axis encloses with the microscope tip. The experimental force data are reproduced by model calculations that consider the CO rotational motion in a harmonic potential and the molecular orientation in the Pauli repulsion term of the Lennard-Jones potential.

O 5.5 Mon 10:30 P

First-principles study of the coexistence of a chemisorption and physisorption state of CO on Au(111) — •Svenja M. Janke[1,2] and Reinhard J. Maurer[2] — [1]Institute of Advanced Studies, University of Warwick, Coventry, UK — [2]Department of Chemistry, University of Warwick, Coventry, UK

Accurate representation of the potential energy landscape for a molecule on a metal surface is essential to model energy transfer between the molecule and the surface, but not always straightforward. Recent experiments suggest the presence of a chemisorption and a physisorption state for CO adsorbed on Au(111). Within the all electron electronic structure code FHI-aims, we survey several approximations to Density Functional Theory for their ability to predict the adsorption state of CO on Au(111). In agreement with previous theoretical observations for similar systems, we find that common generalized gradient approximation functionals with van-der-Waals correction lead to overbinding, with the revised Perdew-Burke-Ernzerhof function with van-der-Waals correction coming closest to experimental results. Our results lay the ground work to construct a high-dimensional energy surface to study the nonadiabatic dynamics of carbonyl reactive scattering on Au(111).

O 5.6 Mon 10:30 P

Moving azulene based molecules by STM: The role of dipole moment and field effect — •Tim Kühne[1,2], Kwan Ho Au Yeung[1,2], Frank Eisenhut[1,2], Oumaima Aiboudi[3], Dmitry Ryndyk[2], Gianaurelio Cuniberti[2], Franziska Lissel[3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [3]Leibniz Institute of Polymer Research, 01069 Dresden, Germany

Among the different mechanisms that can be used to drive a molecule on a surface by the tip of a scanning tunneling microscope at low temperature, we used voltage pulses to move azulene-based single molecules and nanostructures on Au(111). Upon evaporation, the molecules partially cleave and form metallo-organic dimers while single molecules are very scarce, as confirmed by simulations. By applying voltage pulses to the different structures in similar conditions, we observe that only one type of dimers can be controllably driven on the surface. This has the lowest dipole moment of all investigated structures. Experiments at different bias and tip height conditions reveal that the electric field is the main driving force of the directed motion. We discuss the different observed structures and their movement properties with respect to their dipole moment and charge distribution on the surface.

O 5.7 Mon 10:30 P

LT-STM investigation of transmitting rotation between molecule-gears on Au(111) — •Kwan Ho Au Yeung[1,2], Tim Kühne[1,2], Frank Eisenhut[1,2], Michael Kleinwächter[3], Yohan Gisbert[3], Roberto Robles[4], Nicolas Lorente[4,5], Gianaurelio Cuniberti[2], Christian Joachim[3], Gwénaël Rapenne[3,6], Claire Kammerer[3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany —

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The realization of a train of molecule-gears working under the tip of a scanning tunneling microscope (STM) requires a stable anchor of each molecule to the surface. Such anchor can be promoted by a radical state of the molecule induced by a dissociation reaction. Our results reveal that such open radical state at the core of star-shaped pentaphenylcyclopentadiene (PPCP) favors the anchoring. Furthermore, to allow the transmission of motion by manipulation, in our case, a tert-butyl group positioned at one tooth end of the gear benefits both the tip-induced manipulation and the monitoring of rotation. With this optimized molecular system, we achieve reproducible rotations of the single gears and transmit rotations up to three interlocked units.

O 5.8 Mon 10:30 P

Fusion of alkyl groups to form phenyl rings: a new on-surface reaction — •Amogh Kinikar[1], Marco Di Giovannantonio[1], Josè Ignacio Urgel[1], Kristjan Eimre[1], Xiao-Ye Wang[2], Zijie Qiu[2], Akimitsu Narita[2], Klaus Müllen[2], Pascal Ruffieux[1], Carlo Antonio Pignedoli[1], and Roman Fasel[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, 8600, Switzerland — [2]Max Planck Institute for Polymer Research, 55128 Mainz (Germany)

On-surface synthesis allows for the design of carbon nanostructures such as graphene nanoribbons with atomic precision. However, the variety of conceivable structures critically depends on the number of available reactions. Here, we present a new surface-assisted reaction allowing for the controlled fusion of two alkyl groups to form a phenyl ring mediated by the activation of alkyl C-H bonds under ultra-high vacuum conditions. Scanning tunneling and non-contact atomic force microscopy images at different stages of the reaction along with DFT simulations allow us to elucidate the reaction mechanism. Furthermore, we study the influence of surface templating by comparing the reaction on Au(111) and Au(110). The selective formation of phenyl rings by the on-surface fusion of alkyl groups is unprecedented, and introduces a powerful new motif for the design of novel carbon nanomaterials while furthering our understanding of the reactive nature of the alkyl C-H bonds.