

O 49: Metal Substrates: Structure, Adsorption and Growth

Time: Tuesday 18:15–20:30

Location: Poster E

O 49.1 Tue 18:15 Poster E

On the microscopic structure of the Ag(441) surface — ●THORSTEN WAGNER, ROBERT ZIMMERLEITER, DANIEL ROMAN FRITZ, and PETER ZEPPENFELD — Johannes Kepler University Linz, Institute for Experimental Physics, Austria

Regularly stepped (vicinal) surfaces provide a convenient path to control the number of defects of a surface. They can be easily prepared by a slight miscut of a low index surface. In the case of an fcc(nn1) surface with small integer n it is even expected that the large number of steps will dominate the surface properties. Here we report on a study of the Ag(441) surface using a combination of scanning tunneling microscopy (STM) and high resolution electron diffraction (SPA-LEED). The STM data suggest a statistical distribution of the step width which can be described by a Γ -probability distribution. In fact, the steps are not randomly distributed but are interacting. The detailed statistical analysis of the images also reveals that the terraces are formed by an integer number of (331) building blocks whereas the actual steps are given by (551) microfacets. In order to compare the electron diffraction data to the real space information from the STM experiment, we carried out simulations of the reciprocal space maps (RSM) in the framework of the simple kinematic approximation. In the case of narrow, interacting steps one has to be cautious to carry out a correct interpretation of the experimental RSM based on the splitting of the rods and their tilt angle, only. Especially the latter is strongly influenced by the correct alignment of the sample.

O 49.2 Tue 18:15 Poster E

DFT-based survey of site dependent interaction of halogen atoms with the (001) surfaces of Cu, Ag, and Au — ●ALEXANDRA C. DÁVILA, LUKAS DEUCHLER, SÖNKE BUTTENSCHÖN, and ECKHARD PEHLKE — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

Diffusion at electrochemical interfaces is a decisive factor for, e.g., metal electrodeposition using halogen ion containing electrolytes [1]. The potential dependent growth has been ascribed to the variation of activation energy barriers due to the interaction of adsorbate-induced electric dipoles with the electric field at the surface [1,2]. In order to identify trends that may be relevant for the diffusion of halogen atoms on coinage metal (001) surfaces, we present a survey based on density functional total energy calculations with VASP [3,4] for the potential energy surface calculated for particular geometries corresponding to halogen atoms at the hollow, bridge, and top sites, and the associated electric dipole moments. Results both for separated halogen atoms and for coverage $\Theta = 0.5$ are compared to DFT data from the literature, e.g. Ref. [5].

[1] M. Ruge, F. Golks, J. Zegenhagen, O.M. Magnussen, J. Stettner, *Phys. Rev. Lett.* **112**, 055503 (2014).

[2] M. Giesen, G. Beltramo, S. Dieluweit, J. Müller, H. Ibach, W. Schmickler, *Surf. Sci.* **595**, 127 (2005).

[3] G. Kresse, J. Hafner, *Phys. Rev. B* **49**, 14251 (1994).

[4] //www.vasp.at.

[5] A. Migani, F. Illas, *J. Phys. Chem B* **110**, 11894 (2006).

O 49.3 Tue 18:15 Poster E

Diffusion properties of lithium studied using DFT: growth phenomena and the effect of an electric field — ●MARKUS JÄCKLE^{1,2} and AXEL GROSS^{1,2} — ¹Helmholtz Institut Ulm - Elektrochemische Energiespeicherung, 89069 Ulm, Germany — ²Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

The formation of dendrites poses a big problem in batteries and can lead to short-circuits during battery operation. As metal growth processes are intimately linked to diffusion, we have extended our initial theoretical first-principles study of the self-diffusion properties of lithium [1], in order to enhance our understanding of a possible explanation for this phenomenon which may help avoiding battery failure due to dendrite growth.

According to our calculations, the previously established picture of an inhomogeneous lithium surface [1] is correct. The new results further suggest that the (011) surface of lithium may have an important role in facilitating the growth of dendrites and that the effect of an electric field on lithium self-diffusion is rather small.

[1] M. Jäckle and A. Groß, *J. Chem. Phys.* **141**, 174710 (2014).

O 49.4 Tue 18:15 Poster E

Growth and potassium doping of ultrathin layers of picene on Ag(100) — ●MARTIN HAUFERMANN¹, TOBIAS HUEMPFNER¹, ROMAN FORKER¹, and TORSTEN FRITZ^{1,2} — ¹Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — ²Osaka University, Graduate School of Science and Institute for Academic Initiatives, Department of Chemistry, 1-1 Machikaneyama, Toyonaka 560-0043, Osaka, Japan

Superconductivity in polycyclic aromatic hydrocarbons (PAH) was discovered in alkali-metal-intercalated solid picene [1]. A more recent study questions the very superconductivity in K₃picene and calls for more accurate structural characterizations of such systems, especially of their low-dimensional structures [2]. In this contribution we investigate ultrathin films of potassium-doped picene on Ag(100) to obtain a deeper understanding of the mechanisms causing the superconductive properties of PAHs. To analyze the growth of the pristine picene layers as well as the potassium-doping process we used scanning tunneling microscopy (STM) and distortion-corrected low-energy electron diffraction (LEED). We determined that the epitaxy of the picene monolayer on Ag(100) exhibits a point-on-line coincidence, and that the lattice parameters correspond to a bulk-like unit cell consisting of two molecules, one flat lying and one tilted with respect to the substrate surface. Potassium intercalation into one monolayer picene on Ag(100) led to the formation of a new commensurate phase.

[1] R. Mitsuhashi *et al.*, *Nature* **464**, 76 (2010).

[2] S. Heguri *et al.*, *Phys. Rev. B* **92**, 014502 (2015).

O 49.5 Tue 18:15 Poster E

Thin epitaxial films of tetraphenyldibenzoperiflanthene (DBP) on Ag(111) — ●TINO KIRCHHUEBEL¹, MARCO GRUENEWALD¹, FALKO SOJKA¹, SATOSHI KERA^{2,3,4}, FABIO BUSSOLOTTI², TAKAHIRO UEBA^{2,3}, NOBUO UENO⁴, GAËL ROUILLE⁵, ROMAN FORKER¹, and TORSTEN FRITZ¹ — ¹Institute of Solid State Physics, Friedrich Schiller University Jena, Germany — ²Institute of Molecular Science, Myodaiji, Okazaki, Japan — ³SOKENDAI, The Graduate University of Advanced Studies, Okazaki, Japan — ⁴Graduate School of Advanced Integration Science, Chiba University, Japan — ⁵Institute of Solid State Physics & Laboratory Astrophysics Group of the Max Planck Institute for Astronomy, Friedrich Schiller University Jena, Germany

We investigated epitaxial tetraphenyldibenzoperiflanthene (DBP) thin films grown on Ag(111). Structural characterization using LEED and STM revealed a well-ordered flat-lying thin film grown in a herringbone arrangement within the first monolayer. In order to trace the development of the optical properties *in situ* differential reflectance spectroscopy (DRS) was performed. A strong interaction between molecules in contact with the Ag(111) surface was found. Depending on the coverage two distinct spectral fingerprints of DBP molecules on top of the first monolayer arise, indicating a transformation from DBP monomers to aggregates. Ultraviolet photoelectron spectroscopy (UPS) measurements reveal two distinct sets of peaks for the occupied states of DBP multilayer samples on Ag(111), being indicative of an individual alignment of electronic states for each DBP species.

O 49.6 Tue 18:15 Poster E

A Giant Molecular Spoked Wheel — ●STEFAN-SVEN JESTER, ROBERT MAY, and SIGURD HÖGER — Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn

The modular synthesis of a defined, rigid molecular spoked wheel structure with the sum formula C₁₈₇₈H₂₆₈₂ and a diameter of about 12 nm is described. The attached 96 dodecyl side chains provide the solubility of the 25260 Da compound in common organic solvents. At the octanoic acid/highly oriented pyrolytic graphite interface, the molecules self-assemble to form an ordered 2D lattice, which is investigated by scanning tunneling microscopy, displaying their structure with sub-molecular resolution. [1] R. May, S.-S. Jester, S. Höger *J. Am. Chem. Soc.* **2014**, *136*, 16732-16735.

O 49.7 Tue 18:15 Poster E

Nanopatterning by rod-bridge-rod-shaped molecules — ●STEFAN-SVEN JESTER, MELISSA HÜNDGEN, KATHARINA ANNA WEIS,

and SIGURD HÖGER — Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn

The supramolecular self-assembly of arylene-alkynylenes with a rod-bridge-rod geometry is investigated at the solution/solid interface. Scanning tunneling microscopy provides a submolecularly resolved insight into the 2D nanostructures that are formed on the graphite surface, which acts as a template. We focus on how the nanopatterns depend on their molecular building blocks. In particular, we investigate how shape and shape-persistence of the backbones, their alkyl/alkoxy side-chain periphery and the rod end groups influence the pattern structures.

O 49.8 Tue 18:15 Poster E

Structure and electronic properties of triazatruxene layers on Ag(111) studied by LT-STM — ●ANJA BAUER¹, FLORIAN SINGER¹, PHILIPP ERLER¹, MARKUS MAIER², RAINER WINTER², LUCA GRAGNANIELLO¹, and MIKHAIL FONIN¹ — ¹Fachbereich Physik, Universität Konstanz, Konstanz, Germany — ²Fachbereich Chemie, Universität Konstanz, Konstanz, Germany

We present a study of triazatruxene (TAT) molecules deposited on Ag(111) by means of electrospray ionization in ultra high vacuum. We investigated the structural and electronic properties of TAT molecules at different coverages by means of low temperature scanning tunneling microscopy (STM) and spectroscopy (STS). For coverages far below one monolayer we observe the molecular superstructures which are stabilized by long-range repulsive intermolecular interaction. High-resolution STM imaging reveals three different types of intramolecular structure, which are possibly due to different site-specific interaction between the molecule and the substrate. At coverages close to one monolayer we observe the formation of self-assembled structures. Here, three different packing types are observed. Depending on the exact surrounding of each molecule within the layer a strong variation in the orbital structure of the molecules is observed. We attribute this findings to a strong surface-enhanced dipole-dipole interaction between the molecules.

O 49.9 Tue 18:15 Poster E

Adsorbate nanomesh causes lateral segregation: Ab-initio based Monte-Carlo study for *h*-BN on Pt₅₀Rh₅₀(111) — ●WOLFGANG HECKEL¹, TOBIAS C KERSCHER¹, ROLAND STANIA^{2,3}, THOMAS GREBER², and STEFAN MÜLLER¹ — Hamburg University of Technology, Institute of Advanced Ceramics — ²Universität Zürich, Physik-Institut — ³Paul Scherrer Institut Villigen, Swiss Light Source

Surface segregation in metal alloys and its adjustability by adsorbates is a well-known phenomenon [1]. In our study, Pt-Rh serves as a substrate for a self-assembled 2d boron nitride (*h*-BN) layer. The experiments on *h*-BN/Pt₅₀Rh₅₀(111) show a corrugated, honeycombed 11 × 11 nanomesh adsorbate layer caused by the lattice constant mismatch of substrate and adsorbate [2].

Using a combined DFT-cluster-expansion approach we elucidate the laterally periodic segregation profile of PtRh(111) caused by *h*-BN. Our results perfectly confirm the experiment: Beneath pores of the nanomesh the segregation profile shows a strong Rh enrichment, while beneath wires the topmost layer favors platinum.

To quantify the Pt/Rh content per surface layer, we conducted Monte-Carlo simulations accommodating the chemical potential difference of the alloy constituents and the quenched Pt/Rh interdiffusion at low temperatures. In agreement with the experiment, we find that a further Pt enrichment in the top surface layers is favored at elevated temperatures.

[1] Kerschler et al., Phys. Rev. B **86**, 195420 (2012)

[2] Stania et al., submitted.

O 49.10 Tue 18:15 Poster E

Vacuum Synthesis of Magnetic Aluminum Phthalocyanine on Au(111) — CHAO LI and ●YONGFENG WANG — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China.

Air-unstable magnetic aluminum phthalocyanine (AlPc) molecules are prepared by an on-surface metalation reaction of phthalocyanine with aluminum (Al) atoms on Au(111) in ultrahigh vacuum. STM/STS experiments and DFT calculations show that an unpaired spin is located on the conjugated isoindole lobes of the molecule rather than at the Al position. These results demonstrate the success of the vacuum synthesis of an air-unstable magnetic molecule. It is interesting

and important to synthesize other pristine reactive MPc molecules and study their particular properties.

O 49.11 Tue 18:15 Poster E

A first-principles study of chemo-mechanical coupling for hydrogen on Ir(111) — ●ANJA MICHL, GREGOR FELDBAUER, and STEFAN MÜLLER — Hamburg University of Technology, Institute of Advanced Ceramics

Mechanical strain has an impact on the energetics of adsorption and transition states of chemical reactions on surfaces. Therefore, it is possible to tune the reactivity by changing the lattice parameter of the catalyst's surface. Since the interaction of hydrogen with iridium surfaces is relevant for a wide range of catalytic reactions, H/Ir(111) was chosen as a model system.

We use density functional theory (DFT) in conjunction with the cluster-expansion method to investigate the energetics of hydrogen adsorption on Ir(111) and its response to strain. DFT data for various configurations with different H coverages and adsorption sites serve as input for a cluster expansion. This approach allows for an exhaustive scan of the configuration space and thus to identify the most favorable structures as a function of coverage. While top-site adsorption is preferred, the system exhibits only a weak tendency for ordering. Moreover, biaxial strain in the surface plane is applied to different configurations to elucidate the correlation between adsorption energies and mechanical strain. In order to gain further insight into the underlying mechanisms, we also analyze the adsorbate induced work function change and its relation to charge transfer.

O 49.12 Tue 18:15 Poster E

High precision structuring of plan and cylindrical metal surfaces of for printing and packaging applications — ●LUKAS BAYER¹, MARIO GATTNER², PIERRE LORENZ¹, MARTIN EHRHARDT¹, KLAUS ZIMMER¹, and MICHAEL MÄSER³ — ¹Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany — ²Beuth Hochschule für Technik Berlin University of Applied Science, Luxemburger Straße 10, 13353 Berlin, Germany — ³SWG, Badstraße 9, 09669 Frankenberg, Germany

Advanced printing and packaging technologies request improvements in resolution and quality as well as in environmental sustainability due to applications for functional surfaces, security printing and advertising. The conventional laser-based production of such tools is subjected to melting effects causing strongly limited results and cost-intensive post processing. Hence, ultra-short laser pulses were used for engraving that can reduce or eliminate those problems. However, high power 1064 nm ps-laser sources must be combined with high speed scanning to avoid heat accumulation and particles shielding. Finally two applications are presented to demonstrate the possibilities of laser engraving. The first shows the production of high quality intaglio printing plates. Here not only the plates but also the printing results are investigated. The second application is the production of laser-induced periodic surface structure (LIPSS). This ripple structures can be produced in short time on large scale cylinders and the distinct optical diffraction effect of the resultant structures can be used for different applications.

O 49.13 Tue 18:15 Poster E

Design and installation of a thermal hydrogen atom source — ●MARIE SCHMITZ¹, DOMINIQUE KRULL^{1,2}, CHRISTOPH KEUTNER^{1,2}, PHILIPP ESPETER^{1,2}, ULF BERGES^{1,2}, and CARSTEN WESTPHAL^{1,2} — ¹Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund, Germany — ²DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund, Germany

We report on the design and installation of a thermal hydrogen atom source.

The source includes a tungsten capillary, heated radiatively by electron bombardment.

Hydrogen atoms are of substantial interest in surface science, especially for thin layer experiments, semiconductor materials science, and technology.

Atomic hydrogen is not only used for surface cleaning, but also to cover surfaces in studies of adsorption, recombination, and desorption. Furthermore, it is crucial for growing layers within thin film deposition.

In this study, the hydrogen source is installed in a UHV-chamber for experimental analysis of adsorption and interaction on Si(100) surfaces, observed by scanning tunneling microscopy (STM). It can also be used for the passivation of Si-substrates. A residual gas analyser is used to assess the performance of the source.