

## O 44: Metal Substrates: Structure, Epitaxy and Growth

Time: Tuesday 18:30–20:30

Location: P1A

O 44.1 Tue 18:30 P1A

**On the Thin Film Growth of Two Isomers of Dibenzopentacene on Ag(111)** — ●TOBIAS HUEMPFNER, LENNART VORBRINK, FELIX OTTO, MAXIMILIAN SCHAAL, BERND SCHROETER, ROMAN FORKER, and TORSTEN FRITZ — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

We report on the thin film growth of two isomers of the molecule dibenzopentacene (DBPen) deposited on a Ag(111) surface. The different molecular configurations, namely 1,2,8,9-DBPen (trans) and 1,2:10,11-DBPen (cis), differ only in the position of one of the additional benzene rings relative to the pentacene backbone. The optical properties during the growth were measured via differential reflectance spectroscopy (DRS) and interpreted by comparing to calculated excitation spectra obtained from time-dependent density functional theory (TD-DFT) of the isolated molecule. Furthermore, the films were characterized structurally via low-energy electron diffraction (LEED) and low-temperature scanning tunneling microscopy (STM) for different film thicknesses. While the optical properties of the two isomers hardly differ in the visible region, the structural properties vary significantly. The first monolayer of the trans-isomer grows in a highly ordered structure. In contrast, for the monolayer of cis-DBPen no well-defined adlayer exhibiting translational order was observed, although first-order LEED-spots occur owing to the preferential molecular alignment with the substrate.

O 44.2 Tue 18:30 P1A

**Surface Chemistry and Growth of SnCl<sub>2</sub>Pc on Ag(111)** — ●CHRISTIAN ZWICK, ROMAN FORKER, and TORSTEN FRITZ — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Tin(IV) phthalocyanine dichloride (SnCl<sub>2</sub>Pc) is an n-type semiconductor already used in organic field-effect transistors [1], but still very little is known about the actual interface formation when SnCl<sub>2</sub>Pc is deposited onto a substrate. This molecule is not planar owing to its two protruding Cl atoms. These are known to act as spacers in bulk crystal formation, and thereby significantly influence the intermolecular orbital overlap. On the other hand, Cl is known to be highly reactive in contact with certain metals, for example Ag. Hence, these two opposing effects draw attention towards the adsorption behavior of SnCl<sub>2</sub>Pc on a silver substrate. Here we report on the observed surface chemistry, the partial dechlorination of SnCl<sub>2</sub>Pc on Ag(111), and its role concerning the interface formation on Ag(111). Using in situ differential reflectance spectroscopy (DRS), low-energy electron diffraction (LEED) and low-temperature scanning tunneling microscopy (STM), we investigate the optical and structural properties of SnCl<sub>2</sub>Pc/Ag(111) for effective layer thicknesses up to 2 monolayers. [1] SK. Md. Obaidulla *et al.*, Appl. Phys. Lett. **104**, 213302 (2014).

O 44.3 Tue 18:30 P1A

**X-ray spectroscopy of thin film free-base corroles on Ag(111)** — HAZEM ALDAHAK<sup>1</sup>, MATEUSZ PASZKIEWICZ<sup>2</sup>, FRANCESCO ALLEGRETTI<sup>2</sup>, STEFANO TEBI<sup>3</sup>, ●WOLF GERO SCHMIDT<sup>1</sup>, STEFAN MÜLLEGER<sup>3</sup>, FLORIAN KLAPPENBERGER<sup>2</sup>, EVA RAULS<sup>1</sup>, and UWE GERSTMANN<sup>1</sup> — <sup>1</sup>Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany — <sup>2</sup>Physik-Department E20, Technische Universität München, James-Frank-Str. 1, D-85748 Garching, Germany — <sup>3</sup>Institute of Semiconductor and Solid State Physics, Johannes Kepler University, Linz, Austria.

Corroles are structurally closely related to the well-known porphyrins that possess aromatic tetrapyrrole macrocycles. Compared to the corresponding porphyrins, they have a lower symmetry and a smaller, congested cavity. The latter property and the resulting changes in the electronic structure promote the stabilization of metal ions in exceptionally high oxidation states. X-ray spectroscopy is a powerful tool for the investigation of functional interfaces. For corrolic species, however, the required reference data are missing. The X-ray fingerprints are simulated using the continued-fraction approach within density functional theory (DFT) for extended, (quasi-)periodic molecular structures. The excellent agreement between experimental and theoretical spectra enables a thorough interpretation of the detailed spectral features and proves an accurate description of the free-base corrole electronic struc-

ture within the present DFT approach. The present study provides an ideal starting point for the comprehensive understanding of the complex chemistry of corroles in the adsorbed state.

O 44.4 Tue 18:30 P1A

**Comparison of tin(II)- and lead(II)-phthalocyanine layers adsorbed on 1 ML PTCDA/Ag(111)** — ●PHILIPP MUELLER, MARCO GRUENEWALD, J. PEUKER, F. SOJKA, ROMAN FORKER, and TORSTEN FRITZ — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

We investigate the growth of ultrathin, highly ordered layers of the shuttlecock-shaped molecules tin(II)-phthalocyanines (SnPc) and lead(II)-phthalocyanines (PbPc) on top of one monolayer 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on Ag(111). The films have been characterized structurally by means of low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) as well as optically using differential reflectance spectroscopy (DRS). We find that neither their lateral structures formed nor their fingerprints in optical absorption allow distinguishing between both molecules when they are adsorbed on 1 ML PTCDA/Ag(111). In fact, the condensed phases of both systems yield the same commensurate registries with respect to PTCDA. Even the structures formed for higher film thicknesses are rather similar. Also their fingerprints in optical absorption are almost identical. Here we report a possibility of distinguishing both molecules in the respective monolayer phases by means of their different STM-tip-induced switching behavior: SnPc can easily be switched from Sn-down to Sn-up configuration and vice versa by applying tip voltage pulses, whereas PbPc did not respond to our switching attempts. This provides one method of chemical identification on the molecular scale.

O 44.5 Tue 18:30 P1A

**On the adsorption behavior of cyano-functionalized 2H-tetraphenylporphyrin derivatives on Cu(111): a scanning tunneling microscopy study** — ●MANUEL MEUSEL, MICHAEL LEPPER, JULIA KÖBL, MICHAEL STARK, HANS-PETER STEINRÜCK, and HUBERTUS MARBACH — Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

One important objective within surface science is the bottom-up fabrication of functional nanostructures via self-assembly of molecular building blocks. In this context, we study porphyrins as prototype functional molecules on surfaces and target the controlled modification to tweak their adsorption behavior. One method to tailor the properties of porphyrins is the attachment of functional groups. In this study, we compare the adsorption behavior of differently cyano-functionalized 2H-tetraphenylporphyrin (2H-TTP) derivatives on Cu(111) under ultra-high vacuum conditions by scanning tunneling microscopy. We observe a variety of binding motives ranging from isolated individual molecules over dimer formation to one-dimensional molecular chains. The corresponding adsorption behaviors can be correlated with the number and symmetry of the cyano groups. The results show that the functionalization of supramolecular building blocks is a well-suited method to influence the adsorption behavior. Latest results will be presented and discussed. This work was funded through DFG FOR 1878 (funCOS) under grant MA 4246/2 -1.

O 44.6 Tue 18:30 P1A

**Silver segregation near oxygen chain structures on a gold-silver alloy surface: A cluster expansion study combined with ab initio MD simulations** — ●SANDRA HOPPE<sup>1</sup>, YONG LI<sup>2</sup>, LYUDMILA V. MOSKALEVA<sup>2</sup>, and STEFAN MÜLLER<sup>1</sup> — <sup>1</sup>Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — <sup>2</sup>Institute of Applied and Physical Chemistry and Center for Environmental Research, University of Bremen, Bremen, Germany

The high catalytic activity of nanoporous gold has been attributed to its residual silver content originating from the parent Ag-Au alloy. Therefore, the knowledge about the thermodynamically stable positions of silver atoms on the surface of nanoporous gold is crucial for understanding elementary stages of various catalytic processes, in particular, the chemical nature and adsorption properties of active oxygen species. In this study, we investigate the surface segregation of silver in the presence of atomic-oxygen adsorbates arranged in chains on the

stepped and kinked Au(321) surface. Remarkably, we find that up to very high silver surface concentrations, the silver atoms do not occupy positions within the oxide chain, but prefer locations next to it. We identify two effects responsible for this behavior. First, gold is stabilized within the chain by partially covalent bonds with oxygen. Second, silver located in the vicinity of the chain binds stronger to oxygen than gold at the same position does. Ab initio molecular dynamics simulations support our conclusions and reveal that not only silver atoms but also the entire oxide chains may diffuse on the surface to maximize the binding contacts between adjacent silver and oxygen atoms.

O 44.7 Tue 18:30 P1A

**Low temperature bias assisted RF-sputtering process for heteroepitaxial growth of iridium on various oxide substrates**

— •FRANK MEYER<sup>1</sup>, EDUARD REISACHER<sup>1</sup>, JOHANNES PREUSSNER<sup>1</sup>, ANDREAS GRAFF<sup>2</sup>, ALEXANDER FROMM<sup>1</sup>, LUKAS GRÖNER<sup>1</sup>, and FRANK BURMEISTER<sup>1</sup> — <sup>1</sup>Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg i. Br., Germany — <sup>2</sup>Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen IMWS, Halle, Germany

By using the so called bias enhanced nucleation process followed by a growth process in an ellipsoidal reactor, artificial CVD-diamond can be grown on many refractory metal surfaces. The fabrication of single crystal diamond, however requires well-oriented (mostly [100]) substrates with lattice constants close to diamond and high chemical and thermal stability. A suitable candidate is iridium, deposited e.g. on A-plane sapphire [1], yttrium stabilized zirconia (YSZ) (100) [2] or lanthanum aluminate (LaAlO<sub>3</sub>) (100). In related works, we've already established a low-temperature deposition process for the heteroepitaxial growth of iridium (100) on A-plane sapphire. In this study we investigated the influence of different oxidic substrate surfaces on the iridium film characteristics with respect to surface morphology

and growth behavior by characterizing the surface morphology, crystallinity, and growth defects of iridium on LaAlO<sub>3</sub> and YSZ with X-ray diffraction, electron backscattering diffraction, and high resolution transmission electron microscopy. [1] Z. Dai et al., Appl. Phys. Lett., 82, 3847 (2003), [2] S. Gsell et al., Appl. Phys. Lett., 84, 4541 (2004)

O 44.8 Tue 18:30 P1A

**Simulation of TiN crystal growth - a combined ReaxFF+ and Monto-Carlo study.**

— •STEPHAN PFADENHAUER<sup>1</sup> and ROMAN LEITSMANN<sup>1,2,3</sup> — <sup>1</sup>AQcomputare GmbH, Annaberger Straße 240, 09125 Chemnitz Germany — <sup>2</sup>Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz Germany — <sup>3</sup>Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01069 Dresden, Germany

In order to simulate the crystal growth process of TiN on metal substrates one has to treat simultaneously chemical process at very short time scales on the one hand and slow deposition rates on the other hand. To achieve this goal we have combined the reactive force field method ReaxFF+ with a Monte-Carlo approach to simulate the growth of TiN on different metal substrates.

A reliable ReaxFF+ parameter set for titanium und nitrogen has been obtained using the scheme described in [1]. For the investigated metal substrates different growth patterns - namely Frank-van-der-Merwe and Volmer-Weber - could be observed. The obtained results are consistent with [2]. Furthermore, a direct comparison of our theoretical predictions with experimental results [3] could be achieved by calculating a XRD spectra of the obtained structures.

[1] Oliver Böhm et al, The Journal of Physical Chemistry C 2016 120 (20), 10849-10856 [2] Titanitrid- und Titan-Schichten für die Nano-Elektromechanik, Marcus Pritschow, Dissertation 2007 [3] H. Z. Wu et al, Thin Solid Films, 191(1990)