

O 19: Metal substrates: Adsorption of O / H and inorganic molecules II

Time: Monday 17:15–19:00

Location: WIL A317

O 19.1 Mon 17:15 WIL A317

Hydrogen adsorption on sulfur- and chlorine-precovered Pd(100) studied by ab initio molecular dynamics simulations

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The influence of coadsorbates on the adsorption properties of metal surfaces is of considerable technological and fundamental importance. For example, sulfur is well-known as a catalyst poison, i.e. its presence reduces the activity of catalysts. On the other hand, the electrochemical metal-liquid interface is typically characterized by halogen adsorption from the electrolyte. As a model system to understand the effect of such coadsorbates, the adsorption of hydrogen on sulfur- and chlorine-precovered Pd(100) has been studied by ab initio molecular dynamics simulations. The sticking probability has been determined as a function of the kinetic energy, the angle of incidence and the internal degrees of freedom of the impinging H₂ molecules. The results will also be compared to previous quantum dynamical studies on a fixed substrate [1]. It will be shown that sulfur and chlorine affect the adsorption properties of Pd(100) in a rather similar way, but there are also characteristic differences.

[1] A. Groß and M. Scheffler, Phys. Rev. B **61**, 8425 (2000).

O 19.2 Mon 17:30 WIL A317

The influence of monomer size on reaction kinetics and defect density for the synthesis of 2D Covalent Organic Frameworks: a combined Scanning-Tunneling-Microscopy and Density Functional Theory study— ●STEFAN SCHLÖGL^{1,2}, WOLFGANG M. HECKL^{2,3}, and MARKUS LACKINGER^{1,2} — ¹Geowissenschaftliches Institut & CeNS, LMU München — ²Deutsches Museum, München — ³School of Education, Department Physik, TU München

In order to tailor mechanical, chemical, and electronic properties of two-dimensional polymers, a bottom-up surface mediated fabrication process under controlled conditions is very promising. On one hand covalent intermolecular bonds give rise to the strength of 2D materials, on the other hand their irreversible character renders growth associated structural defects permanent. In order to control 'covalent self-assembly', a fundamental understanding of reaction kinetics and defect energetics is necessary.

In this contribution, we study and compare the surface mediated polymerization of 1,3,5-Triiodobenzene (TIB) and 1,3,5-Tris-(4-bromophenyl)benzene (TBPB). Deposition of the monomers onto dense packed metal surfaces under UHV conditions results in full dehalogenation and subsequent addition of the radicals into covalent aggregates. In this talk, we will address the fate of the split-off halogen atom, the topology of resulting covalent aggregates, the role of the organic backbone, and the influence of thermal after-treatments. The structures and energetics are analyzed and discussed by Scanning Tunneling Microscopy and Density Functional Theory calculations.

O 19.3 Mon 17:45 WIL A317

Interaction of H₂O molecules with Fe films investigated with metastable induced electron spectroscopy— ●KAI VOLGMANN^{1,2}, FLORIAN VOIGTS², and WOLFGANG MAUS-FRIEDRICHS^{2,3} — ¹Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover — ²Institut für Physik u. Phys. Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — ³Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld

The formation of an oxide layer on Fe films upon the interaction with H₂O molecules is relevant for both applications and in surface science. This work examines the interaction of H₂O molecules with Fe films grown on a tungsten substrate. X-ray Photoelectron Spectroscopy is used to determine the stoichiometry of the samples, while Ultraviolet Photoelectron Spectroscopy and Metastable Induced Electron Spectroscopy (MIES) are used to analyse their valence band region and to gain information about changes in the work function because of reactions on the surface. All measurements are done at room temperature. MIES is used as a very surface sensitive technique, especially towards hydroxide groups. Only after a high H₂O exposure, we observed the formation of OH groups. Our previous experiments reveal that a passivating oxide layer is formed during oxygen offer to a Fe surface [1]. A similar oxide layer growth may be observed during H₂O offer to iron.

This oxide layer forms prior to the development of any observable OH groups. [1] K. Volgmann, F. Voigts, W. Maus-Friedrichs, Surface Science, **604** (2010), 906-913

O 19.4 Mon 18:00 WIL A317

Constructing the Wetting Layer of H₂O on Pt(111)— ●SEBASTIAN STANDOP¹, GEORGIA LEWES-MALANDRAKIS¹, MARKUS MORGENSTERN², THOMAS MICHELY¹, and CARSTEN BUSSE¹ — ¹II. Physikalisches Institut, Universität zu Köln, Zùlpicher Straße 77, D-50937 Köln — ²II. Physikalisches Institut (IIB), RWTH Aachen, D-52056 Aachen

Adsorption of water molecules on Pt(111) leads to a number of complex superstructures in accordance with scattering experiments. A common and prominent feature of these layers are triangular shaped depressions. On the basis of density functional theory calculation these depressions were predicted to contain flat water molecule hexamers [1]. Through co-adsorption experiments with Xe and CO molecules and artificial manipulation using Scanning Tunneling Microscopy (STM) we directly show that the triangular depressions are indeed hexamers of flat lying water molecules rotated by about 30° with respect to the surrounding host structure of water molecules [2]. Under appropriate STM imaging conditions these hexamers act as nuclei for the growth of the $\sqrt{3} \times \sqrt{3}$ R30° water wetting layer, known to result from electron exposure in LEED experiments. Our observations explain how it is possible for the wetting layer to transform rapidly into this structure. Using graphene flakes grown by ethylene decomposition, we directly compare binding and structure of wetting layers on Pt(111) and on grapheme using thermal desorption spectroscopy and STM.

[1] S. Nie et al., PRL 105 (2010) 026102, [2] S. Standop et al., PRB 82 (2010) 161412(R)

O 19.5 Mon 18:15 WIL A317

Island growth of D₂O on Ag(111) at low temperatures

— ●SARAH-CHARLOTTA HEIDORN, CORD BERTRAM, and KARINA MORGENSTERN — Institut für Festkörperphysik, Abteilung ATMOS, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover

Water is well-known to form hydrogen-bonded networks on metal surfaces, even at low temperatures. We investigate the growth mechanism of D₂O in the submonolayer range on Ag(111) with a low-temperature scanning tunneling microscope. Nucleation and island formation are studied during non-equilibrium growth processes for D₂O pressures between 1·10⁻⁸ mbar and 1·10⁻⁶ mbar and sample temperatures between 17 K and 130 K. The island shapes are analyzed in dependence of temperature and deposition flux. At low deposition rates and low temperature, amorphous, round-shaped islands are formed. At high deposition rates and low temperature, the generated patterns are fractal. At low deposition rates and high temperature, compact islands are grown. Details of the observed structures and mechanism underlying the island formation will be discussed in the presentation.

O 19.6 Mon 18:30 WIL A317

Influencing the bonding and assembly of a multiterminal molecule on a metal surface— ●MAYA LUKAS^{1,2}, KERIN DÖSSEL^{1,2}, ALEXANDRINA SCHRAMM¹, KARIN FINK^{1,2}, OLAF FUHR^{1,2}, CHRISTOPHE STROH¹, MARCEL MAYOR^{1,2,3}, and HILBERT VON LÖHNESEN^{1,2,4} — ¹Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, D-76021 Karlsruhe — ²DFG Center of Functional Nanostructures (CFN), D-76049 Karlsruhe — ³University of Basel, Department of Chemistry, CH-4056 Basel — ⁴Karlsruhe Institute of Technology (KIT), Physics Institute and Institute for Solid State Physics, D-76049 Karlsruhe

The bond of a molecule to a metallic electrode is known to have a crucial influence on the molecular conductance. As electronic functionalities are integrated into molecules or several subunits are connected to a three-dimensional multiterminal molecule, it is not obvious that a "well-known" chemical linker group will lead to the bonding configuration known from simpler molecules.

We investigated a series of tripodal molecules on metal surfaces by STM. The chemical linker groups and the complex connecting the three wire-units are varied. We find that the position of molecules on the surface is governed by a subtle balance of intermolecular and molecule-surface interactions, partly in strong contrast to expectations. This

emphasizes the need to characterize the nature of molecule-electrode contacts along with the investigation of the electronic conductance.

O 19.7 Mon 18:45 WIL A317

CuN structures on Cu(110) — ●MARIELLA DENK, RICHARD DENK, MICHAEL HOHAGE, LIDONG SUN, and PETER ZEPPENFELD — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

Chemisorption of atomic nitrogen on Cu(110) leads, at a saturation coverage of $2/3$, to the formation of a well ordered Cu(110)-(2x3)N reconstruction upon annealing at 650 K [1], [2].

An in-depth study concerning the formation of the nitrogen induced reconstruction has been performed to address open questions regarding the exact structure of the surface at the atomic scale. In case

of an annealing temperature below 550 K, a precursory Cu-N phase which consists of elongated molecule-like structures, termed “CuN compounds”, has been found on the surface by Scanning Tunneling Microscopy (STM). The CuN compounds are characterised by their high mobility on the surface and have been found to be stable up to at least 550 K. The compounds are expected to play a crucial role in the formation of the final (2x3)N phase, as the Cu coverage of the surface layer is increased to $4/3$ compared to the pristine Cu(110) surface. A model structure for the CuN compounds has been derived on the basis of the STM images. The CuN compounds may consist of Cu₄N subunits, which appear as bright dots in the STM images.

[1] D. Heskett, A. Baddorf and E. W. Plummer, Surf. Sci., 195, p. 94 (1988)

[2] A. P. Baddorf and D. M. Zehner, Surf. Sci., 238, p. 255 (1990)