

O 41: Metal Substrates: Adsorption II

Time: Wednesday 15:45–17:30

Location: H39

O 41.1 Wed 15:45 H39

Controllable molecular registration state in self-assembly of 3(5)-(9-anthryl) pyrazole molecule on Ag(111) — •RUIFEN DOU¹, ARNO TILKORN¹, DINGYONG ZHONG¹, WENCHONG WANG¹, YUE WANG², LIFENG CHI¹, and HARALD FUCHS¹ — ¹Physikalisches Institut, Universität Muenster, 48149 Muenster, Germany — ²Key Laboratory for Supramolecular Structure and Materials of Ministry of Education, Jilin University, Changchun 130012, China

The highly-ordered molecular structures of 3(5)-(9-anthryl) pyrazole (ANP) have been investigated on Ag(111) by low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM). Through tailoring film preparation, two different superstructures, α and β , corresponding to two different molecular registration states have been obtained on Ag(111). At the low substrate temperature (229 K), the structure α can be prepared, in which the ANP molecule is adsorbed on the surface with the anthryl-group plane tilting in respect to the substrate surface. After annealing the sample to room temperature, it is found that the structure α gradually evolves into the structure β with four molecules bound together through the hydrogen bonds among them and the anthryl-group plane parallel to the substrate surface to compromise to forming hydrogen bonds. Our analysis reveals a fact that the adsorbate-substrate interaction dominated in the structure α can change into the hydrogen-bonds prevailed over the structure β as mediating the growth temperature, which is responsible for the variation in the molecular registration states from the anthryl-group plane tilting with the substrate surface to parallel to surface.

O 41.2 Wed 16:00 H39

Different assemblies of a phthalocyanine derivative on metal surfaces — •TOMAS SAMUELY¹, MEIKE STÖHR¹, THOMAS JUNG², MARCO HAAS³, SHI-XIA LIU³, and SILVIO DECURTINS³ — ¹Institut für Physik, Universität Basel, Schweiz — ²Paul Scherrer Institut, Villigen, Schweiz — ³Departement für Chemie und Biochemie, Universität Bern, Schweiz

Phthalocyanines have been the subject of intense studies due to their wide range of optical, structural and electronic properties arising from their large π -conjugated system and their assembling into co-facially-stacked arrays. We studied a phthalocyanine derivative which features eight ditertiarybutylphenyl substituents attached over an oxygen atom to the peripheral phenyl rings. Ordered assemblies of the derivative were prepared by thermal evaporation, whereas Ag(111) and Au(111) were used as substrates, respectively. The investigations were carried out by means of STM at various temperatures. For coverage less than one monolayer, two different assemblies were observed. At room temperature, a mobile phase was detected next to the ordered islands. Increasing the coverage results in only one ordered phase, while the second layer begins to form before a full monolayer is completed. Applying different bias voltages had a vast effect on the appearance of the imaged molecules. The assembled domains of the derivative could be suitable for subsequent deposition of various molecules: complexes with interesting magnetic, electronic, redox or photo-active properties could be formed.

O 41.3 Wed 16:15 H39

LEED investigations on SAM of biphenylthiols on Au (111) surfaces — •MICHEL KAZEMPOOR and GERHARD PIRUG — Institut für Bio- und Nanosysteme (IBN3) and Center of Nanoelectronic Systems for Information Technology (CNI), Forschungszentrum Jülich GmbH, D-52425 Jülich

Organic molecules of 4'-methyl-1,1'-biphenyl-4-alkanethiols (BP_n, n = number of alkane spacer) are known to form well ordered so called self-assembled monolayer (SAM) structures on metal surfaces. Characterizing the ordering and packing behaviour of BP_n is essential for the understanding of the electronic and optical properties. BP_n structures are predominantly characterized by STM measurements. In addition a $(2\sqrt{3} \times \sqrt{3})$ structure has been proposed for BP3, based on a diffuse LEED pattern (Azzam et. al., Langmuir 19 (2003) 8262). However, there is still an ongoing discussion about different unit cells of BP_n molecules on Au (111). In principal, LEED should allow a reliable identification of the unit cell and the determination of its lattice vectors. Therefore we studied the adsorption of BP3 and BP4 on Au(111) surfaces using a micro channel plate (MCP) LEED system, which al-

lows a more gentle examination with reduced electron beam current in the pA regime. The samples were exposed at room temperature to BP_n molecules by gas phase deposition. After subsequent annealing up to 423 K we observed unit cells corresponding to a $c(16 \times 2\sqrt{3})$ and $(5\sqrt{3} \times \sqrt{3})$ structure for BP3 and BP4, respectively. Structure models will be discussed under consideration of recent STM findings.

O 41.4 Wed 16:30 H39

Temperature programmed desorption of oligopyridine molecules on HOPG — •MICHAEL ROOS, HARRY E. HOSTER, and R. JÜRGEN BEHM — Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm

As shown in previous STM studies, bis(terpyridine)derivatives (BTP) form highly ordered hydrogen bonded networks on HOPG at the solid/liquid and the solid/gas interface. A reliable method to attain these monolayer networks in UHV is vapor deposition, followed by the desorption of excess material. In this study, we systematically investigate the thermal desorption behavior for varying initial BTP coverage. For a comprehensive understanding, the experimental spectra are compared with spectra attained by simulations based on different models, and are in addition linked to STM images of BTP layers on HOPG with different coverage.

O 41.5 Wed 16:45 H39

Formation of tetrachloroplatinate complexes on Pt(110). — ENRICO DONÀ¹, •MICHAEL CORDIN¹, CESARE FRANCHINI², JOSEF REDINGER², and ERMINDAL BERTEL¹ — ¹Institute for Physical Chemistry, University of Innsbruck, Innrain 52a, A-6020 Innsbruck, Austria — ²Center for Computational Material Science, Gumpendorferstraße 1A, A-1060 Vienna, Austria

The chemisorption of Cl and Br on Pt(110) has been studied as a function of coverage by variable-temperature scanning tunneling microscopy (VT-STM) and low-energy electron diffraction (LEED). For a coverage (Θ) of 0.5 monolayers (ML) Cl and Br form a $p(2 \times 1)$ and a $c(2 \times 2)$ structure, respectively, occupying each second short-bridge (SB) site on the close-packed Pt-rows of the (1×1) -Pt(110) surface. Increasing the coverage leads to the formation of a (3×1) and a (4×1) phase for $\Theta = 0.66$ ML and $\Theta = 0.75$ ML respectively, where both SB and long-bridge (LB) sites are occupied. While these two structures are stable for Br, they are only metastable in the case of Cl. Upon soft annealing ($300\text{K} < T < 670\text{K}$) a transition into a phase with (4×2) periodicity is observed. This phase is characterized by cross-shaped structures, imaged as "clusters" with five bright protrusions by STM. An interpretation of these protrusions entirely in terms of Cl atoms can be excluded by coverage considerations. On the basis of both, experimental arguments and theoretical results the clusters can be identified as tetrachloroplatinate complexes, with the central Pt atom occupying a four-fold hollow site. This implies the onset of Cl induced corrosion on the Pt(110) surface.

O 41.6 Wed 17:00 H39

Racemic mixing in 2D molecular self-assembly — •THORSTEN KAMPEN¹, ROCIO CORTES², PHILIPP MARTIN SCHMIDT¹, HUGO DIL¹, ARANTZAZU MASCARAQUE², and KARSTEN HORN¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ²Depto. Física de Materiales, Universidad Complutense de Madrid, Madrid, Spain

Inherently achiral molecules may become chiral when adsorbed on surfaces, through the loss of symmetry elements in a 2D structure. Here we show how this effect leads to chiral supramolecular assemblies in 4,4'-stilbene dicarboxylic acid (DCSB) on Cu(110) using scanning tunneling microscopy. DCSB molecules are found to adsorb on Cu(110) surface via bonding of all four oxygen atoms of the deprotonated carboxylic end-groups to next-neighbour Cu atoms. In the 2D environment of a surface the molecule assumes to enantiomorphous orientation, that is, the molecules become chiral. Due to the chiral character of the adsorbed molecule and intermolecular interactions two chiral adsorption phases are found, namely a cubic and a herringbone phase. While in the metastable "rectangular" phase consists only of right- or left-handed molecules, i.e. each domain is enantiomorphously pure, the "herringbone" phase is a "racemic mixture" built up of left- and right-handed molecules. The formation of the herringbone phase is

thermodynamically preferred since it decreases the free enthalpy of the self-assembled DCSB islands.

O 41.7 Wed 17:15 H39

On the accuracy of first-principles lateral interactions: Oxygen at Pd(100) — •YONGSHENG ZHANG, VOLKER BLUM, and KARSTEN REUTER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

We employ a first-principles lattice-gas Hamiltonian (LGH) approach to determine the lateral interactions between O atoms adsorbed on the Pd(100) surface. With these interactions we obtain an ordering behavior at low coverages that is in quantitative agreement with ex-

perimental data. Uncertainties in our approach arise from the finite LGH expansion and from the approximate exchange-correlation (xc) functional underlying the employed density-functional theory energetics. We carefully scrutinize these uncertainties and conclude that they primarily affect the on-site energy, which rationalizes the agreement with the experimental data. We also investigate the validity of the frequently applied assumption that the ordering energies can be represented by a sum of pair terms. Restricting our LGH expansion to just pairwise lateral interactions, we find that this results in effective interactions which contain spurious contributions that are notably larger than any of the uncertainties e.g. due to the approximate xc functional.