

strate, maximizing the number of N atoms being adsorbed a-top of substrate atoms [3,4]. This simple model fully explains the resulting molecular networks on Ag(111) and Au(111). Its suitability for rationalizing monolayer networks on the (100) surfaces of Ag and Au is tested.

[1] U.Ziener et al., Chem.Eur.J. 8, 951, 2002

[2] C. Meier et al., J.Phys.Chem.B 109, 21015, 2005

[3] H.E. Hoster et al., Langmuir 23, 11570, 2007

[4] M.Roos et al., Phys. Chem. Chem. Phys. 9, 5672, 2007

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Substrate-induced molecular orientation of ClGa-phthalocyanine studied by MAES and UPS — •T. HOSOKAI¹, A. GERLACH¹, H. MACHIDA², Y. SUZUKI², S. DUHM², N. KOCH³, S. KERA², U. NOBUO², and F. SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, Germany — ²Graduate School of Advanced Integration Science, Chiba university, Japan — ³Institut für Physik, Humboldt-Universität zu Berlin, Germany

Understanding the substrate-molecule interactions is a prerequisite for the control of organic film growth. Here we report the substrate-induced molecular orientation of the non-planar chlorogallium phthalocyanine (ClGaPc) molecules on Cu(111) and graphite by means of UPS and metastable atom electron spectroscopy (MAES). In the monolayer MAES shows distinctively different features on Cu(111) and graphite: On the Cu(111) surface bands corresponding to non-bonding orbitals of the Cl-atom, i.e. those largely distributed parallel and perpendicular to the molecular plane, are not observed, whereas on the graphite both bands can be found. Because of the high surface sensitivity of the MAES technique these results indicate a different orientation of ClGaPc on Cu(111) and graphite. On Cu(111) ClGaPc molecules orient with the Cl-atom directed towards the Cu surface, whereas on the graphite ClGaPc molecules orient with the Cl-atom directed towards the vacuum. Although it is often found that Pc molecules orient to maximize the overlap with the substrate electrons, we show that the central atoms also play a role for the orientation of polar Pc molecules on different substrates.

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Organic and Metal-Organic Networks Based on NC - Ph - CN — •MATTHIAS MARSCHALL¹, JOACHIM REICHERT¹, WILLI AUWÄRTER¹, KNUD SEUFERT¹, FLORIAN KLAPPENBERGER¹, SVETLANA KLYATSAKYA², MARIO RUBEN², ALEXANDER WEBER-BARGIONI³, and JOHANNES V. BARTH¹ — ¹Physik Department, TU München, Germany — ²Institut für Nanotechnologie, Karlsruhe, Germany — ³Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada

The assembly of metal-organic networks is a promising method to fabricate well defined, highly stable supramolecular nanostructures. We investigated the molecular structures by means of Scanning Tunneling Microscopy (STM) and Near Edge X-ray Adsorption Fine Structure (NEXAFS). A systematic investigation of such a metal organic network on Ag(111) and Cu(111) revealed several highly ordered and complex networks. The complexity and the variety of the observed molecular networks is presumably caused by the numerous degrees of freedom of the investigated molecules. Upon adsorption the molecules obtain a surface induced chirality and their supramolecular assemblies were studied in dependence of the coverage and preparation parameters. At certain conditions even highly stable macromolecules were formed.

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Conformation-controlled networking of H-bonded assemblies on surfaces — MANFRED MATENA¹, MIHAELA ENACHE¹, ANNA LLANES-PALLAS², DAVIDE BONIFAZI², THOMAS A. JUNG³, and •MEIKE STÖHR¹ — ¹University of Basel, Switzerland — ²University of Trieste, Italy — ³Paul-Scherrer-Institute, Switzerland

In order to prepare networks that could undergo phase transitions through a thermally-induced inversion of the molecular conformation leading to a variation of the intermolecular interactions, directional intermolecular forces can be regarded as promising candidates. In particular, H-bonding interactions will be exploited since their intermolecular interaction strength and geometry can be controlled by the number and arrangement of available H-bonding donor or acceptor moieties. We studied the 2D self-organization of a conjugated molecule bearing terminal 2,6-di(acylamino)pyridine moieties [1], which are well-known to form H-bonds, on a Ag(111) surface by STM. The hexagonal porous network, which is formed for room temperature deposition, is transformed into a close-packed rhombic pattern by a thermally induced

trans-cis inversion of the terminal groups. This transformation can be explained by the fact that the system wants to minimize its energy: at the same time the free surface energy is minimized while the number of H-bonds per terminal group is doubled from two to four. [1] A. Llanes-Pallas et al., Angew. Chem. Int. Ed. 2008, 47, 7726

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Porphine on Copper (110) - Adatoms make the difference — •ABEL ROBIN, MATTHEW STEPHEN DYER, SAM HAQ, MATS PERSSON, and RASMITA RAVAL — University of Liverpool, Liverpool, U.K.

We have studied the adsorption of free-base (H₂-P) and copper porphine (Cu-P) molecules on a Cu(110) surface.

Using scanning tunnelling microscopy (STM), reflection absorption infrared spectroscopy (RAIRS) and density functional theory (DFT) calculations we gain insight into the details driving the adsorption and organization of porphine molecules on metal surfaces. Interestingly, we find Cu-P molecules organizing upon adsorption in regular 2D assemblies whereas H₂-P only exhibits local ordering - even after annealing.

Experiments and calculations reveal another major difference between the two investigated systems, that is Cu-adatoms are attracted by H₂-P molecules; a process not observed for Cu-P adsorption. The adatom-attachment to H₂-P has - next to a number of interesting features - an influence on the ability of the porphine molecule to self-assemble into a regular structure. Metallization experiments of H₂-P do not lead to a significant improvement in molecular ordering, suggesting that the molecules do remember the original adsorption environment, therefore, the adatom attachment to H₂-P induces irreversible adsorption features.

Finally, we will present experimental and theoretical details of the highly organized Cu-P assembly. This structure is promising for technological applications since it does not require complicated functional groups attached to the porphyrin molecule for self-assembly.

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Self-assembly of highly ordered ferrocenyl nanostructures monitored by second harmonic generation — •ROBERT OSSIG¹, FLORIAN VOGEL¹, JENS HOSSBACH², ULRICH SIEMELING², and FRANK TRÄGER¹ — ¹Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel — ²Institut für Chemie and Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel

Custom-made molecules are ideal candidates to prepare stable self-assembled monolayers (SAM), which yield a wide range of applications, for example, as electronic or sensoric devices. In this contribution we present two recently synthesized ferrocene-functionalized tripod ligands with ferrocene as a reactive head group. The anchor groups of the ligands consist of three thioether-chains, each with 8 or 12 carbon atoms, respectively. Due to their structure, these molecules show a very high rigidity, which is an important pre-condition to form stable SAMs. To monitor the SAM formation, second harmonic generation (SHG) has been applied. The in situ SHG measurements show an initial fast decrease of the signal followed by a slower decrease as a function of immersion time. For a deeper insight of the involved processes, concentration dependent measurements have been performed. From these measurements we conclude that the SAM formation of both molecules occurs in a two-step process, a fast adsorption and a subsequent slow ordering. Further ex situ measurements (ellipsometry and scanning-tunneling-microscopy) confirm the formation of highly ordered monolayers.

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Diffusion of 1,4-butanedithiol on unreconstructed Au(111) — ANDREAS FRANKE and •ECKHARD PEHLKE — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

Extending our previous density-functional studies on the diffusion of alkanethiols on gold surfaces, we now focus on more complex sulfur anchored molecules diffusing on the unreconstructed Au(111) surface. As a benchmark system we choose 1,4-butanedithiol radicals (BDT: S-(CH₂)₄-S) which bind to the gold surface via two sulfur atoms. Molecules that bind to the surface via more than one site are expected to show diffusion properties beyond isotropic diffusion of single adsorbate atoms (e.g. [1]). Unreconstructed Au(111) exists under certain electrochemical conditions [2]. Density functional calculations are carried out using the VASP code by Hafner, Kresse *et al.* [3]. We compare various adsorption geometries of one BDT per (4x3) unit cell. For the most favourable geometry both S-atoms bind close to fcc-hollow sites with d_{S-S}=4.9Å. Taking the free, spinpolarized radical as reference, the