

O 37: Nanostructures at Surfaces III

Time: Tuesday 14:00–16:00

Location: S054

Invited Talk

O 37.1 Tue 14:00 S054

Metal Complexation of Sulfur on Coinage Metal Surfaces — ●PATRICIA THIEL¹, HOLLY WALEN¹, YOUSOO KIM², JUNEPYO OH², HYUN JIN YANG², and DA-JIANG LIU³ — ¹Iowa State University, Ames, Iowa USA — ²RIKEN Surface and Interface Science Laboratory, Wako, Saitama Japan — ³Ames Laboratory, Ames, Iowa USA

It is well known that chemisorbed chalcogens (oxygen, sulfur, selenium) on metal surfaces can induce or lift surface reconstruction. Less well-known is the fact that they can form metal-chalcogen complexes in which the source of metal atoms is the surface itself. Chalcogens can also impact the formation of metal nanostructures during metal deposition, as well as the stability of such nanostructures. We focus on behavior for sulfur (S) on Cu, Ag, and Au surfaces at low coverage (less than 0.1 monolayer) to avoid competition from surface reconstructions, and at low temperature to ensure immobilization. Under these conditions, complex formation is prominent for (111) surfaces of Cu and Ag, where they are proposed to result in a strong destabilization of monolayer islands by providing an alternative vehicle for efficient surface mass transport. For Au(111), S lifts the herringbone reconstruction, but does not produce complexes at low coverage. From these and other studies, a common structural motif emerges: a S-M-S staple-like unit that may be the dominant mass carrier at realistic temperature.

O 37.2 Tue 14:30 S054

Bromine-functionalized pyrene derivatives on metal surfaces: self-assembly and on-surface polymerization — ●BAY V. TRAN¹, TUAN ANH PHAM¹, FEI SONG¹, MANH THUONG NGUYEN², MILAN KIVALA³, LUTZ H. GADE⁴, and MEIKE STÖHR¹ — ¹Zernike Institute for Advanced Materials, University of Groningen, the Netherlands — ²The Abdus Salam International Center for Theoretical Physics, Italy — ³Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Germany — ⁴Anorganisch-Chemisches Institut, University of Heidelberg, Germany

On-surface polymerization under ultrahigh vacuum conditions, an alternative method compared to solution-based synthesis, is considered as a promising route in the bottom-up approach for constructing novel 1D and 2D materials. One of the intriguing materials which can be reliably obtained through on-surface polymerization based on Ullmann coupling is graphene nanoribbons. On the other hand, the controlled construction of sufficiently large 2D polymer networks still represents a challenge.

In this work, we report on both the self-assembly as well as the on-surface polymerization of bromine-functionalized pyrene derivatives on Au and Cu surfaces. The experiments (combining scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS) measurements) were performed under UHV conditions. Insight was obtained with respect to the structural and electronic properties of the as-deposited molecular monomers as well as the polymer networks generated through thermal annealing.

O 37.3 Tue 14:45 S054

Properties of self-assembled molecular structures formed by triarylamine derivatives on the KBr(001) surface — ●MARTIN GURRATH¹, CHRISTIAN STEINER², SABINE MAIER², and BERND MEYER¹ — ¹Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — ²Department of Physics, FAU Erlangen-Nürnberg

Non-contact AFM measurements show that triarylamine molecules with different functional end and side groups form a variety of 1D, 2D and 3D molecular assemblies on a KBr(001) substrate.

Using density-functional theory calculations we analyzed the molecule–molecule and molecule–substrate interactions that lead to the different growth modes.

First, a series of gas phase calculations of dimerization energies was performed to determine the molecule–molecule interaction strength for π -stacking and different hydrogen bonding motifs.

Then, the binding configuration and binding strength of the molecules on the KBr(001) substrate were determined by calculating the adsorption energies of single molecules and dimers.

Finally, monolayer arrangements were derived from the most favorable dimer structures.

The analysis of the different contributions to the adsorption energy allows us to rationalize why specific structures are formed by the molecules on KBr(001) and enables us to predict, how molecule–molecule and molecule–substrate interactions can be tuned in order to achieve 1D, 2D or 3D assembly of the molecules.

O 37.4 Tue 15:00 S054

Pyridyl-functionalized triarylamines self-assembled on Au(111) — ●LEONID SOLIANYK¹, JUAN CARLOS MORENO-LÓPEZ¹, JUN LI¹, STEFANO GOTTARDI¹, UTE MEINHARDT², MILAN KIVALA², and MEIKE STÖHR¹ — ¹Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — ²Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Germany

The formation of 2D molecular architectures on surfaces with both a predefined structure and desired catalytic/electronic properties is of potential interest for the usage in future nanoelectronic devices while self-assembly is a valuable tool for building these nanostructures. In our work, we investigated the self-assembly of pyridyl-functionalized triarylamines on the Au(111) surface by scanning tunneling microscopy at 77K and low energy electron diffraction. For deposition of submonolayer coverage onto Au(111) held at room temperature, a close-packed phase as well as a hexagonal nanoporous network were observed to co-exist. The close-packed phase is stabilized by hydrogen bonding while the nanoporous network is held together by metal-ligand interactions with native gold atom(s). Thermal annealing at 180°C results in the exclusive formation a second hexagonal nanoporous network with a larger pore size. The structural models and the intermolecular as well as the molecule substrate interactions are discussed for the mentioned structures.

O 37.5 Tue 15:15 S054

Self-assembly and on-surface coupling of a carbonyl-bridged triphenylamine derivative — ●MAXIMILIAN AMMON¹, ZECHAO YANG¹, TIM SANDER¹, PATRICK SEITZ¹, MILAN KIVALA², and SABINE MAIER¹ — ¹Department of Physics, FAU Erlangen-Nürnberg, Germany — ²Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg, Germany

Carbonyl-bridged triphenylamines are versatile planar π -systems for the formation of self-assembled and covalent honeycomb networks. Here we present a low-temperature scanning tunneling microscopy (STM) study on the self-assembly of amino-functionalized carbonyl-bridged triphenylamine derivatives. On Au(111), we find hydrogen-bonded porous networks after evaporation at room temperature. The bonding motif is similar to the one expected in gas phase, which demonstrates a weak molecule–surface interaction. In contrast on Ag(111) the strong interaction between the carbonyl groups and the metal promotes metal–ligand bonded networks at room temperature. The bridging carbonyl groups are suitable for Schiff-base type coupling reactions, which proceed, compared to the Ullmann coupling, at lower temperatures and leave no reaction side products on the surface [1]. We will discuss results on the covalent coupling by post annealing on both surfaces.

[1] S. Weigelt, C. Busse, C. Bombis, et al., *Angewandte Chemie* 119, 9387-9390 (2007)

O 37.6 Tue 15:30 S054

On-Surface Reductive Coupling of Aldehydes on Au(111) — ●OSCAR DÍAZ ARADO^{1,2}, HARRY MÖNIG^{1,2}, JÖRN-HOLGER FRANKE³, ALEXANDER TIMMER^{1,2}, PHILIPP HELD⁴, ARMIDO STUDER⁴, and HARALD FUCHS^{1,2} — ¹Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Deutschland — ²Center for Nanotechnology (CeNTech), Münster, Deutschland — ³Department of Physics, Université Libre de Bruxelles, Bruxelles, Belgium — ⁴Organisch-Chemisches Institut, Westfälische Wilhelms-Universität, Münster, Deutschland

The on-surface covalent coupling of organic molecules has been shown to have great potential as a promising approach for the bottom-up design of novel functional organic nanomaterials. Herein we report the C-C coupling of a terephthalaldehyde to produce polyphenylene vinylene oligomers on a Au(111) surface. Scanning tunneling microscopy and photoelectron spectroscopy experiments revealed the success of the covalent coupling after oxygen dissociation and subsequent desorption from the surface. These results, together with density functional theory calculations, showed that the typical diolate-mediated

reaction mechanism for the reductive coupling of carbonyls does not apply in this case. Instead, the reaction proceeds after C-H activation of the aldehyde moiety followed by a two-step deoxygenation process involving reactive sites on the substrate. With this on-surface synthesis approach, nanostructures with tunable optoelectronic properties on substrates can be developed, thus increasing the existing pool of suitable reactions for the growth of organic nanostructures on surfaces.

O 37.7 Tue 15:45 S054

Disaccharide self-assembly on metal surfaces — •SABINE ABB¹, LUDGER HARNAU¹, CHRISTIAN SCHÖN¹, JUAN CORTÉS², STEPHAN RAUSCHENBACH¹, and KLAUS KERN^{1,3} — ¹Max Planck Institute for solid state research, Stuttgart, Germany — ²Centre national de la recherche scientifique, LAAS, Toulouse France — ³Ecole Polytechnique Fédérale de Lausanne, Switzerland

Saccharides are involved in almost every biological process, including signal transducing, cell-adhesion and differentiation. However, the in-

teractions of saccharides adsorbed on a surface are not well understood on a molecular level. While the physical properties differ, the chemical structure of the monosaccharide building blocks is very similar - they all are structural and stereo isomers of the chemical sum formula $C_6H_{12}O_6$. Their vastly different behavior follows from rather subtle differences in the placement of OH-groups in the molecules.

In this study we investigate the self-assembly of the disaccharides sucrose and trehalose on Cu(100) by STM. Electropray ion beam deposition (ES-IBD) enables us to deposit these non-volatile molecules on the surface in ultra-high vacuum as negatively charged molecular ions. After deposition of a submonolayer coverage, we observe self-assembly of ordered 2D nanostructures as well as single molecules.

Based on our observations combined with molecular dynamics and energy landscape calculations, we can propose a model for the different disaccharide assemblies elucidating the influence of the isomers on the assembly behavior. Moreover, imaging of saccharides may be applicable to characterize branched polysaccharides.