O 100: Nanostructures at surfaces: Dots, particles, clusters II

Time: Thursday 15:00–17:00 Location: MA 141

Invited Talk O 100.1 Thu 15:00 MA 141

Suitably functionalized molecules on surface: from self-assembly to chemical reactions — •Shi-Xia Liu[1], Jascha Repp[2], Ernst Meyer[3], and Silvio Decurtins[1] — [1]Department of Chemistry and Biochemistry, University Bern, Freiestrasse 3, CH-3012 Bern, Switzerland — [2]Fakultaet fuer Physik, Universitaet Regensburg, D-93040 Regensburg, Germany — [3]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

A significant progress in the fields of surface science and nanotechnology has mainly been facilitated by single-molecule characterization techniques such as atomic force microscopy (AFM) and scanning tunneling microscopy (STM). Since chemical structures of individual molecules were resolved by AFM via the functionalization of the tip, identification of individual molecules on surfaces in various contexts including charge distribution, self-assembled structures and in situ visualization of on-surface chemical reaction products, have been highly motivated. This presentation puts emphasis on self-assembly and on-surface chemical reactions as well as electronic structures of appropriately functionalized molecules on surfaces.

O 100.2 Thu 15:30 MA 141

Studying Copper Growth on Zinc Oxide Utilizing a Neural Network Potential — •Martín Leandro Paleico and Jörg Behler — Universität Göttingen, Theoretische Chemie, Tammannstr. 6, 37077 Göttingen, Germany

The catalyst used in the industrial synthesis of methanol is composed of large copper and zinc oxide nanoparticles. Studying this system requires a simulation method capable of handling thousands of atoms with ab initio accuracy, but with computational efficiency comparable to classical force fields. For this purpose, a Neural Network Potential (NNP) has been trained to reproduce the potential energy surface of the system, making use of DFT calculations as reference data.

The current work focuses on the initial results for the ternary copper-zinc oxide system. Specifically, we investigate the growth of copper clusters and films on zinc oxide surfaces using basin hopping Monte Carlo simulations, utilizing a NNP to provide the required energies and forces.

O 100.3 Thu 15:45 MA 141

Highly reproducible surface-enhanced Raman scattering substrate for detection of phenolic pollutants — •Zhiqiang Zeng[1,2], Rui Xu[1], and Yong Lei[1] — [1]Technische Universität Ilmenau, 98693, Ilmenau, Germany. — [2]South China Normal University, 510006,Guangzhou, China.

The ordering degree of nanostructures is the key to determining the uniformity of surface enhanced Raman scattering (SERS). However, fabrication of large-area ordered nanostructures remains a challenge, especially with the ultrahigh-density. Here, we report a fabrication of large-area ultrahigh-density ordered Ag@Al2O3/Ag core-shell nanosphere (NS) arrays with tunable nanostructures. The ultrahigh-density ordered NS arrays over a large-area capability (diameter >4.0 cm) enable the uniform SERS signals with the relative standard deviation of less than 5%. The as-fabricated highly reproducible SERS substrate can be applied to detect trace phenolic pollutants in water. This work does not only provide a new route for synthesizing the ultrahigh-density ordered nanostructures, but also create a new class of SERS substrates with high sensitivity and excellent reproducibility.

O 100.4 Thu 16:00 MA 141

Probing water in confinement: a FT-RAIRS study of D2O nano clusters on a graphene-iridium moiré superstructure — •Robert Taube[1,2], Heshmat Noei[1], Marcus Creutzburg[1,2], and Andreas Stierle[1,2] — [1]DESY NanoLab, Deutsches Elektronensynchrotron (DESY), Hamburg, Germany — [2]Institute of Nanostructure- and Solid State Physics, University of Hamburg, Germany

Confined water is highly interesting due to its unique properties regarding the molecular arrangement, electronic structure and the interaction with its neighboring environment. In this work, periodically arranged D2O nano droplets of about 1 nm size were generated on top of a graphene-iridium moiré superstructure and probed by a state-of-the-art Fourier transformation reflection absorption infrared spectrometer under UHV at 117 K. The infrared bands of the heavy water clusters differ significantly from those observed for amorphous solid or crystalline phases, showing a characteristic gap at 2500 cm-1 between two stretching bands. Furthermore, two features of dangling deuterium atoms originating from undercoordinated water molecules are present in the infrared spectrum. One of these features is located at noticeable lower wavenumbers than reported thus far, which is presumably the result of a rearrangement effect triggered by the coalescence of the droplets. The other feature originates from threefold coordinated water molecules at the surface of the water clusters and the film.

O 100.5 Thu 16:15 MA 141

General geometry DLVO model for particle deposition on patterned surfaces — •Joakim Löfgren, Johnas Eklöf, Kasper Moth-Poulsen, and Paul Erhart — Chalmers University of Technology, Gothenburg, Sweden

Molecular electronics holds the key to the continued miniaturization of transistors and diodes, and thus provides a pathway to next-generation electronics. In this context, the deposition of nanoparticles onto surfaces with pre-patterned features is currently being investigated as an efficient means for assembling circuits. Here, predictive modeling of the deposition process would provide an invaluable tool in designing optimized manufacturing protocols. Deposition problems are typically studied within the confines of DLVO theory, where interaction energies are given by analytical expressions but the geometry of the interacting entities is restricted to simple shapes such as spherical particles or flat surfaces, which renders them unsuitable for describing the deposition on patterned surfaces.

In this work we seek to remedy this situation by combining a general-geometry extension of DLVO theory with a random sequential adsorption algorithm to model the deposition onto pre-patterned surfaces. Finite-size effects are taken into account by modeling the geometry of the surface as a collection of virtual particles that interact with the deposited particle. The interaction potentials are based on analytical DLVO expressions and are fitted to reproduce the proper limiting forms. Using this approach we are able to predict optimal surface patterns for capturing particles in various pre-defined geometries.

O 100.6 Thu 16:30 MA 141

STM investigation of cluster-molecule hybrid systems deposited on the Si(111)$\sqrt{3}\times\sqrt{3}$ R30°-B surface — •Tim Amrhein[1], Martin Franz[1], Andre Knecht[2], Andrea Merli[2], Carl Frederic Ussling[2], Thomas Möller[2], and Mario Dähne[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik — [2]Technische Universität Berlin, Institut für Optik und Atomare Physik

Porphyrin based cluster-molecule hybrid systems may find application in constructing two-dimensional cluster arrays formed on a porphyrin template as well as give rise to new materials with tailored optical or electronic properties.

Here the cluster-molecule hybrid system Cu_3(Cu(OEP)) was prepared by combining Cu(II)Octaethylporphyrin with Cu_3^+-clusters in the gas phase, followed by a characterisation using mass spectroscopy and optical excitation. For further investigations of the atomic structure and electronic properties using STM, they were deposited onto a Si(111)$\sqrt{3}\times\sqrt{3}$ R30°-B surface, which was used because of its unique property of being passivated and semiconducting at the same time. To acquire the soft landing regime it was necessary to alter the kinetic energy of the positivly charged hybrids by applying an adjustable electric field. For the transport from the hybrid source to the STM a newly commissioned portable UHV-suitcase was used to preserve the UHV-conditions. First STM results of structures found on the surface will be presented.

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O 100.7 Thu 16:45 MA 141

Characterization of Soot Particles by Helium Ion Microscopy — •André Beyer[1], Daniel Emmrich[1], Maurin Salamanca[2], Lena Ruwe[2], Henning Vieker[1], Katharina Kohse-Höinghaus[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems and Surfaces, Bielefeld University, 33615 Bielefeld, Germany — [2]Department of Chemistry, Bielefeld University, 33615 Bielefeld, Germany

Complementary techniques for the characterization of soot particles are needed to gain insight into their formation processes. In this contribution, we focus on Helium Ion Microscopy (HIM) which allows high contrast imaging of soot particles with sizes down to 2 nm. Soot formation was realized with well-defined model flames from different fuel compositions. The particles were sampled on silicon substrates at different positons within the flame which allows choosing the particles degree of maturity. Large numbers of particles were recorded with a single HIM image in a relatively short time. A number of such images were combined to obtain meaningful particle size distributions. In addition, the following geometric properties of soot particles were evaluated: sphericity, circularity, and fractal dimension. Comparison with other experimental techniques as well as theoretical model calculations demonstrate the strength of HIM as a soot characterization method [1-3].

[1] M. Schenk et al., ChemPhysChem 14 (2013) 3248.
[2] M. Schenk et al., Proc Combust Inst 35 (2015) 1879.
[3] C. Betrancourt et al., Aerosol Sci. Technol. 51 (2017) 916.