

O 3: Metal substrates: Adsorption of organic / bio molecules I

Time: Monday 11:15–12:45

Location: PHY C213

O 3.1 Mon 11:15 PHY C213

Electronic structure of a graphene quantum well system: highly ordered coronene and hexa-peri-hexabenzocoronene films on Ag(111) — ●MICHAEL WIESSNER¹, SOFÍA RODRÍGUEZ¹, JOHANNES ZIROFF¹, SOPHIA HUPPMANN¹, FRANK FORSTER¹, PETER PUSCHNIG², ACHIM SCHÖLL¹, LUKAS DÖSSEL³, KLAUS MÜLLEN³, and FRIEDRICH REINERT¹ — ¹Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg — ²Chair of Atomistic Modelling and Design of Materials, University of Leoben, 8700 Leoben, Austria — ³MPI für Polymerforschung, Ackermannweg 10, D-55128 Mainz

We present angular resolved photoemission measurements of highly ordered monolayer thin films of coronene and hexa-peri-hexabenzocoronene (HBC) on the single-crystalline Ag(111) surface. Coronene and HBC molecules can be viewed as finite pieces of a graphene layer containing 7 and 13 honeycomb rings, respectively, terminated by hydrogen atoms. Thus, the photoemission signal in these systems can be explained by the formation of quantum well states derived from graphene wave functions which are laterally confined by the spatial extension of the molecules. We also calculated the electronic structure of coronene/HBC by density functional theory (DFT) assuming a free molecule. The Fourier-transformed molecular orbitals are shown to reproduce the angle dependent intensity distribution thereby providing a tool to identify different types of orbitals. In conclusion, the solid state derived quantum well states as well as the molecular based DFT orbitals are both applicable to explain the electronic structure of extended aromatic molecules.

O 3.2 Mon 11:30 PHY C213

Incorporation dynamics of molecular guests into 2D supramolecular host-systems at the liquid-solid interface — ●GEORG EDER¹, STEPHAN KLOFT¹, NATALIA MARTSINOVICH², WOLFGANG M. HECKL^{3,4}, and MARKUS LACKINGER^{1,3} — ¹LMU Munich, Germany — ²University of Warwick, UK — ³Deutsches Museum, Munich — ⁴TUM School of Education, Munich

Self-assembly of threefold symmetric tricarboxylic acids at the liquid-solid interface can yield crystalline nanoporous monolayers. Prominent examples are 1,3,5-tricarboxylic acid (TMA) and 1,3,5-benzenetriphenylbenzoic acid (BTB), which both form hydrogen bonded porous structures at the nonanoic acid-graphite interface with pore sizes of ~1.0 nm and ~2.8 nm respectively. It has been shown - also for many other systems - that such nanoporous networks can be utilized as host-networks for the incorporation of molecular guests.

Up to now, predominantly the initial and final structures have been characterized by in-situ Scanning-Tunneling-Microscopy but very little is known about the dynamics. In order to gain a deeper understanding of the incorporation dynamics, we developed an injection system which allows us to simultaneously image the monolayers with submolecular resolution while the guests are introduced to the liquid phase. Even with the modest time resolution of the STM, for coronene guests important differences were revealed for different solvents and different pore sizes. Supported by Molecular Mechanics Simulations, the nature of a comparatively long lived intermediate state could be identified.

O 3.3 Mon 11:45 PHY C213

Robust metal-organic networks with carbonitrile group functionalized polyphenyl backbones — ●MATTHIAS MARSCHALL¹, JOACHIM REICHERT¹, FLORIAN KLAPPENBERGER¹, WILLI AUWÄRTER¹, KNUD SEUFERT¹, SVETLANA KLYATSKAYA², MARIO RUBEN^{2,3}, and JOHANNES V. BARTH¹ — ¹Physik Department E20, TU München, James Frank Str., D-85748 Garching — ²Institut für Nanotechnologie, Karlsruhe Institute of Technology, D-76021 Karlsruhe — ³Université de Strasbourg, IPCMS, 22, Rue de Loess, F-67034 Strasbourg

During the last years metal directed assembly has been used to fabricate robust supramolecular nanostructures on metal surfaces. To determine the relevant interactions in the realized coordination networks scanning tunneling microscopy (STM) has been employed at low- and

at room-temperature. Herein we report on structural changes in the 2D pattern formation on Cu(111) and Ag(111) induced by the position of functional carbonitrile groups in polyphenyl backbones. The observed structures range from highly ordered metal-organic honeycomb lattices to 2D random networks. A complex interplay of molecular interactions, substrate templating effects and molecular degrees of freedom steer the self assembling process in the observed structures and controls the coordination number of the metal coordination center.

O 3.4 Mon 12:00 PHY C213

Ab initio study of a mechanically gated molecule: From weak to strong correlation — ANDREAS GREULING¹, ●MICHAEL ROHLFING¹, RUSLAN TEMIROV², STEFAN TAUTZ², and FRITHJOF ANDERS³ — ¹Fachbereich Physik, Universität Osnabrück, Germany — ²Peter Grünberg Institut, Forschungszentrum Jülich, Germany, and JARA — ³Fakultät für Physik, TU Dortmund, Otto-Hahn-Straße 4, Germany

The electronic spectrum of a chemically contacted molecule in the junction of a scanning tunneling microscope can be modified by tip retraction. We analyze this effect by a combination of density functional, many-body perturbation and numerical renormalization group theory, taking into account both the non-locality and the dynamics of electronic correlation. Our findings, in particular the evolution from a broad quasiparticle resonance below to a narrow Kondo resonance at the Fermi energy, correspond to the experimental observations.

O 3.5 Mon 12:15 PHY C213

Spectroscopy of STM-induced light emission from a molecular double decker on Ag(111) — ●NATALIA L. SCHNEIDER¹, FRANCESCA MATINO¹, GUILLAUME SCHULL², SANDRO GABUTTI³, MARCEL MAYOR³, and RICHARD BERNDT¹ — ¹Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — ²Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, 67034 Strasbourg, France — ³Department of Chemistry, University of Basel, St. Johannsring 19, CH-4056 Basel, Switzerland

A low-temperature scanning tunneling microscope (STM) is used to investigate the electronic states and the STM-induced light emission from naphthalenediimide cyclophane molecules on Ag(111). The cyclophane consists of two parallel π -systems, one of which is adsorbed directly at the metal substrate while the other chromophore is hoped to be partially decoupled from the surface. This intra-molecular decoupling scheme complements previous approaches where molecular multilayers or dielectrics were used. Spectra of the light emission from a single cyclophane layer exhibit molecule-related features and provide information on the excitation processes involved.

O 3.6 Mon 12:30 PHY C213

Electronic Mapping of Molecular Orbitals at the Molecule-Metal Interface — MARIA CHRISTINA LENNARTZ, ●VASILE CACIUC, NICOLAE ATODIRESEI, SILVIA KARTHÄUSER, and STEFAN BLÜGEL — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In the present contribution we report on a combined experimental and theoretical study aimed to investigate the electronic structure of an aromatic organic molecule like pyridine-2,5-dicarboxylic acid ($C_7H_4NO_4$) chemisorbed on the Cu(110) surface. From experimental point of view, the electronic structure of the molecule-Cu(110) was determined by performing scanning tunneling spectroscopy (STS) measurements which enabled us to map the molecular orbitals as a function of tip position. By comparing the experimental differential conductance curves with the calculated density of states for different conformers of this organic molecule on Cu(110), the character (σ or π) of the individual molecular orbitals probed in STS could be clearly identified.

[1] M. C. Lennartz, V. Caciuc, N. Atodiresei, S. Karthäuser, and S. Blügel, Phys. Rev. Lett. **105**, 066801 (2010).