

## O 78: Metal substrates: Adsorption of organic / bio molecules IV

Time: Thursday 16:00–17:45

Location: A 053

O 78.1 Thu 16:00 A 053

**1D growth of  $\alpha$ -Sexithiophene on Au(110)** — ●RENE HAMMER<sup>1</sup>, TOBIAS LEOPOLD<sup>1</sup>, and WOLF WIDDRA<sup>1,2</sup> — <sup>1</sup>Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — <sup>2</sup>Max-Planck Institut für Mikrostrukturphysik, D-06120 Halle, Germany

The quality of the interface between a metal electrode and the organic semiconducting device is a central issue in organic electronics. Typically the structures of the first layers are quite different from its bulk single crystal structures. However for the growth of  $\alpha$ -Sexithiophene (6T) on Au(110) a rather bulk like interface has been proposed [1].

Here we present a scanning tunneling microscopy study of the 6T adsorption on Au(110) at 300K. At low coverages (0.05 monolayer (ML)) the growth of one-dimensional(1D) chains of molecules in [1-10] direction is observed. The structures are 2 molecules wide and several 100nm in length. This chain formation is independent of step edges. At coverages close to a ML a packing of the 1D structures with distances of 4, 5 and 6 Au lattice constants is observed

Single molecular rows grow by a zipper-like mechanism: A topmost atomic row of the (2x1) Au(110) reconstruction shifts by one lattice constant, which leads to a local (1x1) Au(110) micro-facet. These are the preferred adsorption sites of the 6T molecules, in contrast to the previously proposed model [1].

[1] Prato et al., J. Phys. Chem. B 103 (1999)

O 78.2 Thu 16:15 A 053

**Single-molecule spectroscopy of terthiophene adsorbed on Au(111): electronic and vibronic properties** — ●BERNDT KOSLOWSKI, NORBERT MAURER, ANNA TSCHETSCHETKIN, and PAUL ZIEMANN — Institute of Solid State Physics, University of Ulm, D-89069 Ulm, Germany

Because of their expedient properties and their diversity, oligo- and polythiophenes are among the most investigated organic semiconductors. We investigated the adsorption of terthiophene molecules (3T) on Au(111) at low temperature by means of Scanning Tunneling Microscopy and Spectroscopy. 3T adsorbs preferentially in the fcc regions and orients perpendicularly to the soliton walls of the herringbone reconstructed Au(111). Tunneling spectroscopy in the center of the molecule shows the broad LUMO of the molecule at +2.3 eV on a background resembling properties of the gold surface. The HOMO was determined to lie at -1.3 eV leaving the optical gap unchanged as compared to the gas-phase molecule. dI/dV maps reveal a very inhomogeneous distribution of the LUMO/HOMO across the molecule indicating a significant interaction of molecular states with the substrate [1]. By inelastic electron tunneling spectroscopy we find very rich vibrational spectra on the molecules containing more than 30 modes. We analyze the vibronic spectrum and compare it to spectra expected for the free molecules and other experimental results. [1] Koslowski et al., Beilstein J. Nanotechnol. 2, 561-568 (2011).

O 78.3 Thu 16:30 A 053

**Using polarized light in photoelectron emission microscopy** — ●THORSTEN WAGNER<sup>1</sup>, ZDENA DRUCKMÜLLEROVA<sup>1,2</sup>, DANIEL ROMAN FRITZ<sup>1</sup>, and PETER ZEPPENFELD<sup>1</sup> — <sup>1</sup>Johannes Kepler University Linz, Institute of Experimental Physics, Linz, Austria — <sup>2</sup>Brno University of Technology, Institute of Physical Engineering, Brno, Czech Republic

Photoelectron emission microscopy (PEEM) combines a high lateral resolution with the capability to monitor processes at surfaces in real-time. For experiments in the lab, unpolarized light of a Hg lamp is commonly used to excite the photoelectrons. In this case, valuable information about the optical anisotropy of the surface under investigation is lost. On the other hand, techniques like reflectance difference spectroscopy (RDS) which are focussed on this anisotropy have proven to be useful tools to study thin adsorbate films of organic molecules. So why not combining both in a single experiment? In this presentation we will show, how polarized light can be used to study the growth of  $\alpha$ -sexithiophene on silver and nickel oxide surfaces. As the ionization potential of the molecules is higher than the photon energy, the light of the Hg lamp only excites electrons from the metal-organic interface. In this case, no direct response of the molecules to the polarized light can be expected in the PEEM image. Nevertheless, the molecules are

optical anisotropic and act as dichroic filters for the incident light. This effect can actually be used, e.g., to probe the orientation of the molecules even during growth.

O 78.4 Thu 16:45 A 053

**Theoretical Insight into the Growth Mechanisms of 6P Monolayers on Copper Substrates** — ●GIULIO BIDDAU<sup>1</sup>, PETER PUSCHNIG<sup>1</sup>, MARGARETA WAGNER<sup>2</sup>, STEPHEN BERKEBILE<sup>2</sup>, ALEXANDER FLEMING<sup>2</sup>, FALKO NETZER<sup>2</sup>, MICHAEL RAMSEY<sup>2</sup>, and CLAUDIA AMBROSCH-DRAXL<sup>1</sup> — <sup>1</sup>Chair of Atomistic Modelling and Design of Materials, Montanuniversitaet Leoben, Austria — <sup>2</sup>Institute of Physics, Surface and Interface Physics, Karl-Franzens University, Graz, Austria

We present a multi-technique study of the deposition and adsorption of para-sexiphenyl (p-6P) on the Cu(110) substrate and of its first monolayer (1ML) growth at high coverage, while at low coverages the adsorbed molecules repel forming a dense wetting monolayer. The characterization has been carried out by low-temperature STM experiments and Density Functional Theory calculations, performed using the generalized gradient approximation and considering van der Waals interactions with the DFT-D2 approach. Insight in the diffusion barriers is obtained by the Nudged Elastic Band method and the comparison with experimental STM results carried out with the Tersoff-Hamann approximation. We show that island growth occurs through diffusion of ad-molecules deposited in the second monolayer along [110] directions in a 2D Frank-van-der-Merwe layer by layer behavior. We show that molecules of the 1ML, efficiently screen the interaction of 2ML molecules with the metallic substrate. Thus, the weakly bound 2ML ad-molecules are allowed to diffuse with low Ehrlich-Schwoebel barrier along [110], favoring the formation a high-density reconstruction.

O 78.5 Thu 17:00 A 053

**The role of molecular orbitals in scanning tunneling induced luminescence** — ●CHRISTOPH GROSSE<sup>1</sup>, THERESA LUTZ<sup>1</sup>, CHRISTIAN DETTE<sup>1</sup>, ALEXANDER KABAKCHIEV<sup>1</sup>, KLAUS KUHNKE<sup>1</sup>, UTA SCHLICKUM<sup>1</sup>, and KLAUS KERN<sup>1,2</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — <sup>2</sup>Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

The plasmonic light spectrum of pristine metals excited by scanning tunneling microscopy (STM) can be affected in many different ways by the adsorption of organic molecules. In this study we elucidate the role of molecular orbitals in the light emission process and employ STM to investigate the optical and electronic properties of individual *fac*-Ir(ppy)<sub>3</sub> molecules on top of a C<sub>60</sub> monolayer on Ag(111). In this binary system, the C<sub>60</sub> monolayer acts as a molecular decoupling layer. Compared to this, the light excitation on the Ir(ppy)<sub>3</sub> molecules increases locally by half an order of magnitude due to a more efficient excitation of tip induced plasmons. Mapping the molecular orbitals by differential conductance (dI/dV) images reveals three distinguishable molecular orbitals. A comparison of their shape with sub-molecular resolved light excitation maps shows a clear correlation between the light enhancement and the orbital closest to the Fermi energy of the substrate.

O 78.6 Thu 17:15 A 053

**Controlled rotation of single molecules and sub-ångström determination of intrinsic molecular elasticity** — ●RÉMY PAWLAK<sup>1</sup>, SWEETLANA FREMY<sup>1</sup>, SHIGEKI KAWAI<sup>1</sup>, THILO GLATZEL<sup>1</sup>, HONGJUAN FANG<sup>2</sup>, LESLI-ANNE FENDT<sup>2</sup>, FRANÇOIS DIEDERICH<sup>2</sup>, and ERNST MEYER<sup>1</sup> — <sup>1</sup>Depa/Departement of Physics, University of Basel, Switzerland/tement of Physics, University of Basel, Switzerland — <sup>2</sup>Laboratorium für Organische Chemie, ETH Zürich, Switzerland

Directed molecular repositioning is a key step towards the built-up of molecular machines. To artificially generate and control motion on a surface, molecules are generally excited by an exchange of light, chemical or electrical energy. Although the elasticity of molecular structures plays a role in all diffusion processes, such intrinsic properties are rather poorly known. Here, we explore by scanning probe microscopy directed manipulations of single porphyrin derivatives equipped with peripheral carbonitrile end groups confined on Cu(111). Using 3D-spectroscopic measurements with sub-ångström precision, these chemical end-groups have been accurately identified as four reactive centers.

By attaching the tip to one of them, a mechanical stress is applied until a directed motion of the whole molecule is induced. Depending on the selection of one of the CN end-groups, the molecule is either rotated clockwise or anticlockwise in a controlled way. The energy transferred between the molecule and the tip during this mechanically-induced manipulation, which is closely related to its diffusion energy, are directly quantified.

O 78.7 Thu 17:30 A 053

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