

## O 65: Metal substrates: Adsorption of organic / bio molecules VII

Time: Thursday 11:15–13:00

Location: PHY C213

O 65.1 Thu 11:15 PHY C213

**Coverage dependent isomerisation behaviour of tetra-*tert*-butyl-imine on Au(111)** — ●FELIX LEYSSNER, MATTHIAS KOCH, STEPHAN MEYER, and PETRA TEGEDER — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, D-14195 Berlin

High resolution electron energy loss spectroscopy (HREELS) is employed to analyze thermally activated changes in the geometrical structure of the photochromic molecular switch 3,3',5,5'-tetra-*tert*-butyl-imine (TBI) adsorbed on Au(111). Measurements have been performed for two coverage regimes: The monolayer and the bilayer regime. For both coverages all molecules are found in the *trans* state after deposition at sample temperatures of  $T=210\text{K}$ , but conformational changes upon heating are observed, which are assigned to a *trans* to *cis*-isomerization. When heating the sample to  $T=440\text{K}$  two different conformations are observed depending on the initial coverage. Annealing of a monolayer leads to an increasing number of *cis* isomers, pointing towards an inverted thermal isomerisation behaviour of TBI, since the *trans*-isomer is the more stable compound in solution. Whereas for a bilayer the temperature induced isomerization of the TBI can be monitored as well, but desorption of the second layer at  $T=440\text{K}$  leads to the formation of a *trans*-monolayer. The fact that different molecular configurations are found for equal coverages annealed at the same temperature is highly surprising and shows that collective effects may govern the switching properties of molecular switches on surfaces.

O 65.2 Thu 11:30 PHY C213

**Switching behavior of double-decker single molecule magnets on a metal surface** — ●YINGSHUANG FU<sup>1</sup>, JOERG SCHWOEBEL<sup>1</sup>, ANDREW DILLULO<sup>2</sup>, GERMAR HOFFMANN<sup>1</sup>, JENS BREDE<sup>1</sup>, SVETLANA KLYATSKAYA<sup>3</sup>, MARIO RUBEN<sup>3,4</sup>, and ROLAND WIESENDANGER<sup>1</sup> — <sup>1</sup>University of Hamburg, Hamburg, Germany — <sup>2</sup>Ohio University, Athens, USA — <sup>3</sup>Karlsruhe Institute of Technology, Karlsruhe, Germany — <sup>4</sup>Université de Strasbourg, Strasbourg, France

Single molecule magnets (SMM) are most promising materials for spin based molecular electronics. Due to their large magnetic anisotropy stabilized by inside chemical bonds, SMM can potentially be used for information storage at the single molecule level. For applications, it is of importance to adsorb the SMM onto surfaces and to study their subsequent conformational, electronic and magnetic properties.

We have investigated the adsorption behavior of Tb and Dy based double-decker SMM on an Ir(111) surface with low temperature scanning tunneling microscopy and spectroscopy. It is found that Tb double-decker molecules bind tightly to the Ir(111) surface. By resonantly injecting tunneling electrons into its LUMO or HOMO state, the Tb double-decker molecule can be switched from a four-lobed structure to an eight-lobed structure. After switching, energy positions of the HOMO and LUMO states both shift closer to the Fermi level. Dy double-decker molecules also exhibit the same switching properties on the Ir(111) surface. The switching behavior of the molecules is tentatively attributed to a conformational change of the double-decker molecular frame.

O 65.3 Thu 11:45 PHY C213

**Simulation of vibrational spectra of self-assembled monolayers on metal surfaces** — ●KATRIN TONIGOLD and AXEL GROSS — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Vibrational spectroscopy is a common and valuable experimental tool to analyze the chemical composition as well as the orientation of self-assembled monolayers (SAMs) on metal surfaces [1]. The simulation of such vibrational spectra might be helpful for the analysis of experimental spectra and further information might be gained by the theoretical insight in the vibrations occurring at the surface.

In this study vibrational spectra of thiolate-based SAMs on Au(111) have been simulated by means of DFT-GGA-calculations employing two different methods: a harmonic approach using finite differences is compared to an approach using *ab initio* molecular dynamics simulations showing the influence of temperature and anharmonicity. The impact of different conformers and coverages on vibrational spectra has been considered. Furthermore, the influence of defects such as adatoms or vacancies in the gold surface on the structure of the SAMs and their vibrational spectra is discussed.

[1] Xia Stammer *et al.*, PCCP **12**, 6445-6454 (2010).

O 65.4 Thu 12:00 PHY C213

**The effect of molecular vibration on the Resonant Auger Raman spectra of Sn-phthalocyanine thin films** — MARC HAEMING<sup>1</sup>, JOHANNES ZIROFF<sup>1</sup>, LOTHAR WEINHARDT<sup>1</sup>, ●ACHIM SCHÖLL<sup>1</sup>, and FRIEDRICH REINERT<sup>1,2</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg — <sup>2</sup>KIT, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe

On the example of epitaxially grown layers of Tin-phthalocyanine (SnPc) as well as ultrathin SnPc layers adsorbed on a monolayer of PTCDA/Ag(111) we demonstrate the capabilities of Resonant Auger Raman Spectroscopy in analyzing the electron-vibration coupling in thin films of large organic molecules and at their interfaces. The constant initial state signal of particular SnPc levels is substantially enhanced by autoionization and participant decay of the core excited state. We show that the fine structure of the autoionization signal can differ significantly from that of the direct photoemission signal, which is related to electron-vibration coupling. Moreover, continuous modifications of the vibronic fine structure of the autoionization spectra are observed when tuning the excitation energy through an absorption resonance. By comparing SnPc in multilayer samples to SnPc on PTCDA we can demonstrate that these effects are obviously very sensitive to the molecular environment, even in case of weak, predominantly non-covalent interaction. Therefore Resonant Auger Raman Spectroscopy can provide new insight into electron-vibration coupling and into intermolecular interaction in films of organic molecules.

O 65.5 Thu 12:15 PHY C213

**Systematic studies of bonding distances of diindenoperylene on noble metal surfaces** — ●CHRISTOPH BÜRKER<sup>1</sup>, ALEXANDER GERLACH<sup>1</sup>, TAKUYA HOSOKAI<sup>1</sup>, JENS NIEDERHAUSEN<sup>2</sup>, BLANKA DETLEFS<sup>3</sup>, NORBERT KOCH<sup>2</sup>, and FRANK SCHREIBER<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — <sup>2</sup>Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — <sup>3</sup>ESRF, 38043 Grenoble Cedex, France

The interaction of organic semiconducting molecules with different substrates is essential for the understanding of these systems and for possible applications in organic electronic devices. Diindenoperylene (DIP) is one promising semiconductor and has been studied widely in the recent years concerning its growth and ordering behavior on different substrates as well as electronic properties [1]. Despite these efforts the bonding distance  $d_0$  and thus the coupling to the substrate is still an unknown key parameter of DIP adsorption.

Here we present a systematic study of  $d_0$  of DIP on Cu(111), Ag(111) and Au(111) surfaces, determined by the X-ray standing wave (XSW) technique [2]. Different bonding distances for different substrates indicate a substrate dependent interaction strength. Our results are compared with the well-established bonding distances and interaction strength of PTCDA on the same noble metal surfaces. Interesting similarities as well as differences between the two molecules are discussed.

[1] A. C. Dürr *et al.*, Phys. Rev. B **68**, 115428 (2003)[2] A. Gerlach *et al.*, Phys. Rev. B **71**, 205425 (2005)

O 65.6 Thu 12:30 PHY C213

**Transfer of chirality from individual helicene derivatives into 2D supramolecular structures on Cu(111)** — ●MEIKE STÖHR<sup>1</sup>, SERPIL BOZ<sup>2</sup>, MICHAEL SCHÄR<sup>3</sup>, FRANCOIS DIEDERICH<sup>3</sup>, MANH-TUONG NGUYEN<sup>4</sup>, DANIELE PASSERONE<sup>4</sup>, and THOMAS JUNG<sup>5</sup> — <sup>1</sup>University of Groningen, Netherlands — <sup>2</sup>University of Basel, Switzerland — <sup>3</sup>ETH Zürich, Switzerland — <sup>4</sup>EMPA, Switzerland — <sup>5</sup>Paul-Scherrer-Institute, Switzerland

The investigation of chiral phenomena in two dimensions has increased over the last two decades substantially. Both chiral recognition and transfer of chirality are two aspects amongst others which spurred fundamental research in this area. With STM, insight into the processes on the (sub)molecular scale can be gained. In addition, information on intermolecular and molecule substrate interactions, which govern the 2D assembly structure and thus, also determine how chiral recognition and transfer of chirality are expressed, are obtained. We investigated the adsorption of a helicene derivative featuring two cyano groups which are in opposition to each other on Cu(111) with UHV-STM.

Through the functional cyano groups, the guided arrangement in 2D supramolecular structures is enabled. For the adsorption of both the racemic mixture and the enantiopure forms, a transfer of chirality into well-ordered structures is observed. The adsorption of one enantiomer results in structures which are mirror images of those obtained after deposition of the opposite enantiomer. By combining STM experiments with DFT calculations, the intermolecular interactions stabilizing the observed self-organized structures were elucidated.

O 65.7 Thu 12:45 PHY C213

**Precursors for sergeant-and-soldiers experiments: dimethyl succinic acid on Cu(110)** — ●CHRYSANTHI KARAGEORGAKI, CHRISTIAN ROTH, MANFRED PARSCHAU, and KARL-HEINZ ERNST — EMPA, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

In order to better understand chiral recognition at the molecular level,

we are currently studying interactions between different chiral butane-dioic acids, like tartaric acid (TA), malic acid (MA) and 2,3-dimethyl succinic acid (DMSU) as well as achiral analogues like succinic acid (SU), meso-TA and meso-DMSU on metal surfaces. This led to first a observation of chiral amplification 2D crystals via the so-called "sergeant-and soldiers effect" [1]. In order to discriminate if through-substrate or lateral hydrogen bonding dominates the chiral recognition at surfaces, we currently synthesize chiral DMSU, i.e., replacing the hydroxyl groups of TA by methyl. Here we present LEED, XPS, TPD and RAIRS results of achiral meso-DMSU ( $\text{HOOC-CH}(\text{CH}_3)\text{-CH}(\text{CH}_3)\text{-COOH}$ ) on Cu(110). Besides coverage-dependent "surface-explosion" decomposition chemistry and ordered  $\text{C}_2$ -symmetric structures, DMSU spontaneously undergoes symmetry breaking, observed as superposition of mirror domains in LEED, which makes this system indeed interesting for doping experiments with chiral DMSU.

[1] M. Parschau, S. Romer, K.-H. Ernst, J. Am. Chem. Soc. 2004, 126, 15398.