

## O 58: Metal Substrates: Adsorption IV

Time: Thursday 15:45–18:15

Location: H39

O 58.1 Thu 15:45 H39

**On the interaction between ethylene and defect-sites on the Cu(111) surface** — MARTIN BINDER, •OLAF SKIBBE, and ANNEMARIE PUCCI — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

It is well-known, that ethylene adsorbed on rough copper surfaces shows a strong chemical enhancement in the surface enhanced Raman scattering (SERS). In former research, these Raman-active vibrational bands also have been detected also with infrared reflection absorption spectroscopy (IRRAS) on cold deposited and hence rough copper films. They were therefore referred to as defect sites (annealable sites). By evaporating small amounts (sub-monolayers) of copper to the cold surface, we could show that the occurrence of such Raman-active absorption bands in IRRAS of ethylene on a smooth Cu(111) surface is related to defect sites. Surprisingly, not only the intensity of the Raman-active bands was increasing with the amount of evaporated copper, but an unforeseen strong decrease in intensity of the infrared-active out-of-plane vibration ( $\text{CH}_2$  wagging mode) was also detected. In order to understand the morphology of the roughened surface and the nature of the interaction between the copper adatoms and the ethylene molecules, we used high-resolution electron energy loss spectroscopy (HREELS) to examine the vibrational modes of the copper adatoms on the surface and those of the adsorbed ethylene. By doing so, we found that the  $\text{CH}_2$  wagging mode of ethylene is still present on the roughened surface. The loss in dipole-activity of this vibration is an unexpected result. We try to give an explanation.

O 58.2 Thu 16:00 H39

**Tuning the interaction of fullerenes with metal surfaces by molecular self-assembly** — •KATHARINA JENNIFER FRANKE<sup>1</sup>, GUNNAR SCHULZE<sup>1</sup>, ISABEL FERNÁNDEZ-TORRENTE<sup>1</sup>, NILS HENNINGSEN<sup>1</sup>, SEBASTIAN ZARWELL<sup>2</sup>, KAROLA RÜCK-BRAUN<sup>2</sup>, NICOLÁS LORENTE<sup>3</sup>, and JOSÉ IGNACIO PASCUAL<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, Fachbereich Physik, Germany — <sup>2</sup>Technische Universität Berlin, Institut für Chemie, Germany — <sup>3</sup>Université Paul Sabatier, Toulouse, France

Frequently, thin insulating layers are used to electronically decouple molecules from metallic substrates. In an alternative approach we show here, that intermolecular interactions can be employed to create supramolecular structures, which decrease the electronic coupling of fullerenes to a metallic substrate. By low-temperature scanning tunnelling microscopy (STM) we find that the co-adsorption of molecular tripods (1,3,5,7-tetraphenyladamantane) and fullerenes on Au(111) leads to the formation of two basic self-assembled building blocks, which hierarchically arrange in larger structures. One of them is a triangular shaped tetramer consisting of three tripods with a  $\text{C}_{60}$  in their centre. The second one results in rows of alternating adamantane and fullerenes. In both cases scanning tunnelling spectroscopy shows that the presence of the tripod linkers modify the electronic configuration of the fullerene cage. In particular, the tunnelling spectra show a negative differential resistance characteristic for a weaker electronic coupling to the Au(111). DFT calculations indicate that the tripods lift the  $\text{C}_{60}$  from the surface, thus allowing the tunability of the fullerene-metal interaction.

O 58.3 Thu 16:15 H39

**Controlled Contact to a  $\text{C}_{60}$  Molecule** — •NEEL NICOLAS, KRÖGER JÖRG, LIMOT LAURENT, and BERNDT RICHARD — Institut für Experimentelle und Angewandte Physik CAU Kiel

The tip of a low-temperature scanning tunneling microscope is approached towards a  $\text{C}_{60}$  molecule adsorbed on Cu(100) to form a tip-molecule contact. Beyond the tunnelling regime the conductance rapidly increases in a transition region to contact regime. At contact formation, a conductance well below a quantum of conductance is observed. The conductance increases slowly upon further approach of the tip until a jump to one quantum of conductance occurs. The contact properties depend on the adsorption geometry of the molecule on the surface. Ab-initio calculations within density functional theory and non-equilibrium Green's function techniques explain the experimental data in terms of the conductance of an essentially undeformed  $\text{C}_{60}$ . The conductance at the transition from tunneling to contact is strongly affected by structural fluctuations which modulate the tip-molecule distance.

O 58.4 Thu 16:30 H39

**Substrate dependent bonding distances of PTCDA - A comparative X-ray standing-wave study on Cu(111) and Ag(111)** — •ALEXANDER GERLACH<sup>1</sup>, STEFAN SELLNER<sup>1</sup>, FRANK SCHREIBER<sup>1</sup>, NORBERT KOCH<sup>2</sup>, and JÖRG ZEGENHAGEN<sup>3</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — <sup>2</sup>Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — <sup>3</sup>European Synchrotron Radiation Facility, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble Cedex 9, France

We study the adsorption geometry of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on Ag(111) and Cu(111) crystals using X-ray standing waves. The element-specific analysis shows that the carbon core of the molecule adsorbs in a planar configuration, whereas the oxygen atoms experience a non-trivial and substrate dependent distortion. On copper (silver) the carbon rings resides 2.66 Å (2.86 Å) above the substrate. In contrast to the conformation on Ag(111), where the carboxylic oxygen atoms are bent towards the surface, we find that on Cu(111) all oxygen atoms are above the carbon plane at 2.73 Å and 2.89 Å, respectively.

O 58.5 Thu 16:45 H39

**Interface characterization of TTF-TCNQ on metal surfaces** — •ISABEL FERNÁNDEZ-TORRENTE<sup>1</sup>, SERGIO MONTURET<sup>2</sup>, KATHARINA JENNIFER FRANKE<sup>1</sup>, NILS HENNINGSEN<sup>1</sup>, NICOLÁS LORENTE<sup>2</sup>, JORDI FRAXEDAS<sup>3</sup>, and JOSÉ PASCUAL<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Germany — <sup>2</sup>Université Paul Sabatier, Toulouse, France — <sup>3</sup>ICMAB, Campus UAB, Bellaterra, Spain

Molecular charge transfer (CT) complexes are defined as the association of donor and acceptor molecules. The self-assembling properties of molecules open the possibility of building different donor-acceptor stacking structures which rule the electronic functionality of the compound. Tetrathiafulvalene 7,7,8,8-tetracyanoquinodimethane (TTF-TCNQ) is an example of a CT complex which shows a metal conducting behaviour. The stacking of TTF and TCNQ forms in bulk one-dimensional partially occupied energy bands that gives rise to the metallicity. By means of Low Temperature Scanning Tunneling Microscopy/Spectroscopy we have characterised for the first time the mixed growth of TTF and TCNQ on a metallic surface in submonolayer and monolayer regimes. The self-assembled growth is governed by donor-acceptor recognition. In particular a one dimensional phase with alternating lines of TTF and TCNQ is formed and can be considered as the precursor stage for the bulk structure. By Scanning Tunneling Spectroscopy we associate electronic resonances with the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) of TTF and TCNQ and the self-assembled TTF-TCNQ.

O 58.6 Thu 17:00 H39

**Copper-Phthalocyanine on Ag(111) - A SPA-LEED study** — •INGO KRÖGER, CHRISTOPH STADLER, CHRISTIAN KUMPF, and EBERHARD UMBACH — Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg

The adsorption of Copper-Phthalocyanine (CuPc) on Ag(111) has been studied by Spot Profile Analysis Low Energy Electron Diffraction (SPA-LEED). Three different phases were found in the submonolayer regime, differing in coverage and temperature.

At coverages below 0.8 layers and at room temperature no long-range order was observed. However, from diffuse rings in LEED we could still determine an average distance between the molecules which decreases *continuously* with increasing coverage.

Between 0.8 and 1.0 layers CuPc forms incommensurate superstructures. The unit cell size shrinks *continuously* from  $216\text{Å}^2$  (0.8 ML) to  $196\text{Å}^2$  (1.0ML). These measurements show that the molecules (at RT) always occupy the maximum surface area, a behaviour which is only compatible with a repulsive intermolecular interaction and a relatively small influence of the substrate.

Furthermore, at coverages between 0.7 -0.8 layers a low temperature phase was found, which is commensurate with the substrate. Very recently the same behaviour was found for SnPc on Ag(111).

O 58.7 Thu 17:15 H39

**Self-organization of cobalt-phthalocyanine on a vicinal gold surface revealed by scanning tunnelling microscopy** — ●J. KRÖGER, H. JENSEN, N. NÉEL, and R. BERNDT — Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Adsorption of cobalt-phthalocyanine on Au(788) in the sub-monolayer coverage regime leads to a preferential occupation of step edges with the molecule plane tilted such as to bridge adjacent terraces. Molecules which adsorb on terraces leave the surface reconstruction of Au(788) unchanged and exhibit the propensity to occupy face-centered cubic stacking domains. Tunnelling spectroscopy in the centre of the molecule reveals cobalt d-orbital related features, while spectroscopy on the benzene rings shows the lowest unoccupied molecular orbital.

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**Conformational switching in the self assembling process of azobenzene on Au(111)** — ●NILS HENNINGSSEN<sup>1</sup>, KATHARINA JENNIFER FRANKE<sup>1</sup>, ISABEL FERNANDEZ-TORRENTE<sup>1</sup>, GUNNAR SCHULZE<sup>1</sup>, BEATE PRIEWISCH<sup>2</sup>, KAROLA RÜCK-BRAUN<sup>2</sup>, and JOSÉ IGNACIO PASCUAL<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Germany — <sup>2</sup>Institut für Chemie, Technische Universität Berlin, Germany

Here we present low temperature scanning tunneling microscopy studies of 3,3'-Carboxymethylester-Azobenzene (CMA) adsorbed on a Au(111) surface. Two different adsorption geometries are observed, which differ from each other by the rotation of one phenylene ring. The two CMA isomers selectively assemble in two different structures: highly ordered densely packed islands and chains of interlocked molecules. Both molecular structures are stabilised by hydrogen bonds. The ratio of the two conformers has been studied dependently of coverage and adsorption temperature and shows that the selective assembly is not only influenced by conformational recognition during diffusion processes but furthermore by conformational changes while assembling. This proves that intra-molecular conformational dynamics can govern self assembly processes.

O 58.9 Thu 17:45 H39

**Tracking the chiral recognition of adsorbed dipeptides at the single molecule level** — ●GIOVANNI COSTANTINI<sup>1</sup>, MAGALÍ LINGENFELDER<sup>1</sup>, GIULIA TOMBA<sup>2</sup>, LUCIO COLOMBI CIACCHI<sup>3</sup>, ALESSANDRO DE VITA<sup>2</sup>, and KLAUS KERN<sup>1</sup> — <sup>1</sup>MPI-FKF, Stuttgart, Germany — <sup>2</sup>Physics Department, King's College London, UK — <sup>3</sup>Fraunhofer IWM, Freiburg, Germany

We report on the direct observation of chiral recognition events of diphenylalanine adsorbed on Cu(110) by scanning tunneling microscopy (STM). We monitor the self-organization of co-deposited di-L-phenylalanine (L-Phe-L-Phe) and its stereoisomer D-Phe-D-Phe and rationalise the observed steps of the system's dynamical evolution using first principles and classical molecular dynamics techniques.

We demonstrate that the adsorbed dipeptides must undergo both a conformational change and a chemical rearrangement (into a zwitterionic form) in order to assemble into stable supramolecular structures. The process is successfully completed if the approaching dipeptides have the same chirality, and fails otherwise, so that the final structures are in all cases strictly homochiral.

Our analysis shows that a static three-point-model is in general not sufficient for a complete description of chiral recognition. We prove the importance of mutually induced conformational changes in the chiral recognition process, thereby visualizing at the single molecule level a 50 years old prediction of L. Pauling.

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**Adsorption von Ethen auf Pt(111)- und Pt<sub>x</sub>Sn- Oberflächenlegierungen. Eine vergleichende HREELS- und DFT-Studie.** — ●JAN MARKUS ESSEN, JAN HAUBRICH, CONRAD BECKER und KLAUS WANDEL — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn

Durch Zulegieren eines Fremdmetalls können die Eigenschaften von Katalysatoren gezielt beeinflusst werden. Es werden unerwünschte Reaktionswege unterdrückt, das Zielprodukt kann so in höherer Ausbeute und Reinheit erhalten werden. Es wurde das Adsorptionsverhalten von Ethen, als kleinster Repräsentant ungesättigter Kohlenwasserstoffe auf Pt(111) sowie den Oberflächenlegierungen Pt<sub>3</sub>Sn und Pt<sub>2</sub>Sn auf Pt(111) mittels thermischer Desorptions-Spektroskopie (TDS) und hochauflösender Elektronen-Energie-Verlustspektroskopie (HREELS) untersucht. Die erhaltenen Adsorptionsenergien und Schwingungsspektren werden mit Ergebnissen von Dichte-Funktional-Theorie (DFT) Rechnungen verglichen und interpretiert. Ethen adsorbiert auf allen drei Oberflächen bevorzugt in einer di-σ -Konformation, zeigt aber ein völlig verschiedenes Desorptionsverhalten. Als Mindermengenspezies konnte durch Vergleich mit den Rechnungen, erstmalig auf diesen Oberflächen eine π -gebundene Ethen Spezies nachgewiesen werden. Durch diese vergleichende Betrachtung der experimentellen Messungen mit den theoretischen Rechnungen können Reaktionswege, Intermediate und Oberflächenspezies aufgeklärt und der Legierungseinfluss des Zinns bei der unterdrückten Dehydrierung des Ethens auf diesen Oberflächen verstanden werden.