Location: SCH A118

O 11: Metal substrates: Adsorption of organic / bio molecules II

Time: Monday 15:00-16:45

O 11.1 Mon 15:00 SCH A118

Molecular chemistry at surfaces: Ring opening reaction of Spiropyrane molecules on a metal surface — •GUNNAR SCHULZE, MARTEN PIANTEK, CRISTINA NAVÍO, JORGE MIGUEL, MATTHIAS KOCH, FELIX LEYSSNER, KATHARINA J. FRANKE, PETRA TEGEDER, WOLF-GANG KUCH, and JOSE IGNACIO PASCUAL — Inst. für Experimentalphysik, Freie Universität Berlin, Arnimalle 14, 14195 Berlin

The ring-opening reaction of spiropyran (SP) to the merocyanine (MC) form is a reversible photochromic process in solution. The interest in this basic reaction stems from the different properties of each isomer, regarding to structure (SP is chiral), electrical dipole moment (MC has a large dipole) and electronic structure (MC is coloured). In solution SP is the thermally stable isomer. Here, we report that on a metal surface, MC turns out to be more stable. We investigate the thermally induced ring-opening transition from the organic photo switch 6-nitro-spriropyran to its merocyanine isomer on a Au(111) surface by means of low temperature scanning tunnelling microscopy (STM), scanning tunnelling spectroscopy (STS) and force-field simulations. In submonolayer coverages, each isomer presents a very distinct behaviour in terms of electronic properties and structure of the self-assembled molecular domains. Once that the merocyanine domains are created by thermal activation, they remain stable, suggesting that the interaction of the conjugated planar backbone with the metal surface helps to stabilize this isomer. The ring opening reaction can be also induced by local electric currents conducted through the molecule by the STM tip.

O 11.2 Mon 15:15 SCH A118

Manipulation of conjugated molecular chains on Au(111) — •LEIF LAFFERENTZ¹, FRANCISCO AMPLE², HAO YU³, STEFAN HECHT³, CHRISTIAN JOACHIM², and LEONHARD GRILL¹ — ¹Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — ²Nanosciences Group, CEMES-CNRS, 31055 Toulouse, France — ³Institut für Chemie, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin

The goal of molecular electronics is to utilize individual molecules as components in electronic devices. These units have to be linked by conducting connections. To achieve this, two conditions have to be met: First, the connections have to be robust while allowing efficient charge transfer. Furthermore, it is necessary to gain a basic understanding of the charge transport, which requires the ability to measure the current through single molecule junctions.

Solidly connected molecular structures of predetermined architecture could be produced with our method of on-surface synthesis [1]. In this way, conjugated chains with lengths of up to over 100 nm were formed from dibromoterfluorene (DBTF) molecules on a Au(111) surface. The chains are characterized and manipulated by means of lowtemperature scanning tunneling microscopy (STM). It will be shown that it is possible to lift part of individual chains off the surface employing vertical manipulation with the STM tip, which opens the exciting possibility to measure currents through this molecular junction.

[1] L. Grill, M. Dyer, L. Lafferentz, M. Persson, M. V. Peters, and S. Hecht, Nature Nanotech. 2, 687 (2007)

O 11.3 Mon 15:30 SCH A118

STM investigation of imine-based molecular switches on Au(111) — •JOHANNES MIELKE¹, YING LUO², RAINER HAAG², and LEONHARD GRILL¹ — ¹Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — ²Institut für Chemie und Biochemie - Organische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

In the field of molecular electronics, molecular switches are highly relevant because they can control the conductance. Switches based on azobenzene molecules have attracted large interest in the last years. A very similar molecular switch can be created by replacing the functional azo group by an imine group, which does not considerably alter the electronic structure of the molecule and conserves the capability of undergoing a reversible trans-cis isomerisation. Such processes have already been studied in solution and the gas phase but not on surfaces.

In this work, imine molecules with four tert-butyl groups were adsorbed on Au(111) and their adsorption and switching behaviour were studied using a low temperature STM. The molecules were found to form two types of ordered islands and an interesting irreversible switching behaviour was observed when looking at their temperature dependence, because the number of trans isomers was reduced upon heating of the sample.

O 11.4 Mon 15:45 SCH A118 Reversible breaking and forming of a metal-ligand bond by STM: PVBA and Cu adatoms on Cu(111) — •ROBIN OHMANN, LUCIA VITALI, and KLAUS KERN — Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Controlling functional properties at the atomic scale is interesting for fundamental research and is a key for creating smaller operational units for computational devices. Recently, strong attention is focused on surface-adsorbed atoms and molecules, which undergo reversible positional or conformational changes. Here, we used 4-[trans-2-(pyrid-4-yl-vinyl)] benzoic acid (PVBA) molecules, which were deposited in ultra high vacuum (UHV) via molecular beam epitaxy on a Cu(111) surface and measured with a scanning tunneling microscope operating at low temperature (6 K). Single PVBA molecules and self-assembled dimers, which are bond together by a Cu atom in the center, are predominantly observed. Although the single molecules show a stable configuration, for the dimers we found that the tunneling current oscillates between two values above a threshold voltage. This random telegraph noise has been investigated as a function of tip-sample distance, applied voltage and lateral position of the tip. By measuring the topography at well defined conditions, we were able to image both states of the dimer and ascribe their origin to a ligand in contact with and detached from the central metal atom.

O 11.5 Mon 16:00 SCH A118

Stilbene - a molecular switch on surfaces — •THORSTEN ULRICH KAMPEN^{1,3}, PHILIPP MARTIN SCHMIDT-WEBER¹, RALPH PÜTTNER², CHRISTINE KOLCZEWSKI¹, KLAUS HERMANN¹, and KARSTEN HORN¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

- $^2 {\rm Freie}$ Universität Berlin, Institut für Experimental
physik, Berlin, Germany- $^3 {\rm SPECS}$ GmbH, Berlin, Germany

We have investigated the potential of Stilbene as a molecular switch on surfaces. In this study, Si(100) and Cu(110) serve as exemplary semiconductor and metal substrates. Using the StoBe software package and performing NEXAFS measurements on the cis and trans isomers in the gas phase, both isomers are clearly identified by the lineshape of the resonances. NEXAFS investigations, aided by the results from photoelectron spectroscopy, showed that the interaction of the orbitals at the C=C bridge of stilbene with the substrate atoms has a direct influence on the isomerisation process. The isomerisation requires an excitation into the unoccupied bridge orbitals. On Si(100), the bonding of the molecules to the surface takes place via this C=C bridge thereby inhibiting the isomerisation. On Cu(110) adsorbate-substrate bonding does not envolve the C=C bridge, and therefore does not inhibit the isomerisation. For different coverages cis-to-trans isomerisation with an overall conversion of about 25% is possible.

O 11.6 Mon 16:15 SCH A118 Structure microscopy attributed to hydrogen — •CHRISTIAN WEISS, RUSLAN TEMIROV, OLGA NEUCHEVA, SERGEY SOUBATCH, and FRANK STEFAN TAUTZ — Institut für Bio und Nanosysteme (IBN-3) and JARA-Fundamentals of Future Information Technology

Condensation of H2 (D2) leads to ultra-high geometrical resolution in low temperature scanning tunneling microscopy. This has been shown for different molecular adsorbates on different metallic surfaces [1]. Geometrical resolution in this context means that ring-structures in which carbon atoms in many organic molecules are arranged can be clearly identified. Strong non-linear behavior in conductance spectra appears simultaneously with high resolution images, when hydrogen is condensed to the tunnelling junction. In this contribution we analyze the relation between spectroscopic features and imaging contrast to elucidate the specific feature that is responsible for the improved resolution. References: [1] R Temirov, S Soubatch, O Neucheva, A Lassise, and F S Tautz 2008 New. J. Phys 10 053012

O 11.7 Mon 16:30 SCH A118 Inelastic electron tunneling spectroscopy in single C_{60} junctions: the role of energy level alignment — •KATHARINA J. FRANKE, GUNNAR SCHULZE, and JOSE IGNACIO PASCUAL — Freie Universität Berlin, Berlin, Germany

Inelastic scattering of electrons has important implications in transport through single molecule junctions as it leads to heating effects [1]. Here, we measure the inelastic tunneling spectra (IETS) of C_{60} molecules adsorbed on different metal surfaces in order to identify the

molecular vibrations playing a role in transport close to the Fermi level. We find that the alignment of the lowest unoccupied molecular orbital (LUMO) has an important effect on the detection of molecular vibrations. When the LUMO exhibits a small tail crossing the metal's Fermi level, we are able to observe all eight H_g modes, exhibiting a strong coupling to the LUMO. The inelastic signal is further analyzed along the transition from the tunneling to the contact regime.

[1] G. Schulze, et al., Phys. Rev. Lett. 100, 136801 (2008)