Surface stress and its consequences: In-situ study of PTCDA induced faceting of vicinal Ag(111) — 

O.8.1 Mon 12:00 — MA 041 

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PTCDA (3,4,9,10-perylene-tetracarboxylic acid dianhydride) monolayers on Au(111) and Ag(111) are widely used model systems in the field of organo-metallic interfaces, featuring the basic adsorption types of physisorption and chemisorption respectively. By the growth of epitaxial layers of Ag on Au(111), the electronic states of the substrate can be modified (depending on the thickness of the Ag film) to become more and more \textit{silver-like}, up to the point where they resemble the (111) surface of bulk silver. This process includes the formation of quantum well states with well characterised charge distribution and electronic properties. Therefore, this system enables experiments in which we control the substrates physical properties in small discrete steps, meanwhile tuning the molecular bonding from van der Waals to covalent.

We will show angle-resolved photoemission spectra of PTCDA monolayers on Ag films of various thicknesses on Au(111), focusing on the valence band and its electronic features, namely the Shockley surface state, higher molecular orbitals (HOMO, HOMO-1) and the so-called former LUMO. We will comment on correlations between the substrates distinctive electronic features and the appropriate interface structure, thus fathoming their role in the bonding mechanism and the formation of new valence electronic states.

Investigation of unoccupied electronic states in PTCDA/Au(111) — 

O.8.5 Mon 13:00 — MA 041 

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In the archetypal system perylene-tetracarboxylic-dianhydride (PTCDA) on single crystal Ag(111) surfaces considerable differences between the electronic states of chemisorbed monolayer films and multilayer films are eminent. These differences, which are due to the altered chemical environment of PTCDA- and as well Ag-derived states between the electronic states of chemisorbed monolayer films and multilayer films are evident. These differences are due to the altered chemical environment of PTCDA- and as well Ag-derived states in the vicinity of the interface, can be tracked with 2PPE. A new unoccupied interface state at the Ag/PTCDA interface with a free-electron like dispersion and comparatively short lifetime is detected that influences the charge injection characteristics considerably. The results of the 2PPE spectroscopy are compared to the results of complementary spectroscopies like UPS, IPES, and STS.
Local control of the conductivity of single atoms and molecules probed by scanning tunneling microscopy and spectroscopy — Lucia Vitali1, Robin Ohmann2, Sebastian Stepanow2, and Klaus Kern1 — 1MPI for Solid State Research, Stuttgart — 2CREA, Barcelona

The implementation of molecule-based electronics is a pressing challenge of nanotechnology. The realization of such a circuit is still facing challenges such as the contact of the molecule to the electrodes. In order to clarify this, we studied the conductivity through single atoms and more complex molecular systems. Here, we present an experimental study of the electronic transport through single C0 atoms and 4-(trans-2-(pyrid-4-yl- vinyl)) benzoic acid (PVBA) molecules adsorbed on Cu(111) studied by local probe spectroscopy at low temperatures. Morphology and electronic structure of atoms and molecules, obtained by conventional scanning tunneling microscopy/spectroscopy, are combined with transport properties measurements extracted from point contact spectroscopy. For C0 single atoms the transport properties are modulated by the Kondo screening. The Kondo temperatures observed in tunneling and in point contact regime are comparable. A general model to explain our experimental evidence is proposed. For the PVBA molecules, the transport properties are strongly affected by the molecule-metal adsorption orientation. This deepens our understanding of the role of the molecular arrangement in the nano-junction and in molecular electronic transport, and addresses the determining role of the molecule-metal contacts.

Electron transport across single phthalocyanine (Pc) molecules — Florian Witt1, Albert Takacs1,2, Tempey Balashov1, and Wulf Wulfhekel1,2 — 1Physikalisches Institut, Universität Karlsruhe, Wolfgang-Gaede Strasse 1, 76131 Karlsruhe, Germany — 2CFN-DFG Centrum für Funktionelle Nanostrukturen

Recently molecular electronics is discussed as a future replacement of semiconductor electronics. A detailed knowledge of the electronic properties of the molecules i.e. the HOMO-LUMO gap, the density of states and the conductance is necessary. Scanning Tunneling Microscopy (STM) in combination with Scanning Tunneling Spectroscopy (STS) has become one of the most important methods for studying these molecular properties. We present results on single molecule contact measurements obtained with STM at 4K. A small amount of H2Pc and CoPc molecules was evaporated on clean Cu(111) and Co/Cu(111). By laterally positioning the STM tip over isolated molecules and approaching the tip towards the molecules we measured the conductance as function of distance. Initially, an exponential increase was observed reflecting electron tunneling. Below a critical distance both H2Pc and CoPc molecules have a tendency to lift from the surface and jump to contact with the tip. After the jump, the conductance only weakly varies with the distance. On Cu(111) typical conductances of 0.1 G0 were found while on Co/Cu(111) the conductance is higher by a factor of 3. STS measurements in the tunneling regime revealed strong vibrational modes located on the organic side groups of Pc which are most likely responsible for the jump to contact.

Low dimensional electronic structure of a metal/organic interface — Isabel Fernández Torrehn1, Nora González Lakunza2, Katharina Jennifer Franke1, Nicolás Lorente3, Andrés Arnau1, and José Ignacio Pascual1 — 1Institut für Experimentalphysik, Freie Universität Berlin, Germany — 2Unidad de Física de Materiales, Centro Mixto CSIC-UPV/EHU, San Sebastián, Spain — 3Instituo de Ciencias de Materiales de Barcelona-CSIC, Barcelona, Spain

The TTF-TCNO charge donor-acceptor complex is a prototypical organic material. In bulk, it crystallizes in a monoclinic structure built up from parallel stacks of TTF and TCNQ, showing anisotropic conduction along the molecular rows. Our aim is to study the interface of a TTF-TCNQ organic film with a metal. By means of Low Temperature Scanning Tunneling Microscopy and Spectroscopy (LT-STM and STS) we characterise the structure and electronic properties of sub-monolayer films of TTF-TCNQ grown on Au(111). Both molecular species adsorb with a planar configuration. Nevertheless there is a strong donor-acceptor recognition and TTF and TCNQ self-assemble in alternating one-dimensional rows. This arrangement modifies strongly the electronic properties of the molecular entities and the surface state inducing the formation of a resonance with one-dimensional nature delocalised along the TCNQ rows. Ab-initio calculations explain the origin of the detected resonances by a strong modification of the surface state of the underlying metal upon hybridisation with TTF on the mixed TTF-TCNQ phase.