O 109: Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures VII

Organizers: Sabine Maier, FAU Erlangen-Nürnberg; Meike Stöhr, University of Groningen

(Synopsis provided with part I of this session)

Time: Friday 10:30–11:45 Location: MA 004

O 109.1 Fri 10:30 MA 004

Insight into the unit cell: Structure of picene thin films on Ag(100) revealed with complementary methods — •Tobias Huempfner, Martin Hafermann, Christian Udhardt, Felix Otto, Roman Forker, and Torsten Fritz — Friedrich Schiller University, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany

We studied the molecular structure of one monolayer of picene on a Ag(100) surface. Low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) experiments show that the molecules arrange in a highly ordered manner exhibiting a point-on-line epitaxy with two differently arranged molecules per unit cell. Besides the structural investigations, we also studied the electronic properties via photoelectron spectroscopy. In particular, we recorded photoelectron momentum maps (PMMs) at different binding energies. PMMs based on molecular orbitals obtained from density functional theory (DFT) calculations of free molecules are simulated for a better understanding of the measured maps. Comparing measured and simulated PMMs allows further conclusions about the composition of the unit cell. The structural basis consists of two parallel molecules; one molecule lies face-on and the other is tilted by 45° around its long axis with respect to the surface normal.

O 109.2 Fri 10:45 MA 004

construction of sierpiński triangles up to the fifth order — Chao Li, Xue Zhang, Na Li, •Jiajia Yang, and Yongfeng Wang — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China

Self-similar fractal structures are crucial in science, mathematics, and aesthetics. Recently, a series of molecular defect-free fractals of Sierpiński Triangles (STs) have been constructed on surfaces. In those previous experiments, the highest order of STs is simply 4th due to the random formation of nucleation centers and the limitation of kinetic growth. The growth mechanism of STs was investigated by low-temperature scanning tunneling microscopy. Here, we used a templating method to guide the formation of nucleation centers and co-assembly method to overcome the kinetic-growth limitation and control the formation of STs. Owing to the templating effect of the reconstructed Au(100)-(hex) substrate, Fe atoms, 4,4"-dicyano-1,1':3',1"terphenyl (C3PC), and 1,3-bis(4-pyridyl)benzene (BPyB) molecules were used to build fractals. According to our experiments, the proper C3PC : BPyB ratio is need to obtain the 5th-order STs. When C3PC molecules dominate, it tends to form a 1D crystalline chain structure. With large rate of BPyB to C3PC, the surface structures are determined by BPyB molecules and only small STs are obtained. The new strategy may be applied to construct various Sierpiński triangles of higher orders.

O 109.3 Fri 11:00 MA 004

Oxygen-triggered electronic and structural decoupling at the PTCDA/Cu(100) interface — •Xiaosheng Yang[1,2], Simon Weiss[1,2], Ina Krieger[3], Timo Heepenstrick[3], Michael Hollerer[4], Philipp Hurdax[4], Daniel Lüftner[4], Peter Puschnig[4], Georg Koller[4], Michael Ramsey[4], Moritz Sokolowski[3], Frank Stefan Tautz[1,2], and Serguei Soubatch[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, Germany — [3]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Germany — [4]Institut für Physik, Universität Graz, NAWI Graz, Austria

The electronic states and geometric vertical structures of perylenetetracarboxylic dianhydride (PTCDA) molecule upon an oxygen-reconstructed $(\sqrt{2} \times 2\sqrt{2})$R45° Cu(100) surface are investigated using ARPES and the NIXSW technique, respectively. The orbital tomography measurement found that, in contrast to PTCDA on intrinsic Cu(100) where strong molecule-substrate interactions are present [1], the oxygen adsorbed on Cu(100) prevents change transfer from metal substrate into the PTCDA molecule. Further, the geometry of the PTCDA layer on the oxygen-recontructed surface is determined to be flat with a high adsorption height. The results corroborate that the oxygen simultaneously induces electronic and structural decoupling at the molecule-metal interface.

[1] D. Lüftner et al., Physical Review B 96, 125402 (2017)

O 109.4 Fri 11:15 MA 004

Thermally-activated Self-assembly and In Situ Oxidation of a Reduced Decaazapentacene — David Miklik[1], •Fatemeh Mousavi[2], Aisha Ahsan[2], Anna Middleton[3], Yoshitaka Matsushita[1], Jan Labuta[1], Paul Karr[5], Pavel Svec[1,6], Filip Bures[7], Gary Richards[1,8], Francis Souza[3], Thomas Jung[1,4], and Jonathan Hill[1] — [1]MANA-NIMS, Tsukuba, Japan — [2]University of Basel, Switzerland — [3]University of North Texas, USA — [4]Paul Scherrer Institute, Switzerland — [5]Wayne State College, USA — [6]Institute of Macromolecular Chemistry, Praha, Czech Rep. — [7]University of Pardubice, Czech Rep. — [8]Ochanomizu University, Otsuka, Japan

The higher pyrazinacenes are a newly synthesized class of molecules which may take an important role in organic semiconductors. This is due to their expected n-type behaviour which complements to the already important p-type pentacene derivatives with their closely related molecular structure. We report on the supra-molecular interactions and self-assembly of octaazatetracene and decaazapentacenes, two different lengths molecules in this class. On atomically clean Cu(111) the initially achiral compounds take a chiral conformation upon adsorption. Both compounds are imaged individually and form structurally related chains. Dehydrogenation occurs upon thermal activation as recognized by its stronger adsorption in the form of individual units. This on-surface reaction is compared to the dehydrogenation in solution. Experimental evidence is provided by Scanning Tunneling Microscopy and X-ray Photoelectron Spectroscopy.

O 109.5 Fri 11:30 MA 004

Aggregation by Metallophilic Interaction — •Michael Györök[1], Sebastian Wolfmayr[1], Petra Gründlinger[1,2], Uwe Monkowius[3], Peter Zeppenfeld[1], and Thorsten Wagner[1] — [1]Johannes Kepler University, Experimental Physics, Linz, Austria — [2]Johannes Kepler University, Inorganic Chemistry, Linz, Austria — [3]Johannes Kepler University, School of Education, Linz, Austra

Metallophilicity describes attractive interactions between two or more metal atoms with closed shell configurations (i.e. d^8, d^{10}). Metal complexes containing gold in the formal oxidation state +I show very strong attractions, which are therefore also referred to as aurophilicity [1,2]. As a result, the aurohilic interactions determine often the arrangement of gold(I) complexes in the solid state. However, there are almost no examples in the literature, where this attractive interaction has been studied on surfaces. 2-naphthyl-isonitrile-gold(I)-chloride is and stable enough to sublime under ultrahigh vacuum conditions at moderate temperatures of 400 K. Ultrathin films of this molecule were prepared by physical vapor deposition on Au(111) surfaces. The deposition was monitored by differential reflectance spectroscopy (DRS) and photoelectron emission microscopy (PEEM). Finally, the structure of the organic film was analyzed by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) confirming an antidimer structure similar to the known bulk structure.

[1] P. Pyykkö, Chem. Rev. 97, 597 (1997).

[2] F. Schwerbaum *et al.*, Angew. Chemie 27, 1544 (1988).