

## O 59: Molecular Nanostructures

Time: Thursday 9:30–12:00

Location: MA 041

O 59.1 Thu 9:30 MA 041

**Organic Molecular Nanowires: N,N'-dimethylperylene-3,4,9,10-bis(dicarboximide) on KBr(001) and NaCl(001)** — ●MARKUS FENDRICH, CHRISTIAN WEISS, MANFRED LANGE, TOBIAS KUNSTMANN, and ROLF MÖLLER — Fachbereich Physik, Universität Duisburg-Essen, D-47048 Duisburg

The growth of N,N'-dimethylperylene-3,4,9,10-bis(dicarboximide) (DiMe-PTCDI) on KBr(001) [1] and NaCl(001) has been studied by frequency modulation atomic force microscopy. On both substrates, DiMe-PTCDI forms molecular wires with a length of up to 600 nm at low coverages. The height of the wires is two or more molecular layers; all wires grow along the [110] and  $\bar{1}$ [10] direction of the alkali halide (001) substrates. There is no wetting layer of molecules: Atomic resolution of the substrates can be achieved between the wires. Due to their size and shape, the molecular nanowires might act as a model system for organic electronics research on insulating substrates. Calculations using empirical potentials reveal possible growth mechanisms for both substrates.

[1] M. Fendrich and T. Kunstmann, Appl. Phys. Lett. 91, 023101 (2007)

O 59.2 Thu 9:45 MA 041

**Structural coherency of graphene on Ir(111)** — ●CORAUX JOHANN, N'DIAYE ALPHA, BUSSE CARSTEN, and MICHELY THOMAS — University of Cologne - Institute of Physics 2, Zuelpicher Str. 77, 50937 Cologne, Germany

We investigate the high structural quality of monolayers of graphene prepared on Ir(111). Using scanning tunneling microscopy, we show that graphene prepared this way exhibits remarkably large-scale continuity of its carbon rows over terraces and step edges. The graphene layer contains only a very low density of defects. These are zero-dimensional defects, edge dislocation cores consisting of heptagon-pentagon pairs of carbon atom rings, which we relate to small-angle in-plane tilt boundaries in the graphene. We quantitatively examined the bending of graphene across Ir step edges. The corresponding radius of curvature compares to those of thin single-wall carbon nanotubes. *J. Coraux, A. T. N'Diaye, C. Busse, T. Michely, submitted.*

O 59.3 Thu 10:00 MA 041

**Orientationally ordered (7×7) superstructure of C<sub>60</sub> on Au(111)** — GUILLAUME SCHULL and ●RICHARD BERNDT — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Long range orientational order within C<sub>60</sub> monolayers on Au(111) is observed with low-temperature scanning tunneling microscopy. A unit cell comprised of 49 molecules which adopt 11 different orientations is found. It can be divided in a faulted and an unfaulted half similar to the (7×7) reconstruction of Si(111). A model is proposed, which shows how through a Moiré-like effect, the substrate induces minute changes in the orientation of the C<sub>60</sub> molecules. Intermolecular interactions are shown to play a major role in stabilizing the superlattice

O 59.4 Thu 10:15 MA 041

**Morphology of C<sub>58</sub> layers deposited on HOPG** — ●STEFAN SVEN JESTER, DANIEL LÖFFLER, PATRICK WEIS, ARTUR BÖTTCHER, and MANFRED M. KAPPES — Institut für Physikalische Chemie, Universität Karlsruhe, 76131 Karlsruhe, Germany

The low energy cluster beam deposition technique, LECBD, has been applied to grow monodisperse layers comprising of mass-selected carbon clusters, so called non-IPR fullerenes, C<sub>n</sub>, 50 < n < 60 [1/]. The morphology of the C<sub>n</sub> layers deposited on HOPG has been studied by applying atomic force microscopy. The deposition has been performed at hyperthermal kinetic energies, E<sub>0</sub>, ranging from 1 - 49 eV. The initial capability of the C<sub>n</sub> cages to adhere to the surface is governed by the lateral density of step edges which act as pinning and nucleation centers for migrating cages. Consequently the surface exhibits large areas of empty terraces and decorated step edges. The flat terraces become decorated by dendritic C<sub>n</sub> islands only in later deposition stages. Both, the mean size of the 2D islands and the mean distance between nearest islands, d, scale with the size of the terraces. The topography of the islands depends sensitively on the primary kinetic energy, E<sub>0</sub>, and the surface temperature, TS. We explain these find-

ings by considering the loss of the primary kinetic energy induced by molecular friction experienced by the C<sub>n</sub> cages during their ballistic sliding/slipping path across the surface [2/].

[1] A. Böttcher, P. Weis, A. Bihlmeier, M.M. Kappes, PCCP 6 (2004) 5213 [2] a) W.D. Luedtke and U. Landman, Phys. Rev. Lett. 82 (1999) 3835, b) E. Molinari, M. Tomellini, Surf. Sci., 601 (2007) 1

O 59.5 Thu 10:30 MA 041

**A scalable open-pore network: melamine and fatty acids on graphite** — ●HERMANN WALCH, ANNE-KATHRIN MAIER, WOLFGANG M. HECKL, and MARKUS LACKINGER — LMU München, Sektion Kristallographie, Theresienstr. 41, 80333 München

Scanning tunneling microscopy (STM) at the liquid-solid interface was utilized to investigate bimolecular open pore networks comprised of melamine and the homologous series of fatty acids extending from pentanoic through dodecanoic acid. Since at room temperature longer fatty acids (from decanoic acid on) are solid a novel heatable sample holder for measuring at slightly elevated temperatures was designed. Structural properties of the self-assembled monolayers (SAMs) were deduced from the STM data and modelled by force field calculations. Melamine is a heterocyclic aromatic molecule consisting of a triazine ring functionalized with three amine-groups at the 2-, 4-, and 6-positions. In this study, the fatty acids serve as a solvent for melamine but are also incorporated into the SAMs. For all solvents hexagonal honeycomb structures were observed, where the lattice parameter increases linearly from 2.8 nm to 3.8 nm with the chain length of the solvent. All networks exhibited a similar architecture: melamine molecules are located at the corner of hexagons and two adjacent melamins are interconnected by fatty acid molecules in head to tail configuration. Each of the connecting fatty acid molecules forms two H-bonds with one of the melamine molecules. Hence, melamine accounts for the symmetry of the structures, whereas the fatty acid molecules act as a spacer, thus giving rise to the remarkable scalability of these bimolecular networks.

O 59.6 Thu 10:45 MA 041

**Aromatic vs. Hydrogen Bonds in Self-Assembled Monolayers of Organic Molecules, a STM-Study** — ●RICO GUTZLER, SOPHIE LAPPE, WOLFGANG M. HECKL, and MARKUS LACKINGER — LMU München, Sektion Kristallographie, Theresienstr. 41, 80333 München

The monolayer structure of two distinct organic molecules is investigated by STM. We demonstrate how a small modification of a polyaromatic molecule, which does not affect the functional groups, can have dramatic impact on the structure of the self-assembled monolayer. Both molecules exhibit C<sub>3</sub> symmetry, have a central benzene ring in common and three carboxylic groups at the 1,3,5 positions, each separated by a rigid spacer. One compound exhibits methyl groups at the 2,4,6 positions of the central benzene ring, the other remains unsubstituted. This change in molecular structure was found to result in completely different self-assembly behaviour at the liquid-graphite interface. The unsubstituted molecule adsorbs in a row structure, where the molecules are stacked with their planes almost perpendicular to the substrate. The methylated molecule self-assembles into a sixfold chickenwire network where the molecules are adsorbed planar. Based on our experimental finding and supported by force field calculations, we propose that in the first case the intermolecular binding is dominated by aromatic interaction between the extended pi-electron systems, whereas in the latter case the chickenwire structure is driven by twofold intermolecular hydrogen bonds between the peripheral carboxylic groups. This finding is explained by weakening of the pi-pi stacking due to steric hindrance imposed by the methyl groups.

O 59.7 Thu 11:00 MA 041

**Template Readout of Hierarchical Coordination Networks at Surfaces** — ●ALEXANDER LANGNER<sup>1</sup>, STEVEN L. TAIT<sup>1</sup>, NIAN LIN<sup>1</sup>, CHANDRASEKAR RAJADURAI<sup>2</sup>, MARIO RUBEN<sup>2</sup>, and KLAUS KERN<sup>1,3</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Stuttgart — <sup>2</sup>Forschungszentrum Karlsruhe GmbH — <sup>3</sup>Ecole Polytechnique Fédérale de Lausanne, Switzerland

Self-assembly of organic molecules into supramolecular networks is an efficient strategy to pattern surfaces with functional nanostructures. Highly ordered architectures can be achieved if the spontaneous self-

organization process is steered by selective and directional non-covalent interactions. Here we demonstrate that from a mixture of organic ligands, several unique structures can be "read out" by adjusting the external environment of the mixture. We report on the self-organization of mixtures of multiple ligands with metal atoms at the Cu(100) surface under ultra high vacuum (UHV) conditions. The generated architectures exhibit a hierarchy of supramolecular interactions: highly stable metal-organic coordination bonding and somewhat weaker hydrogen bonding. With scanning tunneling microscopy (STM) we demonstrate that modification of external parameters, e.g. commensurability with substrate or introduction of guest molecules, causes distinct structural configurations for identical ligand binding units, even leading in some cases to complete ligand segregation. Due to the hierarchy of bonding strengths, it is possible to modify only the lower level of structural organization resulting in new metal-organic architectures with identical primary structural units.

O 59.8 Thu 11:15 MA 041

**Structure and Charge Transfer in Metal-TCNQ Complexes on Cu (100)** — •Tzu-CHUN TSENG<sup>1</sup>, STEVEN L. TAIT<sup>1</sup>, XIONG LIU<sup>1</sup>, NIAN LIN<sup>1</sup>, and KLAUS KERN<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — <sup>2</sup>Institut de Physique des Nanostructures, Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

Organic-based alternatives to conventional magnets offer the possibility to form self-organized nanometer-scale structures at surfaces with specific magnetic properties. For example, coordination compounds of metal ions (M) with the organic molecule 7,7,8,8-tetracyanoquinodimethane (TCNQ) in solution have been shown recently to have a high magnetic ordering temperature for large M:TCNQ ratios (R. Jain et al., Nature 445 (2007) 291-294). A critical issue for the development of metal-organic structures in magnetic or electronic applications is the relationship of electronic configuration to physical structure. Here we correlate structural information of 2D M-TCNQ (M = Mn, Fe, Co, Ni, Cu) networks from scanning tunneling microscopy and low energy electron diffraction with charge transfer information obtained by X-ray photoemission spectroscopy. M-TCNQ mixtures at Cu(100) self-organize into ordered structures, whose coordination ratio and domain size depend strongly on the choice of metal. XPS results identify distinct core level shifts in N 1s spectra of M-TCNQ for 2D coordination to different metal centers compared to neutral TCNQ.

O 59.9 Thu 11:30 MA 041

**Video-STM investigation of the dynamic behavior of bis-terpyridine submonolayers on Ag(111)-oriented films** — •THOMAS WALDMANN, HARRY E. HOSTER, and R. JÜRGEN BEHM —

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We present a quantitative analysis of the dynamic exchange of single molecules between two phases [1] of a bis-terpyridine derivative (2,4'-BTP) [2] adlayer adsorbed on Ag(111)-oriented thin films on Ru(0001). The analysis is based on video-STM measurements in ultra high vacuum at room temperature. The adlayer was produced by evaporation on a highly ordered (111)-oriented Ag film, which leads to the formation of a quasi-quadratic network (QQN) [2, 3]. Via thermal desorption it is possible to create defects in the QQN, which leads to a new disordered phases with a quasi-hexagonal short-range order (QHP). Depending on the BTP coverage 70-90% of the molecules in the QHP are rotating, while the rest exhibits preferred orientations in steps of 30°. At the QQN/QHP phase boundary, we observed molecules jumping back and forth between both phases. From the different probabilities to find the molecules in either phase we estimated the corresponding energy difference via a Boltzmann-approach.

[1] Poster O 18.58

[2] C.Meier et al., J.Phys.Chem.B 109, 21015 (2005)

[3] H.E.Hoster et al., Langmuir 23, 11570 (2007)

O 59.10 Thu 11:45 MA 041

**Bottom-up construction of covalently bound molecular nanostructures** — •LEONHARD GRILL<sup>1</sup>, MATTHEW DYER<sup>2</sup>, LEIF LAFFERENTZ<sup>1</sup>, MATS PERSSON<sup>2</sup>, MAIKE PETERS<sup>3</sup>, and STEFAN HECHT<sup>3</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, Berlin — <sup>2</sup>Department of Chemistry, University of Liverpool, Liverpool L69 3BX, UK — <sup>3</sup>Institut für Chemie, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, Berlin

The ultimate goal of molecular electronics consists in the use of single functionalized molecules for circuits at the atomic scale. In possible future applications, such molecular arrays need to be highly stable and allow charge transport between the molecular building blocks. Hence, covalent bonds are desired for the intermolecular connections. However, up to now only rather weak interactions have been reported for supramolecular networks on surfaces.

We report on the controlled formation of covalently bound networks of porphyrin molecules on a gold surface upon deposition of thermally activated molecular building blocks and their subsequent chemical reaction at predefined connection points [1]. Scanning tunneling spectroscopy measurements, lateral manipulation, and density functional theory calculations unambiguously reveal the covalent character of the intermolecular bonds. Furthermore, we show that the dimensions and shape of these nanostructures can be precisely engineered by controlling the number of bromine substituents of the molecular building block, leading to the formation of dimers, chains and networks.

[1] L. Grill et al., Nature Nanotech. 2, 687 (2007).