

## O 91: Nanostructures at Surfaces: Molecular Systems I

Time: Thursday 10:30–13:00

Location: REC/PHY C213

O 91.1 Thu 10:30 REC/PHY C213

**Synthesis of highly ordered arrays of organic nanowires on a magnetic surface alloy** — ●JENS BREDE<sup>1</sup>, MIKEL ABADIA<sup>1</sup>, CELIA ROGERO<sup>1,2</sup>, IGNACIO PIQUERO-ZULAICA<sup>1</sup>, MAXIM ILYN<sup>1</sup>, and J. ENRIQUE ORTEGA<sup>1,2,3</sup> — <sup>1</sup>Centro de Física de Materiales CFM-MPC(CSiC-UPV/EHU), Paseo Manuel Lardizabal 5, E-20018 San Sebastián, Spain — <sup>2</sup>Donostia International Physics Center, Paseo Manuel Lardizabal 4, E-20018 San Sebastián, Spain — <sup>3</sup>Departamento Física Aplicada I, Universidad del País Vasco, E-20018 San Sebastián, Spain

The transfer of well-established *in-situ* methods for growing covalently bonded macromolecules with atomic precision onto magnetic substrates presents a viable route toward studying emergent intrinsic magnetic properties in these novel structures as well as their magnetic coupling to the underlying substrate. Here, we present a multi-technique characterization of the polymerization of 4,4-dibromoterephenyl precursors into ordered arrays of poly (p-phenylene) chains on top of the bimetallic GdAu<sub>2</sub> surface alloy. The activation temperature for bromine scission and subsequent homocoupling of molecular precursors was followed by temperature dependent XPS. Structural characterizations of the highly ordered molecular and polymeric phases were performed by LEED and STM. The electronic structures of the valence band of the different phases were determined with ARPES and magnetic ordering in the GdAu<sub>2</sub> alloy was established by XMCD during all stages of the reaction.

O 91.2 Thu 10:45 REC/PHY C213

**Light-Induced Translation of Motorized Molecules on a Surface** — ●ALEX SAYWELL<sup>1,2</sup>, ANNE BAKKER<sup>1</sup>, JOHANNES MIELKE<sup>1</sup>, TAKASHI KUMAGAI<sup>1</sup>, MARTIN WOLF<sup>1</sup>, VICTOR GARCÍA-LÓPEZ<sup>3</sup>, PINN-TSONG CHIANG<sup>3</sup>, JAMES M. TOUR<sup>3</sup>, and LEONHARD GRILL<sup>1,4</sup> — <sup>1</sup>Department of Physical Chemistry, Fritz-Haber-Institute of the Max-Planck Society, 14195 Berlin, Germany. — <sup>2</sup>School of Physics & Astronomy, The University of Nottingham, United Kingdom. — <sup>3</sup>Rice University, Houston, Texas 77005, United States. — <sup>4</sup>Department of Physical Chemistry, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria.

A key component of molecular nanotechnology are molecular machines that can perform controlled work. The motion of such machines should be triggered remotely in order to address a large number of molecules at the same time, with light being an attractive stimulus as a single source. Here, we report the photo-induced translation of molecular machines across a surface by characterizing single molecules before and after illumination. Illumination of molecules containing a motor unit results in an enhancement in the diffusion of the molecules. The effect vanishes if an incompatible photon energy is used or if the motor unit is removed from the molecule, revealing that the enhanced motion is due to the presence of the wavelength-sensitive motor in each molecule.

O 91.3 Thu 11:00 REC/PHY C213

**Charge switching in multi-ferrocene molecules observed** — ●MARTIN ONDRÁČEK, PAVEL JELÍNEK, JAN BERGER, OLEKSANDR STETSOVYCH, and MARTIN ŠVEC — Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

The ability to switch between different redox states makes ferrocene molecules an attractive subject of research aiming to nano-scale electronics. Linking several ferrocene units into multi-ferrocene molecules expands the potential functionality, due to the interaction among the individual ferrocene sub-units and the possibility to switch their charge state in a coordinated manner. Our study shows how the charge of bis- and tetra-ferrocene molecules on NaCl substrate can be detected and controlled by an atomic force microscope (AFM). Here, I focus on theoretical explanation of the main features observed in the AFM and electrostatic force spectroscopy (EFM) with these molecules. Especially notable are sharp boundary-like features characterized by increased frequency shift as well as an increased energy dissipation signal. We interpret them in terms of charge transfer among the ferrocene centers facilitated by the AFM tip. Using a modified version of an earlier written simulator [1], we back our interpretation with a model that encompasses the AFM cantilever dynamics and electrons hopping among the AFM tip and ferrocene centers. We supplement our empirical model with DFT-based calculations of the geometry and electronic structure

of the molecules on NaCl.

[1] M. Ondráček, P. Hapala, P. Jelínek, *Nanotechnology* **27**, 274005 (2016).

O 91.4 Thu 11:15 REC/PHY C213

**Electric-field effect on the formation of single-molecule contacts** — ●JONATHAN BRAND, NICOLAS NÉEL, and JÖRG KRÖGER — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau

Pristine and C<sub>60</sub>-terminated tips of an atomic force microscope are used to form contacts to single C<sub>60</sub> molecules adsorbed on Pb(111) and Cu(111). A pronounced variation of the point of contact with the electric potential difference across the junction is inferred from bias-dependent force spectroscopy. The conventional approach to describing forces in atom-scaled junctions by a superposition of van der Waals, electrostatic, and Lennard-Jones forces with a rigid junction geometry fails. Rather, the experimental observations may be rationalized by considering voltage-dependent relaxations of the electrodes.

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O 91.5 Thu 11:30 REC/PHY C213

**Control of charge states within a single molecule** — ●JAN BERGER<sup>1</sup>, OLEKSANDR STETSOVYCH<sup>1</sup>, MARTIN ONDRÁČEK<sup>1</sup>, MARTIN ŠVEC<sup>1</sup>, IRENA G. STARÁ<sup>2</sup>, IVO STARÝ<sup>2</sup>, and PAVEL JELÍNEK<sup>1</sup> — <sup>1</sup>Institute of Physics, ASCR, Prague, Czech republic — <sup>2</sup>Institute of Organic Chemistry and Biochemistry ASCR, Prague, Czech republic

The field of molecular electronics aims at using a single molecule as building block for electronic devices. Ferrocene-based molecules are extremely appealing as they offer prospects of having a built-in charging functionality. They are known of being stable under redox states and therefore promising as candidates for quantum cellular automata units. Previous works demonstrated charging single metal adatoms [1], molecules or their clusters on insulating films [2] as well as charging of large self-assembled islands of molecules by STM or nc-AFM. [3]

Here we will present experimental evidence of controlling multiple charge states on a single 3,6,3',6'-tetraferrocene-9,9'-bis-fluorenylidene, deposited on thin insulating NaCl film, by means of nc-AFM. We succeed to control the multiple charge states within a single molecule including reversible transitions between them. The induced charged states have prominent fingerprints in both the frequency shift and dissipation channels. Moreover, we demonstrate that the charge states can be modified by presence of neighboring charged molecules.

[1]J. Repp et al., *Science* **305**, 493 (2004) [2]W. Steurer et al., *Nature Comm.* **6**:8353 (2015). [3]P. Rahe et al., *Nano Letters* **2**, 16 (2016)

O 91.6 Thu 11:45 REC/PHY C213

**Revealing an atomic nodal plane by LT-UHV-STM investigations on single benzylnaphthoic diimides** — ●RENÉ EBELING<sup>1</sup>, SHIGERU TSUKAMOTO<sup>2</sup>, VASILE CACIUC<sup>2</sup>, NICOLAE ATODIRESEI<sup>2</sup>, STEFAN BLÜGEL<sup>2</sup>, RAINER WASER<sup>1</sup>, and SILVIA KARTHÄUSER<sup>1</sup> — <sup>1</sup>Forschungszentrum Jülich GmbH - (PGI-7), Jülich, Germany — <sup>2</sup>Forschungszentrum Jülich GmbH - (PGI-1/IAS-1), Jülich, Germany

The LT-UHV-STM investigations presented here demonstrate the adsorption behavior and the exact geometry of single target molecules in orbital resolution on atomically flat surfaces of Pt(111). The conformation and the orbital symmetry of single molecules have been deduced. For this purpose N,N'-dibenzyl-naphthoic diimide (BNI), which consists of a large  $\pi$ -conjugated backbone and two phenyl-rings each connected with a methylene-linker to the central part, have been studied. According to the high resolution STM images, the naphthoic diimide backbone of the molecule adsorbs flat on the substrate while the two benzyl groups build one line together with the backbone and the atomic nodal plane can be identified located at the C atoms of the phenyl rings. That points to phenyl groups standing vertically with their phenyl plane on the substrate. The orbital symmetry of the HOMO and the LUMO identified by STM was compared to DFT based calculations on BNI in the gas phase and tunneling transmission calculations which take the 3-dimensional structure of the molecule into account. These calculations agree with the measurements and provide further evidence for the supposed structure of BNI on Pt(111).

O 91.7 Thu 12:00 REC/PHY C213

**Formation of metallofullerene magnetic arrays: theoretical perspectives.** — ●STANISLAV AVDOSHENKO and ALEXEY POPOV — Institute for Solid State Research, IFW, Dresden

Modeling of formation and properties self-assembled monolayer (SAM) is a very challenging task, especially if highly functional-ligands are concerned. It is true, for instance, in the case of endohedral metallofullerene (EMF) based SAM - promising single molecular magnets (SMMs) grids in-making. Properties of such SMM grids would be a function of SAM architecture (attachment types and crowding effects) and innercluster dynamics under these geometrical constrains. Electronic structure complexity of EMFs and structural mobility of ligands in SAMs brings a dual issue. On the one hand, a minimal level of theory to address the magnetic properties of the systems would require "complete active space"- quality methods. On the other hand, while the system dynamic can be approached by less computationally demanding semiclassical or even classical approaches, such methods are unable to give a reliable magneto-physics of the SMM unit. In our report, we will offer a set of concepts to deal with this problem by extensive development of the multiscale methods (MSM), in which the whole system is divided into the regions described with different levels of theory accordingly to its complexity.

O 91.8 Thu 12:15 REC/PHY C213

**Metal-coordinated molecular chains on gold** — ●SUJOY KARAN and JASCHA REPP — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Choosing right precursors (molecules) is a prerequisite for getting desired polymerized structures, be it a graphene nanoribbon or other molecular networks, on surfaces. When metal atoms are incorporated into those structures, the bondings may change to form completely different networks. We show that metal coordination may not only change the structures of the networks but can also have different physical properties.

O 91.9 Thu 12:30 REC/PHY C213

**Tuning the adsorption and self-assembly of terpyridine derivatives: From metal to bulk insulator surfaces** — ●TUAN ANH PHAM<sup>1</sup>, YI LIU<sup>1</sup>, MANH THUONG NGUYEN<sup>2</sup>, and SABINE MAIER<sup>1</sup> — <sup>1</sup>Department of Physics, University Erlangen-Nürnberg, Erwin-Rommel-Str. 1, 91058 Erlangen, Germany — <sup>2</sup>Center for Computational Physics, Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan St., Hanoi, Vietnam

Controlling and understanding the on-surface self-assembly of organic

molecules are of utmost importance for the effective usage of molecular systems in potential applications. On metal surfaces, it is well-known that the structure of the on-surface self-assembly is strongly dependent on the subtle balance between molecule-molecule and molecule-substrate interactions. On bulk insulators, however, the role of the molecule-substrate interaction on the structure formation is widely unexplored.

Herein, we report the self-assembly of terpyridine derivatives, on both, metal (Au and Cu) and bulk insulator surfaces (KBr), by a combination of high-resolution non contact atomic force microscopy at low temperatures and density functional theory. We achieved to selectively tune the dimensionality of the molecular structures depending on the choice of the substrate: monomeric species on Cu(111), linear chains on Au(111), and two-dimensional networks on KBr. Interestingly, we found that the substrate may induce the rotation of pyridine rings around the C-C bond axis in the terpyridine units and thus, generating the formation of H-bonds stabilizing the self-assembled networks.

O 91.10 Thu 12:45 REC/PHY C213

**Metal coordination of tri-cyano-lophine on surfaces** — ●BODONG ZHANG<sup>1</sup>, LI JIANG<sup>1</sup>, YUANYUAN GUO<sup>1</sup>, GUILLAUME MÉDARD<sup>2</sup>, SIMON NADAL<sup>2</sup>, BERNHARD KUSTER<sup>2</sup>, FRANCESCO ALLEGRETTI<sup>1</sup>, JOACHIM REICHERT<sup>1</sup>, ANTHOULA C. PAPAGEORGIOU<sup>1</sup>, and JOHANNES V. BARTH<sup>1</sup> — <sup>1</sup>Chair of Molecular Nanoscience & Chemical Physics of Interfaces (E20), Department of Physics, Technical University of Munich, DE — <sup>2</sup>Chair of Proteomics and Bioanalytics, Technical University of Munich, DE

Lophine (2,4,5-triphenylimidazole) and its derivatives are of interest due to their large potential in chemiluminescence, fluorescence, and bioanalytics. To expand the application of lophine derivatives, they have been decorated with various functional groups, such as -H, -OH, -NO<sub>2</sub>, -CN. Cyano groups are known to direct the fabrication of well defined metal coordination structures on surfaces through their interaction with metal atoms.

Here, we study the self-assembly and metal directed assembly of a tri-cyano-lophine on Ag(111), Au(111) and Cu(111) surfaces with scanning tunneling microscopy and X-ray photoelectron spectroscopy. On Ag and Au, well-ordered phases are stabilized by dipolar coupling and attractive interactions between cyano groups and phenyl rings. Addition of Co/Fe atoms leads to three-fold coordination of the terminal cyano groups. However, on Cu a different well-ordered phase forms, exhibiting hydrogen bonding of the C≡N...H-N type. Annealing leads to complete Cu adatom coordination of a terminal cyano group and a deprotonated N atom of the imidazole moiety.