

O 110: Molecular Films: Morphology, Electronics, Photovoltaics

Time: Friday 10:30–13:00

Location: GER 38

Invited Talk

O 110.1 Fri 10:30 GER 38

Ceramics for Metal-Organic Frameworks (MOFs) based devices — ●PAOLO FALCARO — Graz University of Technology — The University of Adelaide — International Institute for Nano/Meso Materials Science

Metal organic frameworks (MOFs) are a class of ultra-porous materials with exceptionally high accessible surface area due to the framework produced by the inorganic nodes coordinated by organic ligands.^{1,2} An increasing number of studies are investigating MOFs for a variety of functional applications including sensing, microelectronics, energy production, drug delivery and microfluidics.³ However, MOF-based device fabrication requires synthetic protocols for the controlled functionalization of the porous crystals and the integration in suitable platforms.⁴ Ceramics have been recently employed for the synthesis,^{5,6} crystal engineering,⁶ functionalization,^{7,8} and patterning^{9,10} of MOFs. This presentation will summarize the recent progress in this emerging field.

References (1) Furukawa et al. *Science* 2013, 341(6149), 1230444. (2) Kitagawa et al. *Angew. Chem. Int. Ed.* 2004, 43(18), 2334. (3) *Chem. Soc. Rev.* 2014, 43 - special issue on MOFs. (4) Falcaro, et al. *Chem. Soc. Rev.* 2014, 43(16), 5513. (5) Buso et al. *Chem. Mater.* 2011, 23(4), 929. (6) Reboul et al. *Nat. Mater.* 2012, 11(8), 717. (7) Doherty et al. *Acc. Chem. Res.* 2014, 47(2), 396. (8) Ricco et al. *J. Mater. Chem. A* 2013, 1(42), 13033. (9) Zanchetta et al. *Chem. Mater.* 2015, 27(3), 690. (10) Okada et al. *Adv. Funct. Mater.* 2014, 24(14), 1969.

O 110.2 Fri 11:00 GER 38

Heterochiral to Homochiral Transition in Pentahelicene 2D Crystallization Induced by Second-Layer Nucleation — ●ANAIS MAIRENA¹, LAURA ZOPPI², JOHANNES SEIBEL¹, ALIX TRÖSTER³, KONSTANTIN GRENADER³, MANFRED PARSCHAU¹, ANDREAS TERFORT³, and KARL-HEINZ ERNST^{1,2} — ¹Empa, Dübendorf, Switzerland — ²University Zürich, Zürich, Switzerland — ³Goethe-Universität, Frankfurt, Germany

Chirality is ubiquitous in the molecular world, but the principles of intermolecular recognition are still poorly understood. A promising approach towards a better understanding of chiral interactions is the study of self-assembly of chiral molecules on surfaces with submolecular-resolution scanning tunneling microscopy.

The self-assembly of helical racemic pentahelicene ([5]H, C₂₂H₁₄) on Cu(111) leads, at very low coverages to formation of non-covalently-bonded homochiral dimers. At coverages close to the monolayer (ML), two distinct long-range ordered structures have been observed. They both have homochiral dimers as building blocks. One structure consists of a conglomerate of homochiral domains, while the second structure is a racemate composed of homochiral pairs with opposite handedness. At full ML coverage only the racemic structure prevails. Above ML coverage, a transition from the denser racemate phase into the less dense homochiral conglomerate phase occurs. The observation of such transition in the 1st layer, induced by 2nd layer nucleation is unprecedented in surface science. It indicates a long-range chiral communication between 2nd layer islands and other areas on the surface.

O 110.3 Fri 11:15 GER 38

Electronic Properties of Tailored Co-Salophene Based Building Blocks on Ag(111) — ●MICHA ELSEBACH¹, EMIL SIERDA¹, BERNHARD BUGENHAGEN², MARC PROSENC², ROLAND WIESENDANGER¹, and MACIEJ BAZARNIK¹ — ¹Institute for Nanostructures and Solid State Physics, University of Hamburg, D-20355 Hamburg, Germany — ²Institute of Inorganic Chemistry, University of Hamburg, D-20146 University of Hamburg, Germany

Spintronic devices based on molecules are a promising approach for the future of information technology. Recently we showed that Co-salophenes can be used for the fabrication of such a device on Au(111) [1]. The basic building blocks for this device are 2Br-Co-salophenes and 3Br-3Co-salophenes. These molecules can be covalently linked by the use of an on-surface Ullmann reaction. On the Au(111)-surface the Kondo effect inhibits the control of the molecules' magnetic centers by an external magnetic field. Therefore we are searching for a different substrate material, on which all properties of the molecules are preserved, excluding the Kondo screening.

In this talk I will present STM studies on the electronic properties

of single molecules as well as molecular chains formed by Ullmann reaction on Ag(111). The results show that the electronic structure of the molecules is promising for a working spintronic device, and that there is no Kondo effect on the Ag(111)-substrate.

[1] Bazarnik et al. *Nano Letters* 2016 16 (1), 577-582

O 110.4 Fri 11:30 GER 38

Single molecule manipulation via inelastic electron tunneling — ●GITIKA SRIVASTAVA¹, TIBOR KUDERNAC², MANFRED PARSCHAU¹, PETER STACKO³, NATSUKI ITO⁴, TAKASHI HIROSE⁴, KENJI MATSUDA⁴, BERNARD LUCAS FERINGA³, and KARL-HEINZ ERNST^{1,5} — ¹Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — ²University of Twente, The Netherlands — ³University of Groningen, The Netherlands — ⁴Kyoto University, Japan — ⁵University of Zürich, Switzerland

Manoeuvring individual molecules over a clean and unmodified surface is challenging, yet possible using surface sensitive techniques like Scanning Tunneling Microscopy (STM). Electronic and vibrational excitation by means of inelastic electron tunnelling from the tip of STM has been observed to have brought out subsequent dynamical processes on surfaces. We investigate the influence of inelastic electron tunnelling on helical molecules and have observed molecular motions like hopping and rotation. First results of single molecular dynamics of these molecules at low temperatures (7K) on Cu(111) and Au(111) surfaces are presented and discussed. In addition, we present latest results on molecular machines, a topic that has been awarded the Chemistry Nobel Prize in 2016.

O 110.5 Fri 11:45 GER 38

Determination of large converse piezoelectric effect on a single molecule — OLEKSANDER STETSOVYCH¹, ●MARTIN SVEC¹, PINGO MUTOMBO¹, ONDREJ KREJCI¹, IRENA STARA², IVO STARY², and PAVEL JELINEK¹ — ¹Institute of Physics, CAS, Praha, Czech republic — ²Institute of Chemistry and Biochemistry, CAS, Praha, Czech republic

The converse piezoelectric effect is a phenomenon, in which a mechanical strain is generated in a material due to an applied electrical field. Demonstration of the piezoelectric effect on nanoscale remains a challenge. In this work, we investigate the piezoelectric effect in single 2,17-Bis(acetylsulfanyl) heptahelicene (BA7H) molecules on Ag(111), using the non-contact atomic force microscopy (AFM). The BA7H on the substrate forms various islands, which can be effectively disassembled to individual molecules by the AFM tip, to exclude collective influence on the piezoelectric measurements. The acetylsulfanyl group at the terminal of the molecule exposed to the tip can be reversibly rotated between two metastable configurations via tip interactions. We characterized the bias-induced deformations of the BA7H and found that the piezoelectric constant is independent of the acetylsulfanyl group conformation, thereby demonstrating the piezoelectric effect is intrinsic to the helicene core. The total energy DFT calculations reveal strong charge transfer between BA7H molecule and the metallic substrate, which gives rise to a vertical electric dipole, which causes together with a soft vibrational mode of the molecule the strong piezoelectric effect.

O 110.6 Fri 12:00 GER 38

Lazarevite-type short-range ordering in ternary III-V nanowires — ●MICHAEL SCHNEDLER¹, ISABELLE LEFEBVRE², TAO XU^{2,3}, VERENA PORTZ¹, GILLES PATRIARCHE⁴, JEAN-PHILIPPE NYS², SÉBASTIEN PLISSARD^{2,5}, PHILIPPE CAROFF^{2,6}, MAXIME BERTHE², HOLGER EISELE⁷, RAFAL DUNIN-BORKOWSKI¹, PHILIPP EBERT¹, and BRUNO GRANDIDIER² — ¹Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Germany — ²Dép. ISEN, Institut d'Electronique, de Microélectronique et de Nanotechnologie, CNRS, UMR 8520, Lille Cedex, France — ³Key Laboratory of Advanced Display and System Application, Shanghai University, PRC — ⁴Laboratoire de Photonique et de Nanostructures (LPN), CNRS, Université Paris-Saclay, Marcoussis, France — ⁵Laboratoire d'Analyse et d'Architecture des Systèmes (LAAS), CNRS, Université de Toulouse, France — ⁶Dep. of Electronic Materials Engineering, Research School of Physics and Engineering, ANU, Canberra, Australia — ⁷Institut für Festkörperphysik, Technische Universität Berlin, Germany

Stabilizing ordering instead of randomness in alloy semiconductor materials is a powerful means to change their physical properties. We used STM and TEM to reveal an unrecognized ordering in ternary III-V materials. The lazarevite short-range order, found in the shell of $\text{InAs}_{1-x}\text{Sb}_x$ nanowires, is driven by the strong Sb-Sb repulsion along $\langle 110 \rangle$ atomic chains during their incorporation on unreconstructed $\{110\}$ sidewalls. Its spontaneous formation under group-III rich conditions of growth offers the prospect to broaden the limited classes of ordered structures occurring in III-V semiconductor alloys.

O 110.7 Fri 12:15 GER 38

All-Carbon Nanocapacitors from Graphene–Carbon Nanomembrane–Graphene Heterostructures — ●EMANUEL MARSCHESKI¹, XIANGHUI ZHANG¹, THOMAS WEIMANN², PAUL PENNER¹, DANIEL EMMRICH¹, PETER HINZE², and ARMIN GÖLZHÄUSER¹ — ¹Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld — ²Physikalisch-Technische Bundesanstalt, 38116 Braunschweig

We demonstrated the fabrication and characterization of all-carbon capacitors (ACCs) composed of multilayer stacks of dielectric carbon nanomembranes (CNMs) that are sandwiched between two CVD graphene sheets that act as conducting electrodes. CNMs were formed from a series of phenylthiol homologues, i.e. biphenylthiol (BPT), p-terphenylthiol (TPT), and p-quaterphenylthiol (QPT). Two-layer and six-layer CNMs were used as the dielectric layer between the top and bottom trilayer graphene electrodes. The junction areas of the nanocapacitors range from 1 to 2500 μm^2 . The frequency response of nanocapacitors has been measured with an LCR meter and the impedance spectra could be analyzed with a simple equivalent circuit. The dielectric constant of oligophenyl-based multilayer CNMs could be determined from the junction capacitance. These results suggest that the combination of graphene and CNMs as well as other 2D materials in nanoscale functional devices may provide a promising approach toward further development of molecular electronics devices.

O 110.8 Fri 12:30 GER 38

Diffusion Properties of Molecular Dopants in Organic Semiconducting Polymers — PATRICK REISER^{1,3}, VIPILAN SIVANESAN^{2,3}, ●SEBASTIAN BECK^{2,3}, WOLFRAM JAEGERMANN^{1,3}, and

ERIC MANKEL^{1,3} — ¹Institute for Materials Science, Technische Universität Darmstadt — ²Kirchhoff-Institut für Physik, Universität Heidelberg — ³InnovationLab GmbH, Heidelberg

In this study we investigate the diffusion of a solution-processable metal-organic molybdenum complex ($\text{Mo}(\text{tfd-CO}_2\text{Me})_3$) acting as p-dopant in Poly(3-hexylthiophen) (P3HT) thin films. In general, doping of organic semiconductors significantly increases the charge carrier concentration and improves transport and injection at contacts. However, in photo-active layers and at donor-acceptor interfaces a molecular dopant can act as exciton quencher. Therefore the diffusivity of molecular dopants is of interest for device stability and lifetime. Here, the dopant diffusion is measured at room temperature in 50nm polymer films using long-term Photoemission Electron Spectroscopy (PES) measurements. Molar surface fractions are derived from characteristic core-level emission lines. A simple analytical model can be employed to determine diffusion coefficients from time-dependent changes in surface doping ratios. We observe an exponential concentration dependency of the diffusion constant, which gives insight into the specific diffusion mechanism.

O 110.9 Fri 12:45 GER 38

Polling Ferroelectric BiFeO₃ Photoelectrodes for Switchable Charge-Transfer in the Photoelectrochemical Energy-Conversion Process — ●NASORI NASORI, DAWEI CAO, ZHIJIE WANG, YANG XU, and YONG LEI — Prof-Schmidt-Strauße 26, 98693 Ilmenau, Institute for Physics & IMN MacroNano Ilmenau University of Technology

We report BiFeO₃ ferroelectric photoelectrodes with switchable charge transfer property to break the limits imposed by conventional semiconductor. Because of the prominent ferroelectric properties, the photoelectrodes are able to tune the transfer of photo-excited charges generated either in BiFeO₃ or the surface modifiers by manipulating the poling conditions of the ferroelectric domains. At 0 V vs Ag/AgCl, the photocurrent can be switched from 0 mAcm⁻² to 10 mAcm⁻² and the open-circuit potential changes from 33 mV to 440 mV, when the poling bias of pretreatment is manipulated from -8 V to +8 V. Additionally, the pronounced photocurrent from charge injection of the excited surface modifiers can be quenched by switching the polling bias from +8 V to -8 V.