

CPP 50: P15: Polymers and Fields

Time: Wednesday 10:00–13:00

Location: Poster A

CPP 50.1 Wed 10:00 Poster A

Molecular structure of azobenzene-containing systems from classical MD simulations — ●OLGA GUSKOVA¹, VLADIMIR TOSHCHEVIKOV¹, JAROSLAV ILNYTSKYI^{1,2}, and MARINA SAPHIANNIKOVA¹ — ¹Leibniz-Institut für Polymerforschung Dresden e. V., Theorie der Polymere, Hohe Str. 6, 01069 Dresden, Deutschland — ²National Academy of Sciences of Ukraine, Institute for Condensed Matter Physics, Svientsitskii Str. 1, 79011 Lviv, Ukraine

Azobenzene-containing side chain polymers [1,2] and molecular glasses based on propeller-like C₃-symmetric azobenzene mesogenes [3] are investigated in classical molecular dynamics simulations. Two length scales are considered: (i) the molecular level with atomistic resolution, where reversible conformational changes of azobenzene chromophores upon light illumination lead to contractions/extensions of low amplitudes due to a limited size of mesogene groups, and (ii) the mesoscopic level, where light-induced molecular movements are observed over larger distances, comparable with the gyration radius of polymer chains. The influence of isomerization and orientation mechanisms on molecular structure and light-induced deformation is elucidated.

[1] J. Ilnytskyi et al., *J. Chem. Phys.* 135, 044901 (2011).

[2] M Saphiannikova et al., *Proceedings of SPIE "Optical Materials and Biomaterials in Security and Defence Systems Technology X"*, 8901, 890138 (2013).

[3] N.S. Jadavalli et al., *Appl. Phys. Lett.* 105, 051601 (2014).

CPP 50.2 Wed 10:00 Poster A

An alternative theoretical description of magneto-sensitive elastomers — ●DIRK ROMEIS and MARINA SAPHIANNIKOVA — Leibniz-Institut für Polymerforschung Dresden e. V.

Magnetorheological elastomers are composites that consist of magnetically permeable particles incorporated into an elastic (polymer) matrix. As a magnetic field is applied to such material a deformation and changes in the mechanical properties take place. In experiments often a stretching of the sample in direction parallel to the external field is reported. In contrast, many theoretical approaches to describe such systems predict a compression in the field direction. We present an alternative microscopic approach for magneto-sensitive elastomers in an external magnetic field and find a behavior in agreement with the experimental observation. For any parameter set our results always predict a stretching in direction of the field.

CPP 50.3 Wed 10:00 Poster A

Multifunctional Magnetic Hydrogel Particles — ●MARCUS WITT, SEBASTIAN BACKES, and REGINE VON KLITZING — Technische Universität Berlin, Physikalische Chemie, Germany

Microgels made of N-isopropylacrylamide (NIPAM) exhibit a volume phase transition temperature (VPTT) which leads to reversible swelling in water. The swelling and shrinking depends on the temperature, and with addition of different co-monomers also on the pH and ionic strength.

With the incubation of magnetic nanoparticles (MNP) such as cobalt ferrite we can obtain ferrogels which are also responsive to external magnetic fields.

Most publications about ferrogels are based on core/shell particles. In contrast, we aim for a homogenous distribution of MNP over the whole hydrogel, so that the ferrogel should respond uniformly to the applied magnetic field. Therefore, we synthesized a homogeneously crosslinked hydrogel by a constant feeding of the reactant. The MNP are then incubated by mixing aqueous solutions of hydrogel and MNP.

We were able to show that the initial thermoresponsive properties of the hydrogel are preserved for ferrogels both in bulk solution and adsorbed on a Si-surface.

Measurements of adsorbed ferrogel particles in an external magnetic field parallel to the surface have been carried out by AFM. First results show an increase of particle height and volume with an increasing magnetic field, whereas the area of the particle changes only slightly.

CPP 50.4 Wed 10:00 Poster A

In situ polymerization of organic conductive thin films — ●JENNY LEBERT and EVA M. HERZIG — TU München, Munich School of Engineering, Lichtenbergstr. 4, 85748 Garching

Organic semiconducting materials can be applied in optoelectronic de-

vices such as organic light-emitting diodes and organic solar cells. The conductivity and optoelectronic properties of polymers strongly depend on their molecular morphology and crystallization behavior. Therefore controlling the thin film morphology is one of the main challenges when it comes to developing fabrication processes that work in small labs as well as in large industrial scales. Moreover, a profitable scale-up requires the use of low-priced and available materials.

In situ polymerization of the active material is a promising approach for the fabrication of conductive thin films, as it combines the use of cheap materials with the possibility to control the film morphology. In this work, different synthetic chemical routines are combined with systematic physical analyses to investigate varying systems. The obtained polymer films are analyzed regarding their optic and optoelectronic properties, their conductivity and morphology. Additionally they are employed as active layers in organic solar cells.

CPP 50.5 Wed 10:00 Poster A

A FM-SFM study of the self-assembly of organic molecules on Au(111) — ●SEBASTIAN SCHNEIDER, KUSHTRIM BYTYQI, MICHAEL MARZ, CARMEN PÉREZ LEÓN, and REGINA HOFFMANN-VOGEL — Karlsruher Institut für Technologie, Physikalisches Institut, D-76131 Karlsruhe

Molecular self-assembly at solid interfaces is governed by the delicate balance between competing molecule-substrate and molecule-molecule interactions. Therefore, the substrate temperature during deposition, post-annealing of the sample and the molecular coverage influence the self-assembly process. Noble metal surfaces are widely used as substrates because of their low chemical reactivity. We have investigated 10,10'-dibromo-9,9'-bianthryl (DBBA) on Au(111) with frequency modulation scanning force microscopy. DBBA is well-known as precursor for graphene nanoribbons [1]. Depending on the coverage, different self-assembled molecular structures are observed on the surface. For low coverage, the molecules arrange along the heringbone reconstruction of the Au(111) (HB-phase). With increasing coverage, a new phase of molecular islands appear coexisting with the HB-phase. These islands display a stripe-like structure of highly ordered molecules.

[1] J. Cai, P. Ruffieux, R. Jaafar, M. Bieri, T. Braun, et al., *Nature* 466, 470, (2010)

CPP 50.6 Wed 10:00 Poster A

A scanning force microscopy study of the growth of organic molecules on Au(111) — ●KUSHTRIM BYTYQI, SEBASTIAN SCHNEIDER, MICHAEL MARZ, CARMEN PÉREZ LEÓN, and REGINA HOFFMANN-VOGEL — Karlsruher Institut für Technologie, Physikalisches Institut, D-76131 Karlsruhe

Recently, J. Cai et al. succeeded in the fabrication of graphene nanoribbons (GNRs) on the crystalline surface of noble metals via on-surface chemical synthesis [1]. They showed that armchair edge GNRs can be grown on Au(111) using 10,10'-dibromo-9,9'-bianthryl (DBBA) as precursor molecules following a three-step process [1,2].

We have investigated the ordering of DBBA molecules on Au(111) by frequency modulation scanning force microscopy at room temperature (RT) in ultrahigh vacuum. The molecules were evaporated on clean Au(111). During deposition, the substrate was either kept at RT and subsequently annealed to ~ 200°C, or was preheated to ~ 200°C. The coverage of the molecules was modified by varying the evaporation time. We have observed different molecular configurations depending on the experimental conditions. Among others, we imaged molecular islands with a stripe-like ordering apparently consisting of two distinct phases.

[1] J. Cai et al., *Nature* 466, 470 (2010).

[2] van der Lit et al., *Nature Commun.* 4, 2013 (2013).

CPP 50.7 Wed 10:00 Poster A

On-surface polymerization of flexible molecular wires — CHRISTOPHE NACCI^{1,2}, FRANCISCO AMPLE³, DAVID BLEGER⁴, STEFAN HECHT⁴, CHRISTIAN JOACHIM⁵, and ●LEONHARD GRILL^{1,2} — ¹Fritz-Haber-Institute, Berlin, Germany — ²Department of Physical Chemistry, University of Graz, Austria — ³IMRE, Singapore — ⁴Department of Chemistry, Humboldt-Universität zu Berlin, Germany — ⁵CEMES-CNRS, Toulouse, France

The on-surface polymerization of molecular building blocks on a Au(111) surface is studied by scanning tunneling microscopy and spectroscopy at low temperatures in combination with calculations. While rather rigid molecular chains, such as graphene nanoribbons, have been grown successfully in the last years, flexible molecular wires remain still a challenge. A key issue is here the charge transport capability through the molecule. Chemical linking is achieved by attachment of halogen

substituent atoms at specific molecular sites in the ex-situ synthesis. After deposition under ultrahigh vacuum conditions onto the surface, the chemical reaction is induced by sample heating. We show the successful formation of a flexible polymer that contains various sub-units with characteristic properties directly on the surface. The electronic structure of the molecular wire is studied by spatial mapping of individual molecules.