

DS 17: Organic Thin Films, Organic-Inorganic Interfaces

Time: Thursday 15:00–16:30

Location: A 060

DS 17.1 Thu 15:00 A 060

Thin Film Growth Simulation Study of Diindenoperylene on aSiO₂ — ●PHILIPP ELSÄSSER and TANJA SCHILLING — Institute of Physics, University of Freiburg, Germany

The understanding of film growth mechanisms is of high technological importance for growing single crystals, coating surfaces, and film production. By now there is a good understanding of the processes involved in the growth of films consisting of spherical objects, like atoms. In contrast, films of elongated molecules behave with respect to some of their properties in different ways due to their additional rotational degrees of freedom.

The organic semiconductor Diindenoperylene (DIP) is a candidate for organic solar cells or OLEDs. We have investigated an amorphous SiO₂ (aSiO₂) substrate with DIP molecules deposited on the surface. For this, we have performed MD simulations to study the clustering of few DIP molecules on aSiO₂, as well as the molecular orientation in larger groups of DIP molecules.

DS 17.2 Thu 15:15 A 060

Towards measuring charge transfer in hybrid structures of sub-monolayer dye films on 2D materials — ●TIM VÖLZER^{1,2}, ERIK VON DER OELSCHNITZ^{1,2}, JULIAN SCHRÖER¹, TOBIAS KORN^{1,2}, and STEFAN LOCHBRUNNER^{1,2} — ¹Institute of Physics, University of Rostock, Germany — ²Department "Life, Light & Matter", University of Rostock, Germany

Coating transition metal dichalcogenides (TMDCs) with dye molecules creates hybrid structures offering a playground for ultrafast charge (or energy) transfer exploitable for optoelectronics. Typically, nanometer molecular films are applied to roughly match the crystal density of states. In this case, however, interfacial transfer processes compete with intermolecular interactions and the dynamics may be limited by diffusion towards the interface. Thus, we apply monomeric dye coatings, where the molecules lie far from and do not interact with each other. We perform transient absorption spectroscopy aiming for the ultrafast hole transfer from the dye Perylene Orange (PO) towards monolayer tungsten diselenide and the electron transfer in the reverse direction. As a reference sample, we use PO on hexagonal boron nitride, where no charge or energy transfer can occur and the slow dynamics of the isolated molecules is represented.

DS 17.3 Thu 15:30 A 060

Ab-initio study on mixed donor-acceptor adlayers: Structure, stoichiometry and electrostatic potential of F4TCNQ and 1H,1 H-[4,4]bipyridinylidene on Cu (111) — ●RICHARD BERGER and OLIVER HOFMANN — Petersgasse 16, 8010 Graz, TU Graz: Institut für Festkörperphysik

Adlayer patterns formed from heterogenous molecular species on a substrate surface are of great interest, especially in the case of 2-dimensional donor-acceptor patterns adsorbed on metal surfaces. Such adsorbed donor-acceptor patterns exhibit various remarkable characteristics, such as their ability to form two-dimensional charge density waves or the possibility of tuning the electron injection barrier at the interface via the stoichiometry of the mixed adlayer. Here, we computationally investigated the exemplary donor-acceptor system of F4TCNQ and 1H,1 H-[4,4]bipyridinylidene on the Cu (111) surface. We predict the thermodynamically stable adlayer structure for different mixing stoichiometries. This allows us to forecast the tunability of the on-surface stoichiometry and structure via the gas phase concentration ratio during the deposition process. Using these predictions, we explore how the complex electrostatic potential of the donor/acceptor mixture affects the barriers for charge injection into subsequent layers.

DS 17.4 Thu 15:45 A 060

Influence of Electrostatic Forces: Molecular Packing in 2D

and 3D Films — ●JAN VINCENT SCHREIBER, MAXIMILIAN DREHER, and GREGOR WITTE — Philipps-Universität Marburg, Molekulare Festkörperphysik, 35032 Marburg, Germany

While packing motifs and crystal structures of van der Waals-bound molecular solids are essentially determined by an interplay of London dispersion and electrostatic forces, the latter often receives only little attention. Using the model system 5,7,12,14-Pentacenetetrone as an example, we use STM measurements to demonstrate the formation of different packing motifs in monolayer and bilayer films on graphite, which can be well explained by optimized electrostatic interactions in two and three dimensions, respectively. This knowledge then enables optimization of growth and the production of highly ordered strain-free films through the application of specific temperature protocols upon growth that abolish the initially formed 2D seed layer structure and yield very smooth, crystalline films with the bulk structure while avoiding dewetting that often occurs at higher temperatures. This result highlights the importance of accurately understanding interfacial properties to obtain crystalline molecular functional films.

DS 17.5 Thu 16:00 A 060

Polarized Raman Imaging of *para*-Hexaphenylene Nanoaggregates — ●FRANK BALZER¹, ROLAND RESEL², and MANUELA SCHIEK³ — ¹Mads Clausen Institute, University of Southern Denmark, Sønderborg, Denmark — ²Institute of Solid State Physics, Graz University of Technology, Graz, Austria — ³Center for Surface- and Nanoanalytics (ZONA), Johannes Kepler University, Linz, Austria

Organic molecular beam deposition of *para*-hexaphenylene (p6P) onto poly-crystalline platinum results in the formation of unique nanoaggregates, predominantly as nanofibers and ribbons. Atomic force microscopy reveals intricate morphological differences. Grazing incidence X-ray diffraction validates multiple crystalline contact faces, with a preference for crystallographic contact planes where molecules are oriented parallel to the substrate surface. No evidence of in-plane templating effects is observed. Uniform and varying optical extinction angles in birefringent aggregates suggest a complex aggregation process. Raman microscopy indicates that the molecular orientation within the aggregates is generally perpendicular to the long aggregate axis, aligning with the aggregate orientation. This finding is significant for applications leveraging p6P's polarized emission properties, such as in photonic and optoelectronic devices.

DS 17.6 Thu 16:15 A 060

Formation of CoS_x in the tribological taper junction of hip implants — ●ADRIAN WITTRÖCK¹, CHRISTIAN BECKMANN¹, MARKUS A. WIMMER², ALFONS FISCHER^{2,3}, CHRISTIAN LIEBSCHER⁴, and JÖRG DEBUS¹ — ¹Department of Physics, TU Dortmund University — ²Department of Orthopedic Surgery, Rush University Medical Center, Chicago, USA — ³Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH — ⁴Structure and Nano-/Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH

Within an artificial hip joint gross slip fretting corrosion occurs, leading to the formation of inorganic-organic tribomaterial which contains compounds of the human body fluid and wear particles from the implant materials. However, little is known about tribo-chemical and -structural processes and the types of organometallic species formed within hip-implant taper junctions. Using confocal Raman microscopy, we show that the tribological fretting gives rise to a denaturation of the albumin, associated with a breaking of sulphur bonds, so that - in turn - sulphur ions are released and react with cobalt ions from the Co-alloy of the hip implant. A thin tribofilm of amorphous/nanocrystalline CoS_x is thus formed, covering approximately 12.2% of the fretting track of the CoCr29Mo6C0.03 surface.