

## O 21: Morphology Prediction at Interfaces: Theory meets Experiment

Time: Monday 18:15–20:30

Location: Poster E

O 21.1 Mon 18:15 Poster E

**Simulating stencil lithography of C60 growth: Impact of localized deposition** — ●B. HARTUNG, N. KLEPPMANN, and S. H. L. KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

Understanding and controlling the assembly of crystalline structures of complex organic molecules is an important aspect of the manufacturing of efficient organic and organic/inorganic hybrid semiconductor devices. In organic molecular beam epitaxy growth scenarios, the structure formation can be manipulated by using stencil masks to restrict the molecular beam to a certain area of the substrate. This technique is known as stencil lithography. To examine the basic effects of the mask on the growth behavior of organic molecules, we use C60 homoepitaxy as a model system, based on previous studies [1, 2]. To this end we perform Kinetic Monte Carlo simulations, where the adsorption of particles is restricted to a quadratic area, which is small compared to the size of the overall substrate surface.

The growth behavior shows a transition from the formation of multilayer-islands (covering only the surface of the deposition area) to the formation of monolayer-like islands, the control parameters being the temperature and the adsorption rate. We discuss this behavior studying layer coverages and geometric aspects of growth.

[1] S. Bommel, N. Kleppmann et al., Nat Comm 5, 5388 (2014), doi:10.1038/ncomms6388

[2] N. Kleppmann, S. H. L. Klapp, J. Chem. Phys. 142, 064701 (2015)

O 21.2 Mon 18:15 Poster E

**Naphthalene's six shades on graphite** — ●FALKO SOJKA<sup>1</sup>, MATTHIAS MEISSNER<sup>1</sup>, TAKASHI YAMADA<sup>2</sup>, TOSHIKI MUNAKATA<sup>2</sup>, ROMAN FORKER<sup>1</sup>, and TORSTEN FRITZ<sup>1</sup> — <sup>1</sup>Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — <sup>2</sup>Department of Chemistry, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan

Naphthalene ( $C_{10}H_8$ ) is the smallest member of the polycyclic aromatic hydrocarbons (PAH). For  $C_{10}H_8$  two commensurate monolayer phases on graphite have been reported so far. By using low energy electron diffraction (LEED) we re-analyze precisely the lattice parameters of these systems. Surprisingly, we found a total of six different phases of which only one exhibits an ordinary commensurate registry with graphite. Two further phases vanish irretrievably upon a change in the temperature, while the other three can be converted into one another reversibly. We studied in detail how to obtain the different phases by varying the amount of molecules deposited as well as the substrate temperature. Eventually, the complex behavior and polymorphism of  $C_{10}H_8$  on graphite is compiled in a phase diagram. We believe that such manifold systems should be taken into consideration for theories which try to predict structures and morphologies of adsorbates on surfaces.

O 21.3 Mon 18:15 Poster E

**Investigation of the lateral and vertical structure of CuPc on Cu(001)** — ●MARKUS FRANKE, SONJA SCHRÖDER, JONAS VAN BEBBER, and CHRISTIAN KUMPF — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich GmbH, Jülich, Germany, and Jülich-Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology

For thin molecular films adsorbed on metal surfaces it has been shown that morphology has a big influence on the electronic properties of the system. To achieve a better understanding of the formation of ordered structures, we investigated the system Copper-II-phthalocyanine (CuPc) on Cu(001).

Depending on the substrate temperature and the (sub-monolayer) coverage the CuPc molecules form several different commensurate structures or, at low coverages, remain disordered. We characterized these different phases using STM and LEED, and in one case also with XSW. The most remarkable result may be the breaking of the fourfold symmetry of the LUMO in one of the structures, caused by the degeneracy of both LUMO states being lifted upon adsorption. This is surprising, since both the Cu(001) substrate and the adsorbed molecules originally have the same (fourfold) symmetry.

O 21.4 Mon 18:15 Poster E

**Free-Base 5,10,15-tris(pentafluorophenyl)corrole adsorption on Ag(111)** — ●HAZEM ALDAHAK<sup>1</sup>, STEFANO TEBI<sup>2</sup>, MATEUSZ PASZKIEWICZ<sup>3</sup>, EVA RAULS<sup>1</sup>, UWE GERSTMANN<sup>1</sup>, STEFAN MÜLLEGGGER<sup>2</sup>, FLORIAN KLAPPENBERGER<sup>3</sup>, WOLFGANG SCHÖFBERGER<sup>4</sup>, and WOLF GERO SCHMIDT<sup>1</sup> — <sup>1</sup>Lehrstuhl für Theoretische Materialphysik, Universität Paderborn — <sup>2</sup>Festkörperphysik, Universität Linz — <sup>3</sup>Physik Department E20, Technische Universität München — <sup>4</sup>Institut für Organische Chemie, Universität Linz

While corroles are structurally closely related to porphyrins, they have lower symmetry, smaller cavities, which enables them to stabilize metal ions in exceptionally high oxidation states. This makes them highly interesting for a variety of applications in medicine, catalysis, sensors as well as for solar cells.

Here, dispersion-corrected density-functional theory (DFT) calculations supported by scanning tunneling microscopy (STM) measurements and X-ray photoelectron spectroscopy (XPS) measurements on the adsorption of the free-base 5,10,15-tris(pentafluorophenyl)corrole on Ag(111) surface are presented. Both, single adsorbed molecules as well as monolayer thin films are studied. Single molecules adsorb with its macrocycle tilted with respect to the surface. The tilted adsorption geometries enable the molecules to aggregate in non-trivial interwoven monolayer structures. The simulated STM data as well as the simulated X-ray photoelectron spectroscopy (XPS) data for the C1s, F1s and N1s edges in conjunction with the measurements nicely confirm the molecular structures concluded from the total-energy calculations.

O 21.5 Mon 18:15 Poster E

**Behaviour of the water lithium niobate interface studied from first principles** — ●REBECCA HÖLSCHER, SIMONE SANNA, and WOLF GERO SCHMIDT — Paderborn University

Lithium niobate ( $LiNbO_3$ , LN) is a frequently used material for optical and acoustic applications due to its strong piezoelectric, pyroelectric, and photorefractive properties. As for other ferroelectric materials, manipulating the polarization can change the surface reactivity. This opens the possibility for the realization of molecular detectors and other devices [1]. The water lithium niobate interface is largely unknown. Moreover, recent results show that basic properties of water such as the freezing temperature are strongly polarization dependent [2]. We present here ab initio calculations on the adsorption of water films on both the positive and the negative Z-cut and the X-Cut surface of LN. The adsorption is modelled by means of density functional theory (DFT) within the generalized gradient approximation [3,4]. The interface atomic structure and dynamics are calculated using Molecular Dynamic simulations at room temperature. The influence of the surface polarity on the water layer is investigated by means of a correlation function analysis.

[1] D. Li, et al., Nature Materials 7 (2008) 473.

[2] D. Ehre et al., Science 327 (2010) 672.

[3] W.G. Schmidt, et al., Phys. Rev. B 77 (2008), 035106.

[4] S. Sanna, A.V. Gavrilenko, W.G. Schmidt, Phys. Stat. Sol. C 7 (2010) 145.

O 21.6 Mon 18:15 Poster E

**Molecular Structures of Dialkylimidazolium Ionic Liquids at the Hydroxylated Solid-Liquid Interface** — ●MICHAEL KLIMCZAK<sup>1</sup>, ZLATKO BRKLJAČA<sup>2,3</sup>, DAVID M. SMITH<sup>2,3</sup>, ANA-SUNČANA SMITH<sup>2,3,4</sup>, and ANDREAS MAGERL<sup>5</sup> — <sup>1</sup>Chair of Crystallography and Structural Physics, FAU, Erlangen, Germany — <sup>2</sup>Division of Organic Chemistry and Biochemistry, Institut Ruder Bošković, Zagreb, Croatia — <sup>3</sup>Cluster of Excellence Engineering of Advanced Materials, FAU, Erlangen — <sup>4</sup>Institute for Theoretical Physics I, FAU, Erlangen, Germany — <sup>5</sup>Chair of Biophysics, FAU, Erlangen, Germany

Dialkylimidazolium-based ionic liquids, salts with a melting point well below room temperature, are a fairly novel class of substances with a broad spectrum of potential applications, most notably as solvents or electrolytes in an electrochemical context. Molecular structuring at the solid liquid interface, oftentimes playing a crucial role in small-scale systems, has previously been observed. Yet, no coherent explanation has been given to provide a better understanding of these phenomena.

Using a complementary approach of experimental X-ray reflectivity

and molecular dynamics, we obtain atomic level detail of structuring at the solid-liquid interface of 1-alkyl-3-methylimidazolium bistriflimide ionic liquids. The interface region is dominated by cations, tightly attached to the substrate via hydrogen bonding and a two-dimensional long-range ordering can be observed. This structure is followed by interface normal, monomolecular layering of alternating anion and cation enrichment/depletion, extending about 40 Å into the bulk.

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**Ab initio electron paramagnetic resonance study of 3C-SiC/SiO<sub>2</sub> interfaces in SiC-nanofiber based solar cells** — •TAUFIK ADI NUGRAHA<sup>1,2</sup>, UWE GERSTMANN<sup>2</sup>, WOLFGANG GERO SCHMIDT<sup>2</sup>, and STEFAN WIPPERMANN<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Eisenforschung, Germany — <sup>2</sup>University of Paderborn, Germany

Semiconducting nanocomposites, e. g. hybrid materials based on inorganic semiconducting 3C-SiC nanofibers and organic surfactants, provide genuinely novel pathways to exceed the Shockley-Queisser limit for solar energy conversion. The synthesis of such functionalized fibers can be performed completely using only inexpensive wet chemical solution processing. During synthesis a thin passivation layer is introduced between the SiC-fiber and surfactants, e. g. the native oxide, whose atomistic details are poorly understood. In this study, we utilize unpaired spins in interfacial defects to probe the local chemical environment with ab initio EPR (Electron Paramagnetic Resonance) calculations, which can be directly compared to experiment. Considering a wide variety of possible interfacial structures, a grand canonical approach is used to generate a phase diagram of the 3C-SiC/SiO<sub>2</sub> interface as a function of the chemical potentials of Si, O and H, to provide favorable interfacial structures for g-tensor calculations. This

study provides directions about specific types of interfacial defects and their impact on the electronic properties of the interface. The authors wish to thank S. Greulich-Weber for helpful discussions.

O 21.8 Mon 18:15 Poster E

**Vibrational properties of Pb/Si (111) from first principles** — •MAEDEH ZAHEDIFAR and PETER KRATZER — Faculty of Physics, University of Duisburg-Essen, Germany

Time-resolved spectroscopic methods hold great potential for the exploration of electronic properties of materials. However, the electronic excitation and relaxation processes are, due to their complexity, incompletely understood at present. Due to their unique electronic properties, ultra-thin metallic films on semiconductor surfaces are an important field of contemporary solid state physics. In particular, we studied Pb metallic films of a few monolayers on silicon as substrate in (111) direction. The quantum well states in these films are ideally suited to study electronic relaxation by time-resolved spectroscopy. Therefore, we employed density functional calculations using the GGA-PBE functional to study various structures of Pb/Si(111) and their stabilities. In our calculations using the Quantum-Espresso and the VASP code, we tested different unit cells:  $1 \times 1$ ,  $\sqrt{3} \times \sqrt{3}$  and  $\sqrt{7} \times \sqrt{3}$  for 1ML, and  $\sqrt{3} \times \sqrt{3}$  for 4 and 5ML. We find that the system in  $\sqrt{3} \times \sqrt{3}$  is more stable than in the other structures. The optical in-plane modes at Pb  $\sqrt{7} \times \sqrt{3}$  are somewhat lower in energy than those of Pb  $\sqrt{3} \times \sqrt{3}$ , in agreement with Raman scattering experiments. That is because the density of the Pb layer in  $\sqrt{7} \times \sqrt{3}$  is less than in the  $\sqrt{3} \times \sqrt{3}$ , expressed as coverage 1.2 ML versus 1.333 ML. Calculations are in progress addressing the electron-phonon coupling.