

CPP 63: Interfaces and Thin Films II (joint session CPP/DY, organized by CPP)

Time: Friday 9:30–12:00

Location: H51

CPP 63.1 Fri 9:30 H51

Ring polymer chains in confined geometries: Massive field theory approach — ●ZORYANA USATENKO¹ and JOANNA HALUN² — ¹Institute of Physics, Cracow University of Technology — ²Faculty of Physics, Mathematics and Computer Science, Cracow University of Technology

The investigation of a dilute solution of phantom ideal and real ring polymer chains with excluded volume interactions in a good solvent confined in a slit geometry of two parallel walls was performed. Taking into account the well known polymer - magnet analogy developed by de Gennes the calculations of the correspondent partition functions, depletion interaction potentials, depletion forces and the forces which exert phantom ideal ring polymer chain on the surfaces were performed in a fixed space dimensions $d=3$ for two repulsive walls, two inert walls and for the mixed case of one inert and one repulsive wall. Besides, for the case of ring polymer chain with EVI confined in a slit geometry of two parallel repulsive walls calculations were performed up to one-loop order. It was found that the confining of ring polymer chain to a slit geometry of two walls leads to the loss of configurational entropy and to arising of the repulsive force which exerts ring polymer chain on the surfaces. Increasing of the slit size leads to decreasing of the value of the exerted force on the surfaces at the same value of the end-to-end distance.

CPP 63.2 Fri 9:45 H51

A theoretical approach to bis-urea molecules that form hydrogen-bonded supramolecular polymers in 2D — ●OLGA GUSKOVA^{1,2} and JENS-UWE SOMMER^{1,2,3} — ¹Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — ²Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany — ³Institute of Theoretical Physics, TU Dresden, Dresden, Germany

Supramolecular polymers, i.e. arrays of low-molecular-weight building blocks, usually held together by hydrogen bonding (HB) or other reversible noncovalent interactions. Bis-urea-based molecules with central bis-urea fragment exhibit the highest supramolecular polymerization ability, affording well-defined supramolecular fibers. In this talk, two major points concerning the arrangement and properties of HB bis-urea molecules on surfaces studied by QM/all-atom MD simulations will be addressed: (i) the ordering dynamics on graphite of two bis-urea molecules which differed only by a single cis-double bond in their side groups [1] and (ii) the electronic properties of isolated molecules, HB dimers and bis-urea tapes in adsorbed state on gold surface [2].

[1] R. Shokri, O. Guskova, A. Jamal, K. Jahanshahi, B. Isare, L. Bouteiller, L. Simon, J.-U. Sommer, G. Reiter, *J. Phys. Chem. C* 119 (39), 22596-22603 (2015).

[2] F. Vonau, R. Shokri, D. Aubel, L. Bouteiller, O. Guskova, J.-U. Sommer, G. Reiter, L. Simon, *Nanoscale* 6 (4), 8250-8256 (2014).

CPP 63.3 Fri 10:00 H51

Towards large area atomically flat n-alkane layers: A real-time study of thermal annealing — ●LINUS PITHAN¹, EDUARD MEISTER², CHENYU JIN³, ANTON ZYKOV¹, WOLFGANG BRÜTTING², HANS RIEGLER³, ANDREAS OPITZ¹, and STEFAN KOWARIK¹ — ¹Inst. f. Physik, Humboldt Universität zu Berlin — ²Inst. f. Physik, Universität Augsburg — ³MPI für Kolloid- und Grenzflächenforschung, Potsdam

Highly anisotropic attachment energies of n-alkanes combined with low surface energies result in their unusual thin films growth and wetting behavior [1]. We analyze the thermal annealing behavior of n-tetradecane (TTC, $C_{44}H_{90}$) in detail with the aim to improve smoothness and to increase the lateral size of crystalline islands of polycrystalline TTC films on SiO₂, a material system also of interest from a device perspective [2]. We use *in situ* x-ray diffraction to find an optimum temperature leading to improved texture and crystallinity while avoiding an irreversible phase transition. Further, we employ real-time optical phase contrast microscopy with sub-nm height resolution [3] to track the diffusion of TTC across monomolecular step edges and show that the lateral island sizes increase by more than one order of magnitude from 0.5 μm to 10 μm . This desirable behavior of 2d-Ostwald ripening and the pronounced smoothing we observe is in stark contrast to many other organic molecular films where annealing

leads to dewetting, roughening, and a pronounced 3d morphology.

[1] L. Pithan *et al.*, *J. Chem. Phys.* 143, 164707 (2015)[2] M. Kraus *et al.*, *J. Appl. Phys.* 107, 094503 (2010)[3] R. Köhler *et al.*, *Appl. Phys. Lett.* 89, 241906 (2006)

CPP 63.4 Fri 10:15 H51

Photo-manipulation of the surface tension anisotropy at a liquid-crystal/ITO-glass interface — HAJNALKA NADASI, ●ALEXEY EREMIN, and RALF STANNARIUS — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany

We report direct measurements of the surface energy anisotropy (anchoring energy) at a glass-nematic liquid crystal interface containing a photo-active azo-dendrimeric surfactant. The photoisomerisation at the surface layer drives an anchoring transition from the homogeneous to the planar state of the liquid crystal. The anchoring energy is measured using the Frederiksz transition as a function of the intensities of the UV and VIS light and is compared with a theoretical model. We also demonstrate optical manipulation of the nematic director field around microspheres and rods dispersed in the liquid crystal. In case of rod-shaped particles, the photo-driven change of the anchoring energy results in a reversible macroscopic rotation of the particles.

CPP 63.5 Fri 10:30 H51

Kinetic Monte Carlo Simulations of Photo-Switchable Molecules Tethered to a Surface — ●RAFFAELE TAVARONE¹, PATRICK CHARBONNEAU², and HOLGER STARK¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany — ²Departments of Chemistry and Physics, Duke University, Durham, North Carolina 27708, USA

Photo-switchable molecules can undergo a light-induced *trans-cis* isomerization. They can be used to build functional monolayers with light-controlled macroscopic properties. A recent experiment [1] showed that, in a monolayer densely covered with photo-switchable molecules, the relaxation of the induced birefringence follows a glasslike power-law dynamics. Furthermore, the relaxation can be efficiently fastened by illumination of the sample with circularly polarized light.

We developed a molecular model for the monolayer in which the *trans* and *cis* isomers are modeled as straight and bent needles, respectively. The needles are allowed to overlap and the system dynamics is generated by a kinetic Monte Carlo algorithm. We demonstrate that the glasslike power-law dynamics can be traced back to spatio-temporal correlations in the local structure of the system, i.e., to the formation of dynamical heterogeneities. Also, we find that the different degree of shape anisotropy of the two isomers has a significant effect on the system dynamics: the nearly isotropic *cis* isomers suppress the formation of extended dynamical domains. As a result, the relaxation is faster and follows a simple exponential decay.

[1] Fang, G. J., *et al.*, *Nature communications* 4, 1521 (2013).

15 min. break

CPP 63.6 Fri 11:00 H51

Modulated structures in complex twist-bend nematic phases in bulk and thin-film geometry. — ●NEREA SEBASTIAN, ALEXEY EREMIN, and RALF STANNARIUS — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany

Twist-bend nematic state (Ntb) has recently been discovered as a complex mesophase intermediate between the cholesteric and a uniform nematic phase. The molecules, being non-chiral, spontaneously form a helical twist-bend structure, where the director is inclined to the helical axis. The phase is believed to be driven by the inversion of the bend elastic constant K_3 . We report on an elastic behaviour in the vicinity of the nematic-Ntb transition and describe the transition between the Ntb and a modulated smectic phase which exhibits intricate labyrinthine structures of the layer dislocations in freely-suspended films. It also forms fluid cylindrical filaments with large slenderness ratios.

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CPP 63.7 Fri 11:15 H51

Properties of a monomolecular water film flowing into a graphene-mica slit pore — ●ANDRÉ SCHILO, NIKOLAI SEVERIN, IGOR M. SOKOLOV, and JÜRGEN P. RABE — Department of Physics, Humboldt-Universität zu Berlin, Germany

Nanoscopically confined water and water adsorbed at interfaces play an important role in e.g. biology, tribology or nanotechnology. Graphene has recently been demonstrated to replicate the substrate topography with a precision down to single macromolecules. Thus the flexible graphene cover provides the possibility of visualizing a water monolayer confined in a slit pore between graphene and mica. However, the phase of the confined water (solid or fluid) is still debated. Here we report high-resolution scanning force microscopy (SFM) imaging of water monolayers flowing into the slit pore. The initially dry pore gets filled upon raising the ambient humidity. We observed a layer of water wetting the sample in reproducible finger-shaped patterns with a step height of 2.8 Å. The flow kinetics are highly dependent on the rate of humidity change. Keeping the humidity constant at a value above the beginning of the wetting process and below the complete wetting, results in a nearly exponential saturation of the finger growth. A further increase of the humidity reactivates the growth of the fingers, eventually leading to a complete monolayer of water. From this we conclude that the confined water monolayer must be fluid.

CPP 63.8 Fri 11:30 H51

A spectroscopic investigation of surface melting of ice — ●M.ALEJANDRA SANCHEZ, MISCHA BONN, and ELLEN H.G BACKUS — Max Planck Polymer Research Institute, Mainz, Germany

In nature, ice is, amongst others, responsible for rock weathering, soil metamorphosis, thunderstorms and the ozone chemistry on stratospheric clouds. It has been generally accepted that from the bulk freezing point down to roughly 240 K, a quasi-liquid-layer is present

on ice. However, the nature of this layer has been intensely debated. We study the nature of the interfacial water on well-defined single crystal ice surfaces. The surface sensitive technique sum frequency generation spectroscopy provides the vibrational spectrum of specifically the interfacial molecules. We find a sudden change in the spectrum around 255 K which is assigned to the phase transition from ice/air to ice/quasi-liquid/air. The experimental results are well reproduced by simulations that allow to relate the observed spectral changes to information on the molecular scale.

CPP 63.9 Fri 11:45 H51

Interfacial Melting in Ice/Nanocomposite Materials — ●HAILONG LI¹, JULIAN MARS^{1,2}, HENNING WEISS¹, THOMAS BUSLAPS³, WIEBKE LOHSTROH⁴, and MARKUS MEZGER^{1,2} — ¹Max-Planck-Institut für Polymerforschung, Mainz, Germany — ²Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — ³ESRF-The European Synchrotron, Grenoble, France — ⁴Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany

The material properties of permafrost strongly depend on the molecular scale structure of the ice/solid interface. Early in 1859, Faraday proposed the existence of a quasi-liquid layer (qll) at ice surfaces. However, the understanding of the interfacial melting of ice and the structure of the qll is still under debate. Layered sheet silicates are ideal model systems to study the interfacial melting of ice in geologically relevant materials. Using x-ray diffraction, we determined the crystalline ice fraction in ice composites with high interface to volume ratio. From the anisotropy of the ice Bragg reflections in textured composite samples we extract the preferred orientation of ice crystals confined between the sheet silicates. Approaching the bulk melting point of ice, we observe a logarithmic growth law of the thickness of the qll. Quasielastic neutron scattering was employed to elucidate the mobility of the qll at hydrophilic and hydrophobic solid-ice interfaces.