CPP 3: Liquid Crystals and Polar Fluids

Time: Monday 10:00–12:30 Location: C 264

CPP 3.1 Mon 10:00 C 264

Controlling Size and Arrangement of Smectic Focal Conic Domains — Wei Guo, Yasutaka Iwashita, Stephan Herminghaus, and •Christian Bahr — MPI for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen

Defect structures in liquid crystals are of interest from both fundamental and applied viewpoints. For instance, topological defects can lead to the self-assembly of two-dimensional nematic colloidal crystals [1].

The present study is concerned with defect structures in smectic liquid crystals, so-called focal conic domains, which consist of a complex arrangement of curved equidistant molecular smectic layers which are wrapped around two singular lines. We describe a method to generate almost arbitrary two-dimensional arrangements of focal conic domains in smectic films. The method is based on the patterning of a silicon substrate with a thin gold layer that is evaporated through a lithographic mask. In smectic films on such substrates, the generation of focal conic domains is confined to the masked areas so that both the size of individual domains and the overall arrangement of many domains can be controlled. We study the generated structures on linearly and circularly patterned substrates by optical, fluorescence confocal, and scanning force microscopy [2], and discuss the use of focal conic domains as matrices for self-assembling microsystems.

[1] I. Muševič, M. Škarabot, U. Tkalec, M. Ravnik, and S. Žumer, Science **313**, 954 (2006).

[2] V. Designolle, S. Herminghaus, T. Pfohl, and Ch. Bahr, Langmuir **22**, 363 (2006).

CPP 3.2 Mon 10:15 C 264

Dielectric relaxation behavior of nematic liquid crystals dispersed in a ferroelectric polymer — •Lakshmi Meena Ganesan, Axel Mellinger, Peter Frübing, Werner Werges, and Reimund Gerhard — Department of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany

Polymer-dispersed liquid crystals (PDLCs) are a class of materials that consists of micrometer-sized liquid-crystal (LC) droplets embedded in a polymer matrix. Here, ferroelectric poly(vinylidene fluoride-co-trifluoroethylene) (P(VDF-TrFE)) (65/35 mol%) was used as the matrix polymer, since the electric field generated by the piezo- or pyro-electric effect of the matrix material could potentially be used to switch the director of the LC. In the absence of an external electric field, the nematic molecules at the interface are oriented spontaneously at a specific angle. The phenomenon of orienting the LC molecules at an interface is called anchoring. By application of an electric field, the nematic molecules can be oriented along the field direction. If the perpendicular refractive index of the liquid crystal matches the refractive index of the polymer matrix, the optical transmission of the PDLC film increases. The anchoring effect can be studied using dielectric relaxation spectroscopy. Two dispersion regions are observed in the dielectric spectra of the pure P(VDF-TrFE) film. They are related to the glass transition and to a charge-carrier relaxation. In PDLC films containing 10 wt% of LC, an additional, bias-field-dependent relaxation peak is found that can be attributed to the motion of LC molecules.

CPP 3.3 Mon 10:30 C 264

Charge transport in discotic liquid crystals: effect of temperature and mesophase symmetry — •Denis Andrienko[1], Valentina Marcon[1], James Kirkpatrick[2], Jenny Nelson[2], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Physics, Imperial College London, Prince Consort Road, London SW7 2BW, United Kingdom

Charge mobilities of several derivatives of discotic liquid crystals have been determined by combining three methods into one scheme: (i) quantum chemical methods for the calculation of molecular electronic structures, reorganization energies, and energetic disorder (ii) molecular dynamics for simulation of the relative positions and orientations of molecules in a columnar mesophase, and (iii) kinetic Monte Carlo simulations and Master Equation approach to simulate charge transport. Applying this scheme to differently substituted hexabenzocoronene derivatives we reproduce the trends and magnitudes of mobilities as measured by PR-TRMC and connect mobility directly to the microscopic morphology of the columns. It is shown that in the herringbone mesophase transfer integrals are higher, but so is energetic disorder. Analysing the temperature dependence of the distributions of charge transport parameters helps to establish a link between the system morphology/mesophase symmetry and charge mobility.

CPP 3.4 Mon 10:45 C 264

AFM Study of Surface-Induced Ordering in Liquid Crystals: Impurity Enhanced Ordering — •Doris Vollmer, Li-Juan Zhang, Michael Kappl, and Günter K. Auernhammer — MPI Polymerforschung, Mainz, Germany

We experimentally investigate surface-induced smectic-like ordering close to the isotropic-nematic phase transition of thermotropic liquid crystals of the n-CB series. Homeotropic alignment has been induced by depositing a lipid monolayer onto the silica surface. As shown by AFM the smectic like ordering alignment vanishes for temperatures a few degree above the phase transition.

Surprisingly, addition of a few percent of alkane to the liquid crystal enhances the presmectic ordering. In case of 4′-n-cyano-4-octylbiphenyl (8-CB) and octane we found maximal ordering at 4 percent of octane. This enhanced ordering depends on the length of the alkane, C_i, compared to length of the carbon tail of the liquid crystal, n-CB.

Probably impurity enhanced ordering is due to a combination of improved molecular packing and enhanced presmectic fluctuations, because addition of octane causes a decrease of the width of the nematic domain.

break

CPP 3.5 Mon 11:15 C 264

Gas-Liquid Phase Behavior of Dipolar Fluids — •Jörg Bartke and Reinhard Hentschke — Bergische Universität Wuppertal, Germany

The gas-isotropic liquid-nematic liquid phase behavior of the Stockmayer fluid is studied using Molecular Dynamics simulation over a wide range of dipole strengths. In our simulations we do not observe the disappearance of the isotropic gas-isotropic liquid coexistence at high dipole strength contrary to earlier findings based on Monte Carlo techniques. Even though the formation of reversible dipole chains strongly affects the location of the critical point, it does not lead to its disappearance. In addition to the simulation results we present a theory explaining the dependence of the gas-liquid critical point in the Stockmayer fluid on the dipole strength. The theory is based on the Flory-Huggins lattice description for polymer systems in conjunction with a transfer matrix model for isolated chains of reversibly assembled dipolar particles. We find that the shift of the critical point as function of dipole strength, also observed in computer simulation, strongly resembles the critical point shift as function of chain length in ordinary linear polymer systems. In particular the decrease of the critical density with increasing dipole strength is a consequence of the existence of reversible chains near criticality.

CPP 3.6 Mon 11:30 C 264

A new approach to the quantitative prediction of phase behaviour of quadrupolar fluids — •Bortolo M. Mognetti[1], Leonid Yelash[1], Peter Virnau[1], Wolfgang Paul[1], Kurt Binder[1], Marcus Mueller[2], and Luis G. MacDowell[3] — [1]Institut für Physik, Johannes Gutenberg–Universität, Staudinger Weg 7, 55099 Mainz, Germany — [2]Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Dpto. de Quimica Fisica, Facultad de Cc. Qumicas, Universidad Complutense, 28040 Madrid, Spain

We investigate the phase behaviour of simple quadrupolar fluid and short alkane in quadrupolar solvents using Grand-Canonical Monte-Carlo simulations. First we carefully investigate Coarse-Grained models for solvents in which molecules are represented by single Lennard-Jones beads plus a quadrupolar moment. We show that these models perform well in predicting equilibria states, also if compared to more realistic (and computationally more expensive) atomistic models. Furthermore we investigate mixtures. Previous investigations have failed to predict the correct type of the binary phase behaviour without modifying the Lorentz-Berthelot mixing rules. We discuss how the new polar coarse grained model for the solvent improves the description of the mixture without any new phenomenological parameter. In order to elucidate the role of quadrupolar interactions we test also the Lorentz-Berthelot rules in some apolar mixtures.

CPP 3.7 Mon 11:45 C 264

Disappearance of ferromagnetic ordering in nanoconfined dipolar fluids

— •Sabine H.L. Klapp[1,2] and R. Andreea Trasca[2] — [1]Institute of Theoretical Physics, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Stranski-Laboratorium of Physical and Theoretical Chemistry, TU Berlin, Strasse des 17. Juni 135, 10623 Berlin, Germany

We present Monte-Carlo (MC) simulation results for dipolar fluid films under strongly coupled conditions where the bulk fluid [1] and films of mesoscopic thicknesses [2] display ferromagnetic ordering. We demonstrate that the ordering persists down to nanoscopic wall separations where the system consists of only four monolayers [3]. For smaller thicknesses we observe stripe-like defects (domains) and finally the breakdown of ferromagnetic ordering for systems close to the two-dimensional limit [3,4]. The results for the liquid phase are supported by MC calculations starting from quasi-crystalline soft-sphere configurations. Our findings are relevant for systems of magnetic colloids but also for the ordering behavior of thin solid-like magnetic films.

[1] D. Wei and G. N. Patey, Phys. Rev. Lett. **68**, 2043 (1992)

[2] S. H. L. Klapp and M. Schoen, J. Chem. Phys. **117**, 8050 (2002).

[3] R. A. Trasca and S. H. L. Klapp, in preparation.

[4] S. H. L. Klapp, Mol. Sim. **32**, 609 (2006).

CPP 3.8 Mon 12:00 C 264

Field–controlled layer formation in dipolar nanofilms

— •Jelena Jordanovic[1] and Sabine H. L. Klapp[1,2] — [1]Stranski-Laboratorium, Technische Universität Berlin, Strasse des 17.Juni 135, 10623 Berlin — [2]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin

Using molecular dynamic we investigate the equilibrium behaviour of a dipolar model fluid confined between two plane parallel walls, focussing on the influence of an additional homogeneous external electric or magnetic field. Structural properties are examined for field directions parallel and perpendicular with respect to the walls. Confinement alone induces already an in–plane orientation of the dipole moments [1] such that a parallel field easily polarizes the system. Moreover, the parallel field enhances the layer structure typical for confined fluids. Contrary to that a perpendicular field gives a new preferential direction which competes with the in–plane orientation observed without field. As a consequence very large fields are required to reach similar polarisation values as with parallel field. A particularly interesting effect is that high fields can generate a new layer in the system accompanied by structural rearrangements within the layer [2].

[1] V. A. Froltsov and S. H. L. Klapp, J. Chem. Phys. **124**, 134701 (2006); *ibid.* **126**, 114703 (2007).

[2] J. Jordanovic and S. H. L. Klapp, in preparation.

CPP 3.9 Mon 12:15 C 264

The impact of substrate-induced molecular orientation on dimerization in nanoreactors

— •Randy Mathes and Martin Schoen — Stranski-Laboratorium, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin

We investigate the impact of substrate-induced molecular orientation on dimerization in nano-confinement. Equilibrium properties are examined for different substrates and bond lengths and are compared to a bulk system. The system under study is a reacting mixture of Lennard-Jones spheres and homonuclear Lennard-Jones diatomics. We use Gibbs ensemble Monte Carlo to examine the bulk phase diagram. Substrate and bond length effects in confinement are studied using grand canonical Monte Carlo. In bulk systems we generally find higher mole fractions of dimers at higher densities and lower temperatures. As expected we find higher mole fractions of dimers in non-orientating confinement compared to a bulk system at fixed chemical potential. We exploit the preferred in-plane orientation of dimers near walls to tune dimer rates in confinement by enforcing molecular orientation perpendicular to the walls. From adsorption calculations we also expect a strong dependence on bond length.