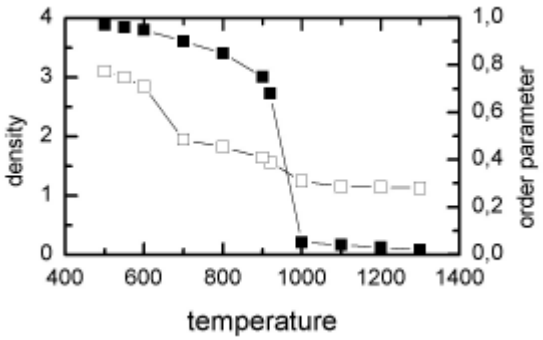
Report on PIRSES visits of A.Trokhymchuk, Institute for Condensed Matter Physics, NANU. (August 2012) to: TUB

Scope of work: Computer simulation of Janus particles using coarse-grained molecular dynamics simulations, first stage.

Simulation of Janus particles, as a part of a current project scope, will have a use of soft coarse-grained model potentials, as a cheaper alternative to the semi-atomistic potentials of Gay-Berne or similar. One of the options is to use the model potential for liquid crystal mesogens, developed by Lintuvuori and Wilson [J.S. Lintuvuori, M.R. Wilson, J. Chem. Phys. 128, 044906 (2008)]. As the first stage of the simulations of Janus particles immersed into a nematic solvent, there is strong need to study the bulk phase diagram for the particles interacting via this soft coarse-grained potential. Preliminary studies can be found in the paper mentioned above, according to these, the model can exhibit both the nematic phase as well as the smectic phase. Since our aim is to apply this model for the simulations of the defects around spherical Janus particle in nematic liquid crystal, we have performed an extensive computer simulation study to locate and define the thermodynamic boundary (temperature and pressure), where a stable nematic phase for this model can be observed.

The simulations have been performed at several fixed pressures in the range from 100 Pa to 5000 Pa. At each fixed pressure we have performed a set of simulation runs varying the temperature. We were interested how properties of the liquid crystalline medium will be changing by lowering the temperature. In each simulation run we we were calculating the full set of properties of this model system, including components of pressure tensor, energy, density, etc. However, the quantity of principal interest in these simulations was the order parameter. In figure we show simulation data for the pressure 1000 Pa.



The figure contains two sets of data – for order parameter (the line with filed symbols) and density (the line with open symbols). From the profile of order parameter we can see that at high temperatures up to 1000 K the model fluid is isotropic, i.e., disordered. However, as the temperature getting lower than 1000 K there is light increase of the density (from 1 to 2). This increase of the density is accompanied by a sharp increase in the order parameter (from 0.05 till 0.7). This is where the nematic phase in this model is located. The nematic phase exists in the temperature window from 900 K till 700 K. Further lowering of the temperature leads to one more jump in the density (from 2 to 3) when temperature is around 600 K. From other hand, order parameter at this temperature conditions shows the tendency to approach its maximal value. We attribute this temperature range to the smectic phase in this model.

Next, we performed modification of the coarse-grained molecular dynamics code for the LC systems to generalize it for the presence of the spherical colloid particles. Specifically, we considered the case of colloid particle split into two hemispheres, each possessing

independent type of anchoring (homeotropic or planar) of variable strength. Possible ways of describing the colloid-liquid crystal interaction and imposing the anchoring are suggested, in particular: (a) scaled sphere-spherocylinder potential plus extra anchoring field acting around certain shell around the collolid; (b) shifted sphere-spherocylinder potential plus extra anchoring field acting around certain shell around the collolid; (c) the shell of (either spherical of spherocylindrical) “phantom” particles on the shell of the colloid. Besides that, the plan for following research is set. In involves several stages: (i) tests on the effectiveness of various colloid-LC potentials outlined above; (ii) writing computer code for building the 2D projection of director orientations; (iii) performing extensive simulations of both non-Janus (uniform colloid) and Janus particles of various types and analyzing the results for the director field. This work will be performed during following visits.