

Report on the activities of Małgorzata Borówko during her visit to the Institute of Condensed Matter of Ukrainian Academy of Sciences in Lviv

January 15 – March 14. 2014

1. Scientific developments

During my stay in Lviv I dealt with two problems - the structure of grafted chain layers and a phase behavior of Janus discs in two-dimensional systems.

First, I have continued study the adsorption-induced changes of the structure of tethered chain layer in various fluids. We used density functional theory to investigate how different parameters affected configurations on grafted chains immersed in an explicit solvent. We concentrated on the effects of the fluid density and temperature. The results will be presented during 9th Liblice Conference on the Statistical Mechanics of Liquids (Czech Republic) I discussed with J.Ilnytskyi numerous aspects of the interplay between fluid adsorption and the structure of the bonded layer. We have also compared the results of his computer simulations with our theoretical predictions.

Second, I have finished the paper 'Phase transitions and self-organization of Janus discs in two dimensions by Monte Carlo simulation'. The study involved the special model of directional interactions between Janus particles. The nature of phase transitions in the selected model systems was analyzed. We found two phase transitions, a first order 'condensation' from a colloidal-poor to colloidal-rich phase and a continuous transition from a disordered fluid to the ordered fluid. We discussed how energy parameters influenced phase diagram topology. We observed a competition between self-organization into complex structures and phase transitions.

2. Meetings and transfer of Knowledge

I took part in seminars for doctoral students of Institute of Condensed Matter of Ukrainian Academy of Sciences and in the seminar by S. Sokołowski 'Confined Janus particles' (2014.02.10). I had also discussions with J. Ilnytskyi, A. Trokhymchuk and other research workers of the host Institute.