

**Report on the activities of Malgorzata Borówko during her visit to the Institute of
Condensed Matter of Ukrainian Academy of Sciences in Lviv.
The visit took place between 20 May and 19 June of 2013.**

1. On May 23 I attended the seminar given by prof. S. Sokołowski on *Electric double layers in slit-like pores: a DFT approach*.
2. Over entire period of the visit I discussed several problems connected with the project with the members of the host Institute. In particular, the discussions have been devoted to the following subjects: the impact of the chemical environment on the structure of polymer brushes, structural transitions in polymer layers, adsorption of chain molecules on the grafted chain layers.
3. During the visit I worked on thermoresponsive tethered chain layers in an explicit solvent. I carried out calculations using the density functional approach applied in our previous papers (J. Colloid and Interface Sci., 356 (2011) 267, J. Phys. Chem. B, 116 (2012) 3115). We introduce the following model. The chains were freely jointed tangent spheres. The grafted chains were inert with respect to the substrate. The fluid molecules interacted with the solid surface via Lennard-Jones (9-3) potential. All segments interacted via Lennard-Jones (12-6) potential. The density profiles of all components and the thickness of the brush have been calculated. The calculations have been carried out for selected model systems. First, we have investigated an influence of temperature on the structure of the grafted chain layer. We have studied the brushes in solvents with different affinities to the grafted chains. We have analyzed how the fluid density, grafting density and fluid-brush interactions affect the brush thickness at selected temperatures. We have considered the brush thickness as a function of temperature. It has been shown that a shape of such a function depended on the fluid density. For low fluid densities the brush height monotonically increases with increasing temperature. On contrary, at high fluid densities the brush thickness decreased. We have shown that at a certain fluid density the brush height was almost independent of temperature. Moreover, it has been shown that an increase of fluid density caused an increase or a decrease of the brush height depending on temperature. Second, we calculated the force acting on a selected segment of a tethered chain that leads to pulling the chain off the wall. The effects due the presence of other chains and fluid molecules, as well as temperature, were considered.
4. Moreover, we have analyzed the results of molecular simulation carried out using dissipative particle dynamic for selected grafted chain layers. We have investigated the influence of different parameters on the structure of the tethered chain layers. We have considered linear chains and the Y-shape molecules. The results were qualitatively consistent with the predictions of the density functional theory.