STEPS Students Report

Anastasia Sorokina (M1)
Faculty of Physics, MSU

I joined the group of Prof. Hiroshi Noguchi in order to study the interaction between lipid bilayers and microgels based on homopolymers and copolymers with different percentage of hydrophobic beads and to define the conditions of different regimes of such interactions by means of computer simulations. Polymer microgels are known to be soft colloidal networks, which possess a high surface activity and therefore can be applied as the effective emulsion stabilizers or as the templates of "smart" membranes. While the behavior of microgels on solid substrates and on liquid-liquid interfaces is well studied, the bilayer-microgel systems have not been studied yet, so it is an actual scientific problem. The motivation of such studies is porous structure of microgel molecules: they can incorporate into the living cell's walls (e.g. lipid bilayers) and thus serve as the responsive channels. Another reason is that microgels absorb drug molecules so these drug nanocarriers can pass through the lipid membrane and deliver drugs into the cell.

First, I learned how to simulate lipid bilayers on mesoscopic level and created the coarse-grained model of bilayer with zero surface tension. I took 23040 lipids consisting of three head segments (hydrophilic) and eight tail segments (hydrophobic). Such model was chosen based on the approach proposed by A. C. Balazs group, where the tension-free bilayer is constructed with 1.6 lipids per unit area. Then, I made the models of microgel particles based on a regular network with diamond-like lattice, where the molecules consist only of hydrophilic and hydrophobic units. The fraction of hydrophobic segments was varied from 0 to 50%.

Further, to simulate the interactions between bilayers and microgels I used dissipative particle dynamic simulation method (DPD). In this well-known method, each group of monomer units is represented by a spherical particle (bead) with a certain mass and cutoff radius. The force acting on each particle consists of three components: conservative, dissipative and random. In a classic DPD approach, the variation of conservative force parameter aij between different types of beads (namely, i and j) varies the character of interaction: for instance, the aij=25 corresponds to the neutral interaction, aij < 25 – to the attraction, and aij > 30 – to the repulsion. On this research step, I varied three interaction parameters: hydrophilic microgel beads – lipid head (from 15 to 25), hydrophilic microgel beads – water (from 25 to 30) and

hydrophobic microgel beads – lipid head (from 30 to 40).

In case of homopolymer microgel systems I have not found yet the conditions under which microgel attaches bilayer, though I have studied only 25-25, 20-25 and 20-30 systems (here the first number is for hydrophilic microgel beads – lipid head interaction, the second number is for hydrophilic microgel beads – solvent interaction). That means, that both for swollen and collapsed (aij= 25 and aij=30 respectively) states the microgel will rather bounce from the bilayer if the attraction between the lipid head and hydrophilic monomers is low. On the contrary, for bilayer – copolymer microgel systems I found that microgel attaches bilayer at 20-25 interaction parameters, and the contact area increases with increase of the hydrophobic fraction in microgel. Also, the contact area becomes smaller with the increase of repulsion between hydrophobic microgel beads and lipid heads. Finally, microgel spreads over bilayer at 15-30 interaction parameters for all systems, which occurs both due to the collapse of hydrophilic microgel beads and due to the attraction between them and lipid heads. Besides, I have calculated surface tension for all systems and revealed its dependence on main interaction parameters in systems.

Thus, during my visit, I have started the research on the complex systems based on microgels and lipid bilayers and I hope that it will eventually lead to the joined publication. I have obtained invaluable experience not only in computer simulation of such polymer and biopolymer systems, but also in communicating with foreign scientists, giving reports and discussing scientific work in English. Also, I hope that we will continue collaboration between the research group of my scientific supervisor and the group of Prof. Noguchi.