The goal of the project is to study self-organization of nanoparticles with modified surfaces. We will investigate two groups of nanoparticles: Janus-like particles and hairy nanoparticles particles. The chosen subject is fascinating from a purely cognitive point of view and touches fundamental problems in physics and chemistry. On the other hand, self-organization is a process of great importance for nanotechnology.

The spontaneous organization of molecules is the basic way of building complex structures in living systems. Inspired by these organizational processes in nature, chemists have recognized opportunities for a new generation of materials via the self-organization of synthetic building blocks. Nanoparticles are particularly promising building blocks with unique physical properties. The controlled assembly of nanoparticles in superstructures is important for realizing their novel applications ranging from medical therapeutics and diagnostics to photonics and electronics.

Among nanoparicles with modified surfaces Janus particles are the most popular. They have been named after two faced Roman god Janus because their surfaces have two patches with distinguishable properties. This special architecture allows them to form various aggregates and complex ordered structures. Similarly, the “hairy” nanoparticles provide unique opportunities for self-assembly into well-defined structures. A hairy particle contains a “core” with attached polymer chains. The “hairy” nanoparticles can be regarded as hybrid building blocks combining the properties of the core and the properties of the polymer brush.

The control of the assembly requires understanding how thermodynamic conditions affect the behavior of nanoparticles. Therefore, we will study effective interactions between the particles, their self-assembly under different conditions, phase transitions, the behavior at interfaces and adsorption of small molecules on nanoparticles.

The formulation of theory for self-organization is a difficult and an interesting challenge. We will use two types of research techniques: computer simulations and the density functional theory. We will carry out simulations using Monte Carlo and Molecular Dynamics methods.

The study should considerably broaden our knowledge on nanoparticles and their self-organization. The results can be used to project various novel “smart” materials.