

Self-assembly is one of the most common phenomena occurring in nature. Chemical molecules undergo this phenomenon, organizing themselves into supramolecular structures. We also observe self-organization on much larger scales: from nanoparticles to colloidal particles on a micro-scale. The spontaneous arrangement of particles into complex structures is ubiquitous in biological systems both at the intra- and extracellular levels.

Scientists working in different fields inspired by self-organization processes occurring in nature discovered the possibilities of producing new materials by synthesizing „building bricks” with specific properties, which then, under certain conditions and in a specific environment can „arrange” into several self-assembled structures with specific symmetry. Despite the thermodynamic principles that control self-organization processes are well-known, the theoretical prediction of the behavior of many particles with different properties and symmetry under different conditions is still a difficult task.

One of the most interesting types of "building bricks" are the so-called "patchy nanoparticles". By "patchy particles" we mean nanoscale objects that are anisotropically patterned, either by chemical modification of their surfaces, or through changes of the particles' shape, or both. Patchy particles have repulsive “core” and several “patches” of different characters allowing their assembly into numerous structures. Particularly, we can highlight the simplest case of patchy particles which are the Janus nanoparticles that consist of two jointed hemispheres that differ in their physical and chemical properties, often contrary in nature (e.g. hydrophilic and hydrophobic parts). The interactions between patches can have different characters, but this project concerns the cases in which only short-range, i.e. van der Waals or associative interactions are present. The method of distribution of patches, i.e. their topography determines the symmetry of the resulting self-organized structures. Patchy nanoparticles are one of the most common models of colloidal nanoparticles, this model can be also used to describe biomolecules

Our project concerns the investigation of adsorption and self-assembly of patchy nanoparticles in contact with walls of different curvatures. We will study the aforementioned processes of such systems and establish the limits of their stability, as well as determine their thermodynamic properties. We will carry out our research in slit-like pores (Fig. 1 a, b), nanotubes (Fig. 1 d-f), as well as in systems in contact with a single wall (flat or curved, Fig. 1 c, g). It has to be emphasized that due to the nanoparticle sizes we will investigate meso- and macropores according to the IUPAC convention which ensures us that they are able to adsorb inside them. We will also change the geometry of patchy nanoparticles due to the change of number, distribution, and chemical character of patches.

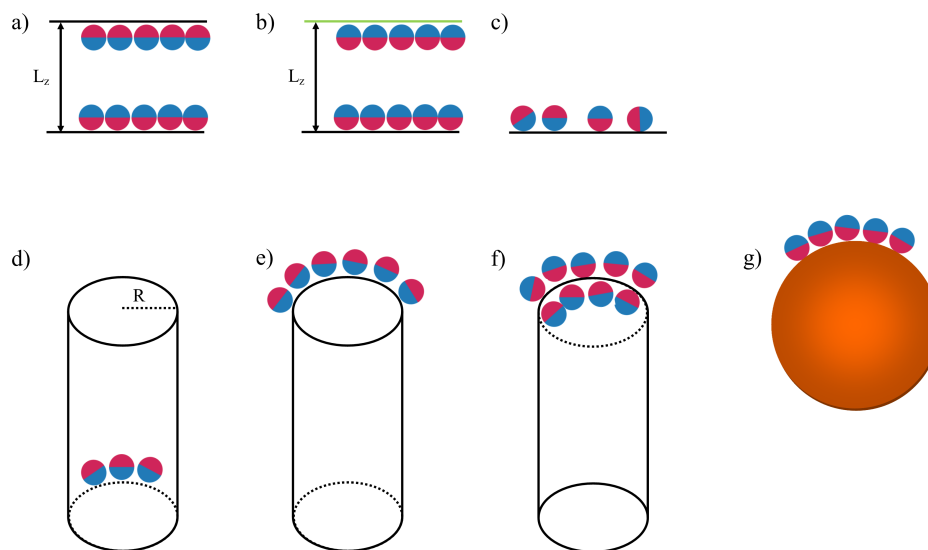


Fig. 1. Schematic representation of different type of confinement conditions and possible aggregation of Janus particles in such systems.

The presented project is mainly cognitive and its aims are determining (a) how the nature of the "patches" and their topography, and (b) how existing geometric restrictions (pore walls) affect their self-organization. We are convinced that the results obtained may be useful for the development of experimental research and nanotechnology.