

Polymers are macromolecular compounds comprised of many repeated elementary subunits called monomers. Polymers are important class of materials belonging to soft condensed matter. Polymers are widespread. Synthetic macromolecules are inevitable ingredients of commonly used materials, including plastics, rubbers, fibers, textiles, resins, glues and many others. Large group of materials which are biological in origin also contains polymers. These are for instance proteins, nucleic acids (DNA) or polysaccharides (starch). Of particular importance for polymer sciences is theoretical description of macromolecule conformation, i.e. spatial polymer configuration. Many physical properties of polymers are manifestations of the underlying structure and dynamics of a single polymer conformation.

The general scientific goal of proposed research is to develop theoretical framework providing deeper insight into dynamics of single (bio)polymers in solutions. The project aims to provide computational methods allowing to study and understand response of single molecules under different state of tension and at different frequencies. These advances will enable for instance to determine from simulations relaxation and frictional properties of single polymers under both equilibrium and nonequilibrium conditions. Since a variety of problems relies on fundamental understanding of polymer micromechanics the impact of this research is diverse from the point of view of basic and applied science. The mechanical properties of synthetic polymers provide the basis for investigating and predicting behavior of various materials. On the other hand molecular mechanics of biopolymers is essential to extend our knowledge about structural phase transitions of these molecules and to better understanding the relationship between their morphology and functionality.