

Nanotechnology is a multidisciplinary science which combines chemistry, physics, biology, medicine, and engineering. Nanotechnology deals with the design, chemical synthesis, and implementation of atomic-scale objects termed nanoparticles. Nowadays, nanotechnology is one of the fastest-developing branch of science and industry. Nanoparticles have been studied since many years ago, because of their unique properties resulting from their small size. As the result of their increasing use in industry, nanoparticles enter the environment and, consequently, living organisms. They are also extensively investigated in the context of the delivery of potential drugs to their targets such as, e.g., cancer cells, which is the domain of nanomedicine. Therefore, a lot of research is focused on the development of nanoparticle drug carriers. Because of the increasing presence of nanoparticles in the environment, their medical use, and their use in everyday life, there is a concern about their toxicity to the living cells and the entire organisms. Because the proteins and peptides present in living organisms are the primary molecules to interact with nanoparticles, studying protein and peptide interactions with nanoparticles is very important to assess their influence on the living organisms and to assess their ability to serve as drug carriers.

The goal of this project is to design and parameterize the coarse-grained models of carbon nanotubes and their interactions with polypeptides. The first component of these models will be the existing coarse-grained UNited RESidue (UNRES) model of polypeptide chains, which enables us to carry out protein simulations on a much longer time- and size-scale than those of the all-atom approaches. Two nanotube models will be designed and parameterized: continuous-tube and granular one. As the initial implementation, association of histidine- and tryptophan-rich peptides with nanotubes (the corona effect) will be and interactions of nanotubes with TLR receptors will be studied.

UNRES provides an about 1000-fold speed-up with respect to all-atom calculations. Therefore, the models developed in this project, will enable us to study peptide- and protein-nanotube system at the time- and size-scale inaccessible to all-atom simulations and to leave out unnecessary details (e.g., to calculate the trajectory of a cannonball, it is not necessary to know the atomic structure of the ball and of the surrounding air). In other words, the calculations will be possible with an off-shelf desktop or laptop computer instead of a dedicated supercomputer machine such as, e.g., ANTON. Such simulation will enable us to determine the mechanisms, thermodynamics and kinetics of interaction between the proteins and nanotubes at low computational cost. Therefore, nanotube toxicity to healthy cells and cancer cell and the affinity for drugs and their transport will be possible to assess and, consequently, the developed models could find use in nanomedicine.