Adsorption of Proteins onto Nanoparticles: Modelling the protein corona

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Cellular responses to materials in a biological medium reflect greatly the adsorbed biomolecular layer, rather than the material itself. Here, we study by molecular dynamic simulations the competitive protein adsorption on surfaces, i.e. the non-monotonic behavior of the amount of protein adsorbed on a surface in contact with plasma as a function of contact time and plasma concentration.

We try to understand the fundamental mechanisms of general competitive protein adsorption on surfaces. We make use of computational models to describe and analyze protein adsorption onto flat surfaces and curved surfaces such as Nanoparticles. This last case is specially interesting in many biological problems, for example NP uptake into cells, and a fully understanding of the dependence on surface curvature, size, or surface chemistry of how do proteins adsorb on NP is very important.

We implement Molecular Dynamics simulations in the NVT ensemble when the number of proteins is fixed or in a pseudo-μVT ensemble keeping constant the concentration of each kind of protein in the bulk when needed. We write high-performance GPGPU codes performing large-scale simulations. We use a coarse-grained model of protein interactions where each protein is described by two characteristic lenght-scales and its binding affinity with the surface. The solvent is also coarse-grained and it is implicit in the parametrization of the interaction forces. The protein-protein interactions are described with a CSW potential and the protein-NP interactions are described within the DLVO theory.

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