Molecular Characterization of the Effects of the Nanoparticle Interface on the Hydration Water

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Abstract

In the framework of a multiscale approach to study the protein-nanoparticle interaction in solution, we study here how to include the effects of the nanoparticle (NP) interface on the hydration water. From atomistic molecular dynamic simulations of a single nanometer-size solute in water, we study the hydration structure of different Silver NP. We analyze the behavior of the dipole moment and the potential energy of water molecules as a function of the distance from the surface, for different NPs shape. We show how our results can be used to tune the interaction parameters of a 3D coarse-grained model for water, in order to account of the interaction of water molecules at the NP surface. Our goal is to develop a coarse-grained model of the NP-protein solution with explicit water that would allow us to perform large scale simulations, something essential to compare simulations with experiments and to lead to useful model.