Molecular dynamics simulations of the spherical electrical double layer of a soft nanoparticle

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Abstract

Molecular dynamics simulations were performed to study the ion and water distribution around a spherical charged nanoparticle (Fig.1). A soft nanoparticle model was designed using a set of hydrophobic interaction sites distributed in six concentric spherical layers. To simulate the effect of charged functionalized groups on the nanoparticle surface, a set of charged sites were distributed in the outer layer. Four charged nanoparticle models, from a surface charge value of −0.035 C m^{-2} to −0.28 C m^{-2} were studied in NaCl and CaCl2salt solutions at 1 M and 0.1 M concentrations to evaluate the effect of the surface charge, counterion valence, and concentration of added salt.

We obtain that Na+ and Ca2+ ions enter inside the soft nanoparticle. Monovalent ions are more accumulated inside the nanoparticle surface, whereas divalent ions are more accumulated just in the plane of the nanoparticle surface sites. The increasing of the salt concentration has little effect on the internalization of counterions, but significantly reduces the number of water molecules that enter inside the nanoparticle. The manner of distributing the surface charge in the nanoparticle (uniformly over all surface sites or discretely over a limited set of randomly selected sites) considerably affects the distribution of counterions in the proximities of the nanoparticle surface.

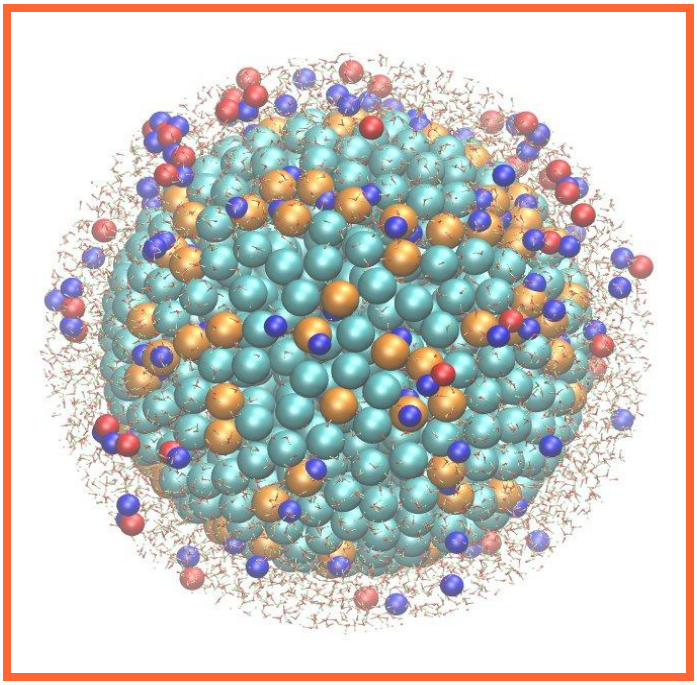

Figure 1: Model of spherical charged soft nanoparticle: water layers, Na^+ ions (in blue), and Cl^- ions (in red) close to 1.0 nm from the nanoparticle surface are displayed.