Overcharging process of spherical nanostructures

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Ionisable interfaces are present in many natural and industrial systems. In particular, numerous physical, chemical, and biological processes are governed by electrostatic interactions between charged colloids, surfactant monolayer, functionalized latex and oxide particles, polyelectrolyte, etc. In all these systems, the appearance of electrical forces is due to the surface charges developed on the interface by different charging mechanisms. Therefore, the presence of this surface charge implicates a distribution of ions around the charged surface, which is normally termed electric double layer (EDL).

The objective of our study is electrostatic properties of a model charged latex particle. In particular, we are interested to find the conditions needed to obtain the overcharging process for this modelled particle. The overcharging phenomenon or charge inversion occurs when the effective charge of a surface exposed to solution reverses polarity due to an excess of counter ions accumulated in the interface.

We have performed MD simulations with the GROMACS package. Different bulk conditions were obtained with different amounts of monovalent (Na+), divalent (Ca++) counterions. The Cl- ions were applied as co ions. The dependency of the colloids inverted charge on the concentration of the additional salt has been studied. The ionic strengths considered in our study were 1.0, 0.4 and 0.2 M.

MD simulations have been performed with GROMACS studying the density profiles and integrated charge distribution functions near nanoparticles bearing mobile unit charges at a variety of solution conditions. In particular, we analyzed the ability to generate particle charge inversion.