

Not accounting for the electronic polarizability due to divalent ions such as  $\text{Ca}^{2+}$  introduces a significant artifacts to force field-based molecular dynamic simulations of biological systems. Two newly developed parameter refinements were used to compute the free energy profile of the  $\text{Ca}^{2+}$ - $\text{Cl}^-$  ion dissociation in aqueous solutions, to be compared with a free energy profile obtained from ab-initio molecular dynamics and to data from neutron scattering.

Next, the computational evidence for the existence of a local free energy minimum representing a guanidinium-guanidinium contact ion pair in aqueous solutions is provided suggesting a global preference for a contact ion pair.

Finally, the passive membrane penetration mechanism of oligoarginines was investigated on a cell membrane model systems - lipid vesicles - by fluorescent spectroscopy. In this study, a mechanistic link between membrane penetration and vesicle aggregation and fusion was found.