Abstract

Molecular dynamics simulations are an important tool for the study of biological systems, such as biomembranes. The missing electronic polarization in classical non-polarizable force fields, however, produces significant inaccuracies in the interactions of membranes with charged particles, such as ions. In this work, we implement the missing electronic polarization effects into CHARMM36 force field for phospatidylcholine lipids. This implementation is done in the mean field way by using electronic continuum correction (ECC) model. We will validate the strength of ion–membrane interactions using the electrometer concept. This concept connects the response of choline order parameters of lipid molecules with the amount of charge present in the surface of the membrane.

Keywords: phosphatydylcholine, calcium ions, sodium ions, electronic continuum correction, electrometer concept