Simulation of processes in cellular membranes

Abstract

Many important processes in cells involve ions, e.g., fusion of synaptic vesicles with neuronal cell membranes is controlled by a divalent cation Ca^{2+}; and the exchange of Na^+ and K^+ drives the the fast electrical signal transmission in neurons. We have investigated model phospholipid membranes and their interactions with these biologically relevant ions. Using state-of-the-art molecular dynamics simulations, we accurately quantified their respective affinites towards neutral and negatively charged phospholipid bilayers. In order to achieve that, we developed a new model of phospholipids termed ECC-lipids, which accounts for the electronic polarization via the electronic continuum correction implemented as charge rescaling. Our simulations with this new force field reach for the first time a quantitative agreement with the experimental lipid electrometer concept for POPC as well as for POPS with all the studied cations. We have also examined the effects of transmembrane voltage on phospholipid bilayers. The electric field induced by the voltage exists exclusively in the hydrophobic region of the membrane, where it has an almost constant strength. This field affects the structure of nearby water molecules highlighting its importance in electroporation.