OVERCHARGING IN BIOMIMETIC MEMBRANES: MOLECULAR DYNAMICS SIMULATIONS

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Ions near membranes play an important role in many processes (transport, recognition,...) and determine the interactions between membranes. Experimentally, it is known that concentrations of divalent ions above certain thresold limits produce overcharging (i.e., charge inversion due to adsorption of counterions) at amphiphilic interfaces[1]. The consequences of membrane overcharging are dramatic. However, the physical mechanisms underliying this phenomenon are not well understood. Several theories propose different mechanisms of charge correlation leading to overcharging [2, 3]. In addition, ion hydration and dielectric overscreening near the membranes may have a decisive role [4]. In this work, we show large-scale molecular dynamics simulations performed in the new BSC spanish national Supercomputing facility showing the physical mechanisms of overscreening in a phospholipid biomimetic membrane. We performed simulations of a $DMPA^{2-}$/water layer in contact with Ba^{2+} counterions and added sat ($BaCl_2$), in conditions similar to those observed experimentally [1]. Our results allow us to identify the physical mechanisms for overcharging in these systems and the role player by Bjerrum correlations and ion hydration.

References

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