

372g Importance of Including Long-Range Interactions in Simulations of Biologically Relevant 2d Surfaces

Jeffery B. Klauda, Xiongwu Wu, Richard W. Pastor, and Bernard R. Brooks

The cell membrane consists primarily of lipids and is biologically important for the transport of substrates into the cell via membrane proteins. For large cells, these membranes are essentially 2-dimensional and are typically simulated in this manner. However, long-range interactions beyond standard cutoffs in molecular dynamics (MD) simulations are important, especially for lipid structure and surface tension. The air interfaces of heptane, hexadecane, and water are simulated with various cutoffs to test the appropriate methods to use in alkane-water and hydrated lipid membrane systems. MD simulations with particle mesh Ewald (PME) were used to test the recently developed Isotropic Period Sum (IPS) method. The IPS method approximates both long-range electrostatic (an alternative to PME) and non-electrostatic energies. We have found that the 2D version of IPS with only a 10 Å cutoff accurately reproduces PME with a necessary cutoff of 25 Å. Simulations with dipalmitoyl phosphatidylcholine (DPPC) using IPS result in an increase in surface tension and change in lipid structure demonstrating the need for both electrostatic and Lennard-Jones long-range interactions using 2D IPS in simulations of lipids. Another advantage of 2D IPS is the ability to simulate lipid monolayers with long-range interactions, where previous methods are unable to simulate these systems.