Bilayer perturbations

Peter Tieleman
University of Calgary, Calgary, Canada

With the decreasing cost of CPU cycles, a number of interesting properties of pure lipid bilayers has become within reach of simulations. These include free energy calculations on the partitioning of small molecules, lipids, and amino acids in membranes, large-scale deformations such as pore formation by electric fields, tension, antimicrobial peptides or surfactants, and phase changes to non-lammelar phases. Several of these processes are of direct interest to a better understanding of the mechanisms of certain membrane proteins. I will focus on recent work on the behavior of small molecules mimicking amino acid side chains, in particular arginine, and on free energy calculations related to the distribution and kinetics of sterol and lipid movement within a membrane.