MAR17-2016-000560

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

All-atom molecular dynamics simulation of lipid bilayers: Recent successes and current challenges

EDWARD LYMAN, Department of Physics and Astronomy, University of Delaware

About twenty years ago, the first molecular dynamics simulations of lipid bilayers revealed dynamics and structure on timescales of a few tens of picoseconds and lengthscales of a few nanometers. In the intervening years, ever increasing computational power has enabled ever more stringent tests of the models. The current generation of models obtains quantitative agreement with experiments for many *thermodynamic* observables for *simple* bilayers — quantities like NMR order parameters, area per lipid, and elastic constants. In this talk I will highlight three challenges that must be met in order for MD simulation to approach the complexity of cell membranes: bilayer asymmetry, lipidomic complexity, and translational dynamics. I will use our own recent work simulating complex lipid mixtures on the Anton computer to highlight two unexpected features of lipidomically complex membranes: Lateral subdiffusion on timescales up to milliseconds, and non-additive curvature energetics of lipid mixtures.