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Monte Carlo Simulation of Coexisting Phases in DOPC/DSPC/Cholesterol Ternary Mixtures REJWAN ALI, Polytechnic Institute of New York University, JIAN DAI, JUYANG HUANG, Texas Tech University — Lipid raft domain has been a topic of current interest in both computational and experimental membrane biophysics. Understanding raft domain will open up path for modeling many cellular phenomena. Extensive studies on model raft consists of DOPC/DSPC/cholesterol ternary system have been reported by many experimental groups. We report Monte Carlo simulation to reconstruct experimental phase diagram. Both pair-wise and multi-body interactions have been used to simulate the phase boundary of liquid-ordered phase and liquid-disordered phase coexistence region. A new algorithm, named the "Composition Evaluation Method," was implemented to determine the compositions of the coexisting phases in simulations. The new method is about 20∼50 times faster in determining phase boundaries, comparing to the traditional free energy calculation. In addition, pair correlation functions were used to map the phase boundaries in the critical region. We found that pair-wise interactions can reproduce the experimental critical point as well as the slope of tie lines, but not the compositions of the coexisting phases. Simulations with multi-body interactions produced a much better fit to the experimental phase diagram.

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