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Molecular simulation studies of tail-length effects in mixed-lipid bilayers JAMES KINDT, JASON DE JOANNIS, FUCHANG YIN, FRANK YONG JIANG, HAO WANG, Department of Chemistry and Emerson Center for Scientific Computation, Emory University — Because lipid lateral diffusion is slow on the time-scale accessible to atomistic molecular dynamics (MD) simulations, equilibrium clustering and segregation in mixed-lipid bilayers are impractical to study through conventional computational approaches. A hybrid MD-Monte Carlo method employing lipid mutation moves within the semi-grand canonical ensemble method has been implemented for mixtures of lipids of differing tail lengths. For DLPC:DPPC mixtures, equilibration is demonstrated during simulation runs nearly two orders of magnitude shorter than estimates for standard MD. Statistical measures of lateral association in bilayer slabs and of partitioning among membrane micro-environments (flat bilayers, inner and outer leaflets of curved bilayers, and bilayer edge) will be presented.

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