493a Simulation of Fluorescence Resonance Energy Transfer in Two-Phase Multi-Component Membranes

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We model bilayer lipid membrane systems using both simulation and semi-analytical methods for a binary phospholipid/cholesterol system containing two (donor and acceptor) lipid-like fluorescent membrane probes. Several compositions inside the liquid-disordered and liquid-ordered coexistence regime were investigated. We develop a model to predict fluorescent resonance energy transfer (FRET) efficiencies while accounting for liquid-ordered domain size. Simulations are carried out for domain sizes of 15, 30, 45, and 60 nm at different cholesterol compositions within the two-phase coexistence regime. Model results produce both qualitatively and quantitatively similar data to that of the simulations. A three parameter fit is performed using the model to estimate the domain diameter and partition coefficients for both fluorescent probes. Using this methodology we estimate liquid-ordered domain sizes for simulated FRET data and demonstrate the effect of probe partition coefficients on the accuracy of these predictions.