Applications of Coarse-Grained Molecular Modeling

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In many materials and biomolecular systems, the problems of interest span time and/or length scales that make traditional all-atom approaches challenging. Coarse-grained (CG) models, where each site represents a collection of atomic or molecular units, have emerged as a valuable alternative to accelerate progress on these challenging problems. In this presentation, I will discuss examples from our group where we have applied CG modeling and advanced sampling techniques to address problems in lipid membranes and DNA. In the case lipid membranes, we show how the cooperative dynamics of lipid molecules naturally give rise to transient clusters of highly mobile and immobile regions of the membrane. We discuss the potential role of such dynamic heterogeneity for biological processes and the potential formation of lipid raft structures. In the case of DNA, we examine the ability of a three-site-per-nucleotide model to mimic the experimentally measured properties of four-way junction DNA, which plays a central role in genetic recombination and DNA repair. If time allows, we will also discuss a more extreme coarse-grained model for DNA that can be used to predict the phase diagram of nanoparticle lattices, where the lattice structure is dictated by DNA linkages between nanoparticles.