

MAR15-2014-020771

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Bridging scales: from atoms to coarse-grained models for soft matter systems

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Molecular simulation has extended to increasingly complex soft matter systems, and time-scale and system-size requirements have instigated the use of simulation models on multiple levels of resolution. On the classical particle-based level, a large variety of methods to develop coarse grained (CG) simulation models has emerged, an important subgroup being those scale-bridging methods where the CG model is derived from and systematically linked to an underlying atomistic description. In my talk, I will introduce a few of these methods, address the underlying concepts as well as some of the ongoing challenges that are inherent to coarse graining. A natural consequence of reducing the level of resolution in a simulation model is a loss of transferability, i.e. a decreasing ability to correctly describe a system at several thermodynamic state points. Intimately linked to this is a loss of the ability to correctly represent all structural, thermodynamic and dynamic properties of the system. Examples for these limitations are easily found in all CG simulations of multicomponent or multiphase soft matter systems – ranging from liquid crystals, biomolecular aggregates, biomaterials to hard/soft nanocomposites. A correct representation of phase transitions, phase coexistence, environment-induced conformational transitions, or effects due to surfaces and interfaces is a severe challenge for bottom-up CG models. Addressing this challenge requires both a method of generating CG potentials as well as finding and rationalizing an appropriate reference state point to start out from. I will illustrate several of these aspects using examples from the biomolecular and (biomimetic-) materials world.