Systematic coarse graining for dynamical simulations of anisotropic particles

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Coarse-grained simulation models, in which several atoms are represented by a single coarse-grained site, are often used to study phenomena on longer length and time scales than are computationally feasible with all-atom models (Baschnagel *et al.* 2000; Saunders and Voth 2013). Almost all coarse-grained models and algorithms to parametrize such models have used spherical sites (Baschnagel *et al.* 2000; Saunders and Voth 2013). While this strategy is generally accurate for flexible molecules, highly anisotropic rigid molecules, such as organic semiconductors (Huang *et al.* 2010; Schwarz *et al.* 2013) used in novel flexible electronic devices, are often not efficiently represented by spheres. I will discuss a new systematic and thermodynamically consistent algorithm that we have developed to parametrize coarse-grained models using anisotropic sites from an underlying all-atom model for use in molecular dynamics simulations. I will also discuss the application of such simulation models to studying the supramolecular ordering of anisotropic particles in the liquid phase.

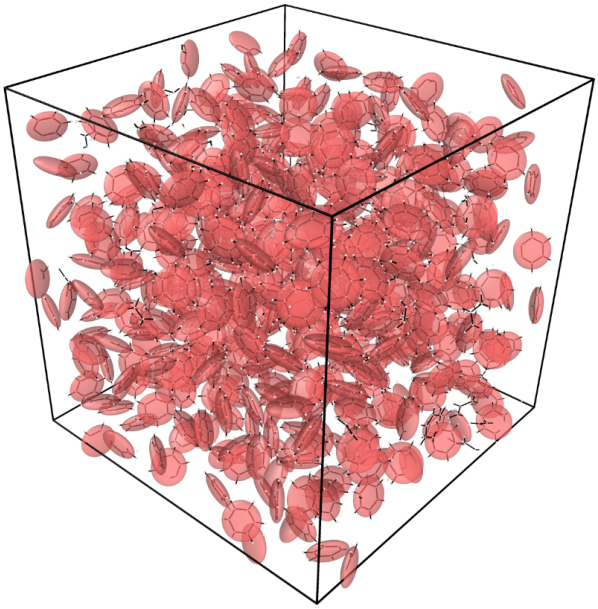

Fig. 1. Mapping from all-atom to anisotropic coarse-grained representation of liquid benzene.

References

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