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Development of Coarse Grained Models for Long Chain Alkanes
GAURAV GYAWALI, SAMUEL STERNFIELD, IN CHUL HWANG, STEVEN RICK, Univ of New Orleans, REVATI KUMAR, Louisiana State University, RICK GROUP TEAM, KUMAR GROUP TEAM — Modeling aggregation in aqueous solution is a challenge for molecular simulations as it involves long time scales, a range of length scales, and the correct balance of hydrophobic and hydrophilic interactions. We have developed a coarse-grained model fast enough for the rapid testing of molecular structures for their aggregation properties. This model, using the Stillinger-Weber potential, achieves efficiency through a reduction in the number of interaction sites and the use of short-ranged interactions. The model can be two to three orders of magnitude more efficient than conventional all atom simulations, yet through a careful parameterization process and the use of many-body interactions can be remarkably accurate. We have developed models for long chain alkanes in water that reproduce the thermodynamics and structure of water-alkane and liquid alkane systems.

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