Developing a Coarse-Grained Model for 1-Alkyl-3-methyl-imidazolium Chloride Ionic Liquids

Because of the sluggish dynamic and complex electrostatic potential networks of ionic liquids, establishing a reasonable and efficient coarse-grained model with enough simulation time is very important for a large system. In this work, novel coarse-grained models of 1-n-alkyl-3-methylimidazolium chloride \([C_{n\text{mim}}][\text{Cl}]\) \((n=4, 6, 8)\) have been developed from the united atom model of ionic liquids. There are two mapping strategies for the ionic liquids coarse graining, one is that the imidazolium cations \([C_{n\text{mim}}]^+\) \((4, 6, 8)\) and \(\text{Cl}^-\) anion are represented as single coarse-grained bead as an ionic model. The other is a pair of ionic liquids mapped to one bead as a molecular model. It was found that both of the coarse-grained models could give a good description of structures and thermodynamic properties for ionic liquids. Moreover, because of the reducing freedom of a coarse-grained model a correction of the results as a united atom force field was established for self-diffusion coefficients which could be reproduced effectively. Notably, the ionic model improves the calculation efficiency up to 9.5 times compared with united atom force field under the same simulation conditions because the electrostatic potentials in the ionic model are highly important for coarse-grained model for ionic liquids. In summary, the coarse-grained models could provide a theoretical basis for large-scale ionic liquids systems.

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