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 [Cnmim][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 ([Cnmim]+ (4, 6, 8)) and 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.

General information
State: Published
Organisations: KT Consortium, CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Bohai University, Chinese Academy of Sciences
Number of pages: 10
Pages: 15206-15215
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: Industrial and Engineering Chemistry Research
Volume: 57
Issue number: 44
ISSN (Print): 0888-5885
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.4 SJR 0.978 SNIP 1.203
Web of Science (2017): Impact factor 3.141
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.95 SNIP 1.155
Web of Science (2016): Impact factor 2.843
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.87 SJR 0.938 SNIP 1.145
Web of Science (2015): Impact factor 2.567
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.85 SJR 1.009 SNIP 1.287
Web of Science (2014): Impact factor 2.587
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.6 SJR 0.975 SNIP 1.232
Web of Science (2013): Impact factor 2.235
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.56 SJR 1.054 SNIP 1.32