

Static and dynamical properties of ionic liquids

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Ionic liquids are liquid of organic salts at room temperature. The melting temperatures of ionic liquids are much lower than that of typical salts (ex. NaCl). This feature is the most characteristic property of ionic liquids. The applications as clean solvent, electrolytes for batteries and electrosynthesis have been extensively investigated. We performed molecular dynamics (MD) simulations of 1-butyl-3-methylimidazolium cation with PF₆, NO₃ and Cl anions to obtain their static and dynamics properties. The parameters of force field for MD simulation were introduced by Lopes et al [1]. We used special purpose computer, MDGRAPE-3, to perform MD simulations of large systems which have up to 4,096 ion pairs system (131,072 particles).

[1] J. N. C. Lopes et al, J. Phys. Chem. B, 108, 2038 (2004)

[2] M. Taiji et al, Proceedings of the SC2003 (2003)