455g Modeling Co_2 Solubility in Ionic Liquids Using Semi-Grand Ensemble Hybrid Monte Carlo

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Ionic liquids have good solvation properties, capable of dissolving polar and non-polar species. Experimentally, it has been found that many gases, including CO_2, are highly soluble in ionic liquids. The solubility of gases in ionic liquids is important, since many applications focus on the use of these liquids as replacement solvents for reactions involving gaseous species and as novel absorbents. To achieve this goal, fundamentals of gas solubility in ionic liquids should be understood. Cadena et al. conducted molecular dynamics simulations[1] and found that the anion is primarily responsible for high CO_2 solubility.

In this work, the semi-grand hybrid Monte Carlo method ($N_{IL}f_gPT$; fixed number of ionic liquid, fixed fugacity of gas, constant pressure and constant temperature ensemble) is described in the simulation of CO_2 solubility in ionic liquids. The simulation system evolves according to the equation of motion through molecular dynamics method. Cavity-bias[2, 3] and configurational-bias[4] methods were applied to increase the insertion acceptance ratio. The computed isothermal results for CO_2 in 1-*n*-butyl-3-methylimidazolium hexafluorophosphate (bmim + PF_6]) are compared with the ones from experiment[5].

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