Calculating Pure and Mixed Gas Isotherms in Ionic Liquids Via Monte Carlo Simulation

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Ionic liquids (ILs) are salts that are liquid at or near ambient temperature. A large number of different cations and anions may be paired to form an IL, and because of this the properties of ILs vary widely. ILs have been shown to have excellent solvation properties, which has stimulated investigations into the use of ionic liquids as solvents and separation media. Given the huge number of ILs available, it is impossible to experimentally test even a small subset of all potential ILs. For this reason, atomistic-based simulations have been used to gain insight into the chemical and structural factors governing solubilities in ILs. In this talk, we show how pure and mixed gas solubilities in ionic liquids can be computed using Monte Carlo simulations. Sampling in these dense, highly charged systems is difficult, so we utilize a recently developed procedure called continuous fractional component Monte Carlo to enable the calculations to be carried out. We demonstrate the accuracy of the simulations by comparing computed isotherms for CO2, SO2, H2O, N2, O2 and NH3 in different ILs against experimental data. We also compute the solubility of gas mixtures, data for which is much harder to obtain experimentally. Finally, we show how the molecular level insight obtained from the simulations can enable us to develop new ionic liquids tailored to have optimal solvation characteristics for applications such as separations and catalysis.