Understanding Phase Separation of Water/O-alkylated Ionic Liquid Mixtures through Molecular Dynamics Simulation

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In this study, the phase separation between water and hydrophobic ionic liquid (IL) composed of amide-based O-alkylated cations (i.e. O-ethyl-dimethylacetamidium (EDEA), O-methyl-dimethylacetamidium (MDEA), O-methyl-dimethylformamidium (MDMF) and O-methyl-1-ethylpyrrolidinonium (MEPyr)) and trifluoromethanesulfonate (TfO-) anion was investigated via molecular dynamics simulations. We found that pcff force field, along with the scaled AM1-BCC charge model, can properly describe the behavior of the ionic liquid, which was validated by the calculated density of each ionic liquid. Phase separation of randomly mixed water-IL systems were observed within dozens of nanoseconds. In order to quantify the miscibility between water and hydrophobic IL, demixing indexes and interaction energies of water-ion were estimated for all water-IL systems. Furthermore, the distribution of ions and water in each phase was analyzed by radial distribution function. This theoretical information about the phase separation could serve as a cornerstone for the extraction of metal ions using IL.