Computational Molecular Design of Ionic Liquids for Carbon Dioxide Capture

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Carbon dioxide is the main greenhouse gas and its major source is the combustion of fossil fuels for power generation. Ionic liquids can be an alternative for carbon capture because they possess several advantages over conventional solvents. The objective of this work is to carry out the design of ionic liquids by computational molecular design (CMD). Their molecular adjustable nature yields a surprising number of possible cation and anion combinations. So the selection of appropriate ionic liquid by molecular design becomes very important. Current focus is on property prediction of ionic liquids using the group contribution method. A region of desirable target properties will be calculated by process simulations. A mixed-integer programming (MIP) formulation for the molecular design optimization of ionic liquids to achieve the targeted properties and cost effectiveness will be presented. This solvent design work is intended to accelerate the experimental trial-and-error approach by searching and providing a smaller set of chemical structures, that are likely to match a set of desired properties and economic targets.