Developing New Ionic Liquids for CO_2 Capture:
A Success Story for Thermodynamics and Computational Molecular Design

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In this talk I will discuss results from a DOE-sponsored research partnership in which our team at Notre Dame, working with various industrial partners, have designed, synthesized and tested new molecules that have the potential to dramatically reduce the cost of post-combustion CO_2 capture. The class of compounds we have investigated are ionic liquids, which are pure salts that are liquid around ambient temperatures. These salts are known to have many favorable properties, including good thermal and chemical stability and essentially no vapor pressure. These properties, along with their ability to be "tuned" to have a wide range of chemical functionality, have made them particularly interesting targets as solvents. Using advanced computational chemistry methods and atomistic based simulations coupled with sophisticated experimental property measurement techniques and process modeling, we have developed a new class of ionic liquids that may have significantly better CO_2 capture economics than conventional amine-based solvents. These liquids have a higher effective capacity for CO_2 than conventional monoethanolamine solvents, and preliminary process modeling suggests that they also have a lower parasitic energy cost.