Liquids that contain charged species, such as electrolytes and ionic liquids, have many important technological applications in fields such as energy storage, separations, and catalysis. By changing the structure of the molecules or employing mixtures, the properties of these fluids can be altered significantly. The key questions are: How should I change the structure of the molecule or ion to get the properties I want? What type of additives should I use to improve performance? To answer these and related questions, we use atomistic-level simulations to compute structural, thermodynamic and transport properties of these systems. We are able to provide molecular-level explanations for experimental observations, and we can predict properties of systems that may not yet have even been made in the laboratory.

In the first part of this talk, I will describe molecular modeling research directed at improving the performance of electrolytes used in next generation “beyond lithium” batteries. Electrolytes are a critical component of batteries, since they transport ions from the cathode to the anode during charging, then in the reverse direction in releasing energy on discharge. Electrolytes play a leading role in a battery’s capacity for energy storage, its lifetime and the safety of the battery. The electrolyte in a conventional lithium-ion battery consists of a lithium salt dissolved in an organic solvent. The electrolytes for next generation “beyond lithium” batteries will require new salt-solvent combinations. Our simulations probe the way in which different electrolyte formulations, charge carriers and additives impact the structure and dynamics of these liquids.

In the second half of the talk, I will show how these same kinds of simulations can be used to develop new ionic liquids that can be used for CO2 separations / capture. Ionic liquids are pure salts that are liquid at ambient temperatures. Because they have essentially no vapor pressure and readily dissolve CO2, people have been interested in using them for carbon capture. I will describe how our simulations have been successful in identifying new ionic liquids with properties tuned for use as conventional liquid absorbents or as supported ionic liquid membranes.

Tuesday, Dec. 5, 2017
Lecture at 4:00 p.m.
Room 1610, Engineering Hall
Refreshments will be served at 3:45 p.m.