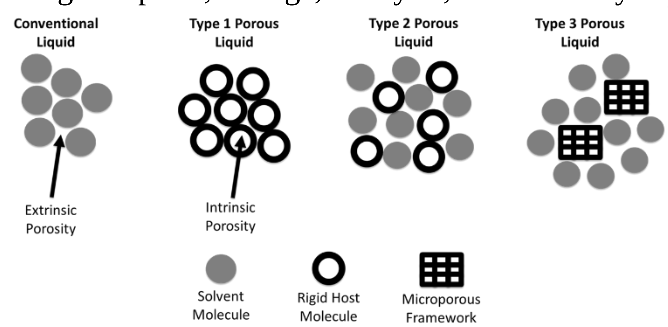
Engineering Porous Liquids for Gas Separations

Much of the CO_2 and greenhouse gases in the atmosphere are emitted from point sources like refineries, power plants, and other large industrial plants. The state-of-the-art technology for capturing CO_2 from these concentrated mixtures is solvents that have high affinity for CO_2. Despite the advances in solvents for CO_2 capture there are inherent disadvantages of these liquid-based systems including low gas capacities, large operating units and capital costs, and high regeneration energy/costs. Solid adsorbent materials have been explored as alternatives. These materials are microporous and can selectively adsorb target molecules from a mixture via a combination of guest-surface interactions and guest confinement. Adsorbents can have much lower volumes and operating costs than solvent systems, but are much more complex to operate than solvent systems. "Porous liquids" offer the opportunity to combine the benefits of mature solvent processes with the benefits of solid adsorbents.

Porous liquids (PLs) are an emerging class of microporous materials where a flowing liquid is imbued with intrinsic and permanent porosity. There are three types of porous liquids: Type 1 porous liquids are porous molecules that flow and maintain their porosity, Type II porous liquids are developed by dissolving a rigid, porous host molecule in a solvent that is too large to penetrate the pores of the host molecule, and Type III porous liquids are developed by dispersing a microporous host molecules in a sterically hindered solvent. In each case a flowing liquid decorated with micropores that are available for gas capture, storage, catalysis, and a variety of other applications is created. The focus of this talk is on the development of Type II porous liquids. Although multiple Type II porous liquids have been reported, there has been little work done to understand the fundamental nature of porous liquids, accelerate the discovery of new PLs, and determine their potential in the separations field.



This seminar will address two main issues, 1) the discovery and characterization of Type II PLs and 2) the potential of Type II PL use in industrial contexts. The thermodynamic properties of PLs are evaluated across multiple PL types and used to determine ideal applications for each type of PL. Partial molar properties of the PLs are used to quickly characterize their porosity which will lead to the accelerated characterization of future PLs. Next, we successfully developed a solvent screening tool in collaboration with computational researchers to accelerate the search for good solvents that can dissolve porous organic cages. As stated before the potential of porous liquids in gas separations has not been explored by engineers yet. A high-level techno-economic analysis of porous liquids in a CO_2 capture process shows that porous liquids have the potential to economically compete with industrial physical solvents while significantly reducing the capital and operating costs of the separation. Industrial separations scenarios present chemically aggressive and complex environments, so post synthetic modification of POCs is conducted to imbue chemical gas stability to the resulting porous liquid.