Molecular Design Strategies for Task-Specific Solvent Technologies

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Abstract

CO_2 capture from power plant exhaust is a complex problem that requires the capture and removal of massive quantities of gases. Solvent technologies for CO_2 capture and conversion have become one of the most promising solutions with aqueous amines being one of the industrial standards. However, their high regeneration costs render them prohibitive for many of the large-scale applications in power generation. My presentation will outline the computational approach used toward the deliberate design of single-molecule CO_2-bidining transformational solvents. These types of solvents constitute an attractive alternative to the water-based solvents, but are hampered by exponentially increasing viscosities at high CO_2 saturation. Using state-of-the-art computational methods, like enhanced sampling methods for reaction free energetics in explicit solvent models using *ab initio* molecular dynamics, we describe the key structural parameters that allowed us to create reduced models for fast screening of solvent libraries. This approach led to tangible hypotheses as to the synthetic protocols that have already identified candidate molecules with appreciable viscosity reductions at target loading levels.

Image

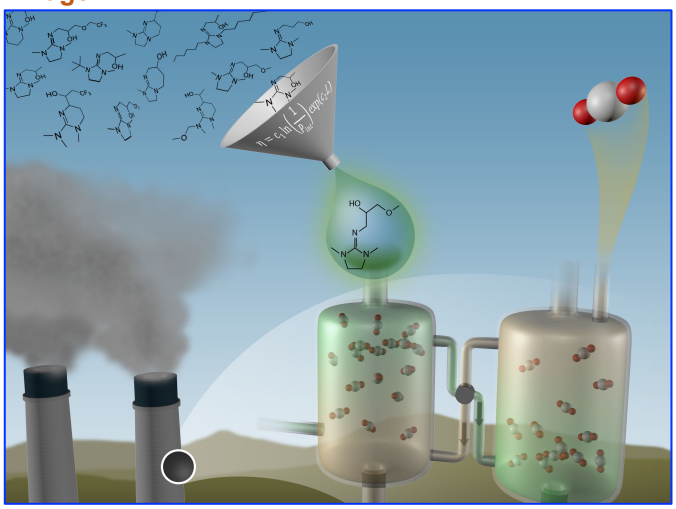


Figure 1. Schematic representation of concerted design efforts to accelerate solvent design for CO_2 capture.

Recent Publications (minimum 5)

1. Cantu D. et al. (2016) Dynamic Acid/Base Equilibrium in Single Component Switchable Ionic Liquids and Consequences on Viscosity. *J. Phys. Chem. Lett*. 7: 1646-1652.
2. Cantu D. et al. (2016) Structure-property reduced order model for viscosity predicition in single-component CO2-binding organic liquids. Green Chemistry 18: 6004-6011.
3. Malhotra D. et al. (2017) Reinveting design principles for developing low-viscosity carbon dioxide binding organic liquids for flue clean up. ChemSusChem 10: 636-642.



Biography

Dr. V.-A. Glezakou is a computational chemist with over 20 years of experience in atomistic simulations, with particular emphasis in transition metals chemistry and condensed phase systems relevant to carbon capture an conversion, catalysis and materials properties. The focus of recent research is in the structure, vibrational spectroscopy and structure/activity correlations in a diverse ensemble of problems such as catalytic activity of metal clusters and oxide supports, transformative solvents for post-combustion carbon dioxide separations, mechanistic studies of MOF nucleation, solvatochromic effects in surface-supported chromophores. She is co-supervising a group of about 10 staff and post-docs that are tasked with the integration of fundamental and applied studies that help accelerate time-sensitive technologies.

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Notes/Comments: