

“Molecule Design Strategies to Reduce the Viscosity of Non-Aqueous Carbon Capture Solvents”

1104 Gilman, Friday, August 26th at 11:00 a.m.



Dr. David Cantu
Pacific Northwest
National Laboratory

The industrial use of non-aqueous solvents for CO₂ capture from power generation sources is primarily limited by the high viscosities of the solvents. Carbon dioxide binding organic liquids (CO₂BOLs) are strong non-nucleophilic bases well suited for binding CO₂ to their aliphatic alcohol group. They become zwitterionic upon reaction with CO₂ but they easily revert to their non-ionic form thermally. Post-combustion capture of carbon dioxide can be performed with solvents that exhibit adequate CO₂ binding capacities, are non-volatile at operating conditions, and have low viscosity. Currently, CO₂BOLs meet only the first two requirements. However, they are still very attractive candidates for CO₂ capture because they require no additional solvents and are liquid at post-combustion conditions, reducing thermal regeneration cost.

I will present our studies of candidate CO₂BOL molecules, in collaboration with experiment, toward the design of low-viscosity compounds. I will introduce key molecular features that control their viscosity and CO₂ uptake kinetics. Ab initio molecular dynamics simulations reveal the mechanism of carbon capture, and a proton transfer equilibrium toward a non-charged acid state. Larger scale classical molecular dynamics simulations, performed at varying carbon loadings, provide estimates of viscosities showing that the hydrogen-bonding network between the two charged functional groups is a key descriptor of solvent viscosity. Based on this result, a quantitative structure-property relation model was developed that predicts CO₂BOL viscosity given a few structural parameters and CO₂ loading. With the model, a high number of candidate compounds were screened to identify promising candidate molecules that are currently synthesized and their viscosities experimentally measured. Two viscosity reduction design strategies are presented: chemically tuning solvent molecules to favor internal hydrogen bonds, and favoring the non-charged acid state of the proton transfer equilibrium.

**Refreshments
will be provided
in 2061 Sweeney
Hall at 10:30 a.m.**

*If you plan to attend,
email a question to
bellinda@iastate.edu
and the speaker will
answer your question!*

**Graduate
Seminar
Series**

2016-2017

www.cbe.iastate.edu/events

IOWA STATE UNIVERSITY

Department of Chemical and Biological Engineering



**Chemical and
Biological
Engineering**