Brennecke Research Group

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Univ. Notre Dame until Summer 2017

The University of Texas at Austin
McKetta Department of Chemical Engineering

Starting August 1, 2017
Labs in EERC

Who am I?

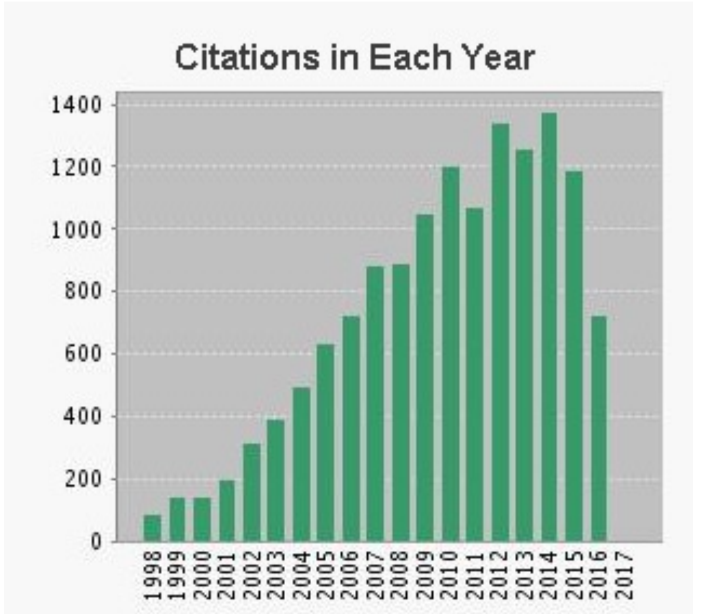
Alumna Joan Brennecke To Join Faculty

The McKetta Department of Chemical Engineering is proud to announce alumna and renowned researcher Joan Brennecke (B.S. '84) will join our faculty as a professor beginning fall 2017.

Brennecke, a leading expert in energy and sustainability, was recruited with key support from Texas Gov. Greg Abbott and his new Governor's University Research Initiative (GURI) grant program. The program aims to bring the world's best and brightest minds to Texas universities to spur innovation and drive economic activity. Brennecke is one of 10 researchers to receive a GURI grant in 2016 to come to Texas universities, marking the program's first round of awards.

Who Am I?

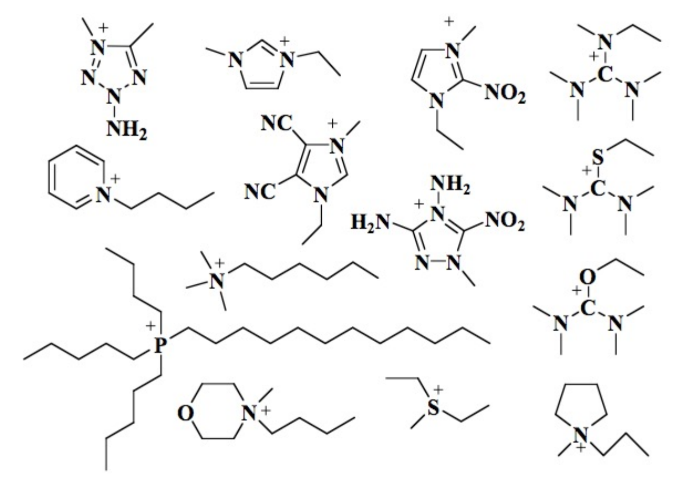
- B. S. UT Austin 1984
- M.S., Ph.D. Univ. Illinois 1987, 1989
- At Notre Dame since 1989
- >160 pubs; >14,000 citations
- H-index 53
- ACS Ipatieff and Murphree, DOE E.O. Lawrence, AIChE Professional Progress
- National Academy of Engineering



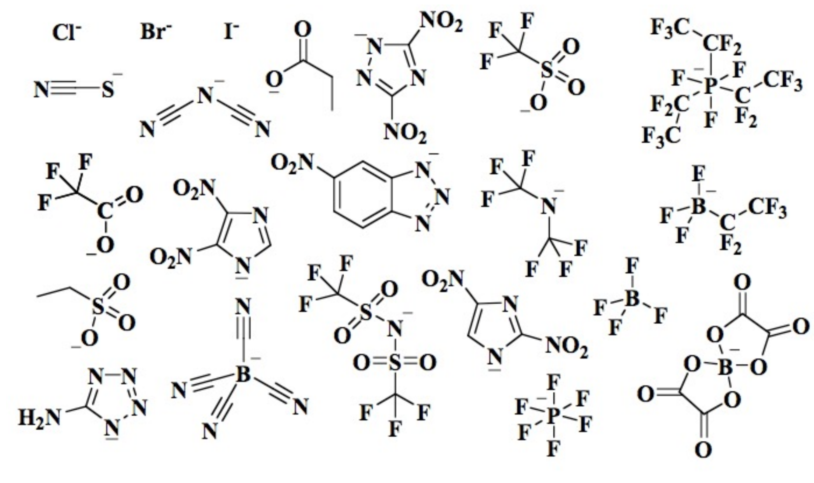
Ionic Liquids

- Pure salts that are liquid around ambient temperature
  - Not simple salts like alkali salts
- Many favorable properties
  - **Low volatility**
  - Anhydrous
  - High thermal stability
  - Huge chemical diversity

Examples of cations



Examples of anions



Overall Hypothesis

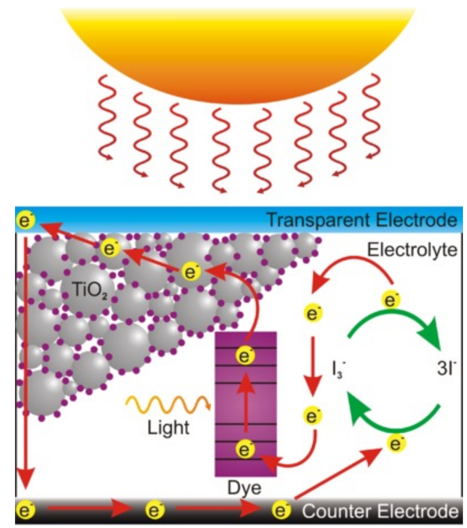
- Relationship between molecular structure and function
  - Enthalpic interactions and entropy
  - Some characteristics like conventional liquids, but some like solids
- If you can specify the desired chemical and physical properties to perform a give function, we can design an IL with those properties

What We Do

- Design, synthesis and purification of new ILs
- Thermophysical properties
  - Melting points, decomposition temperatures, viscosities, densities, ionic conductivities
  - Excess enthalpies
- Phase behavior
  - Gas solubilities, VLE, LLE, SLE
- Electrochemical properties
  - Electrochemical windows, electrochemical reduction of CO_2, electroplating
- Reactivity (with CO_2)
- Macroscopic thermodynamic modeling

Energy Applications

- Separations
  - CO_2 capture
  - Desulfurization
  - Organics from fermentation broths
- Cooling and Heating
  - Absorption cooling
  - Co-fluid vapor-compression refrigeration and heat pumps
- Biomass Processing
- Electrolytes
  - Batteries
  - Fuel cells
  - Supercapacitors
  - Dye sensitized solar cells
- Heat Transfer Fluids



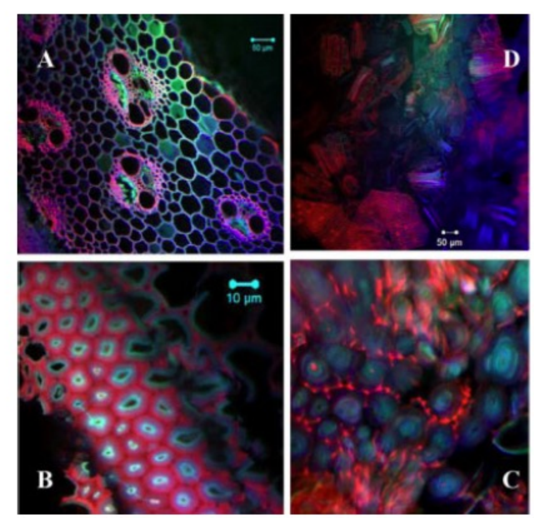
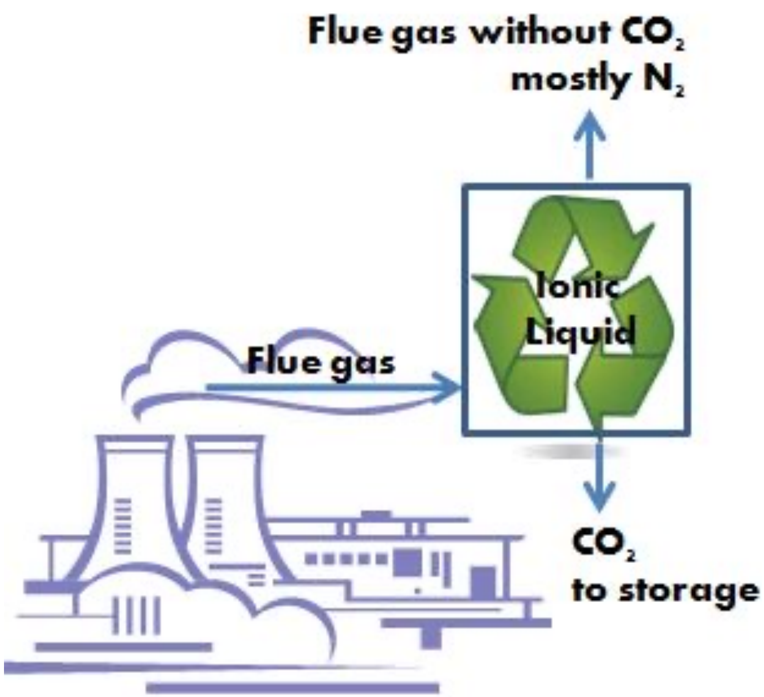


Figure 4. In situ dynamic study of switchgrass dissolution in ethyl methyl imidazolium acetate. Confocal fluorescence images of switchgrass stem section before pretreatment (**a**), and after 20 (**b**) and 50 (**c**) min of pretreatment. Complete breakdown of organized plant cell wall structure (**d**) is observed after 2 h.

ILs for CO_2 Capture



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CO_2 IMPACCT

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

NETL the ENERGY lab
Where energy challenges converge and energy solutions emerge

GCEP

STANFORD UNIVERSITY
GLOBAL CLIMATE & ENERGY PROJECT

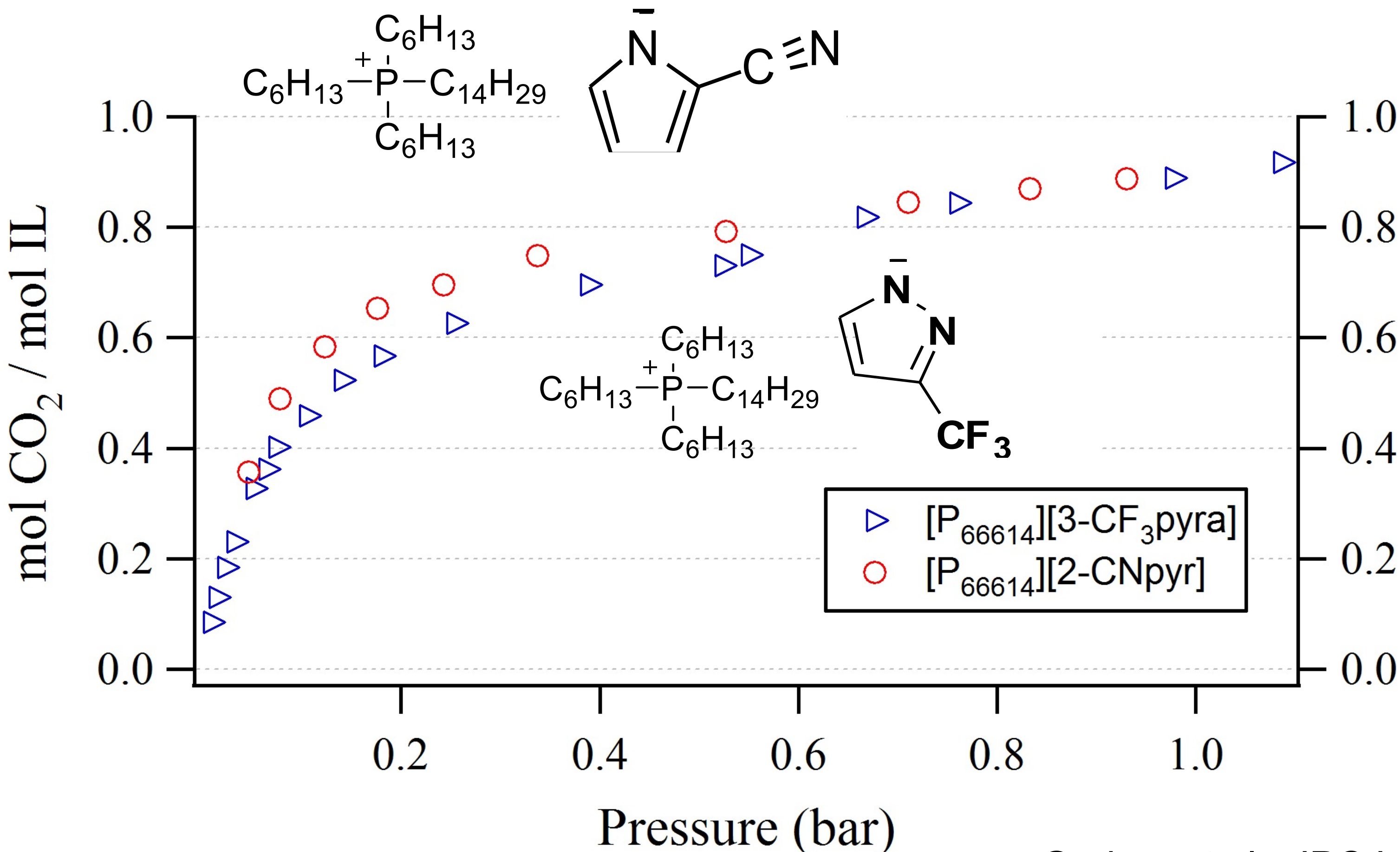
NASA

Ionic Liquids for CO_2 Capture

- Equimolar capacity – 1 mol CO_2/mol IL

AHA – aprotic heterocyclic anions

- Retain amine in ring structure
- Further reduce free hydrogens to reduce hydrogen bonding

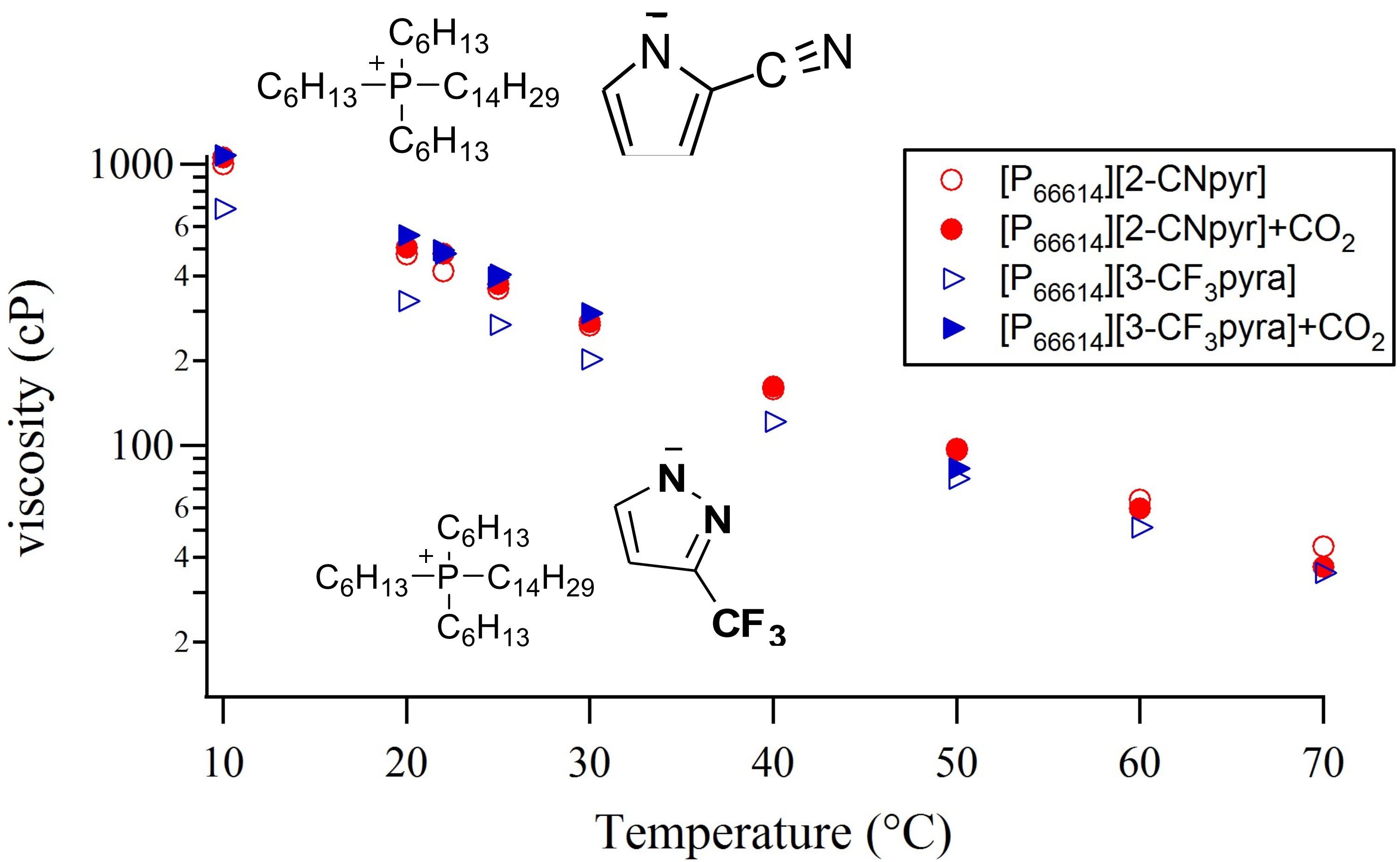


Gurkan et al., JPC Lett, 2010

Ionic Liquids for CO_2 Capture

- Equimolar capacity – 1 mol CO_2/mol IL
- No viscosity increase upon reaction with CO_2

Eliminate Viscosity Increase by Using AHA – aprotic heterocyclic anions

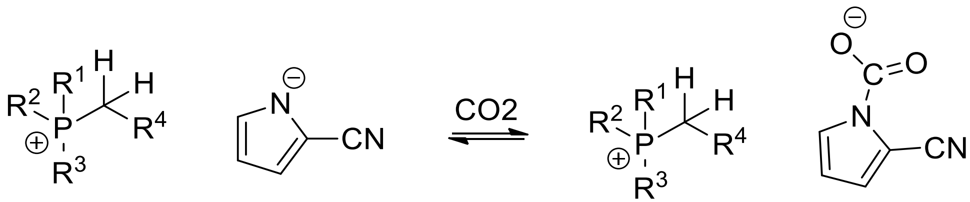


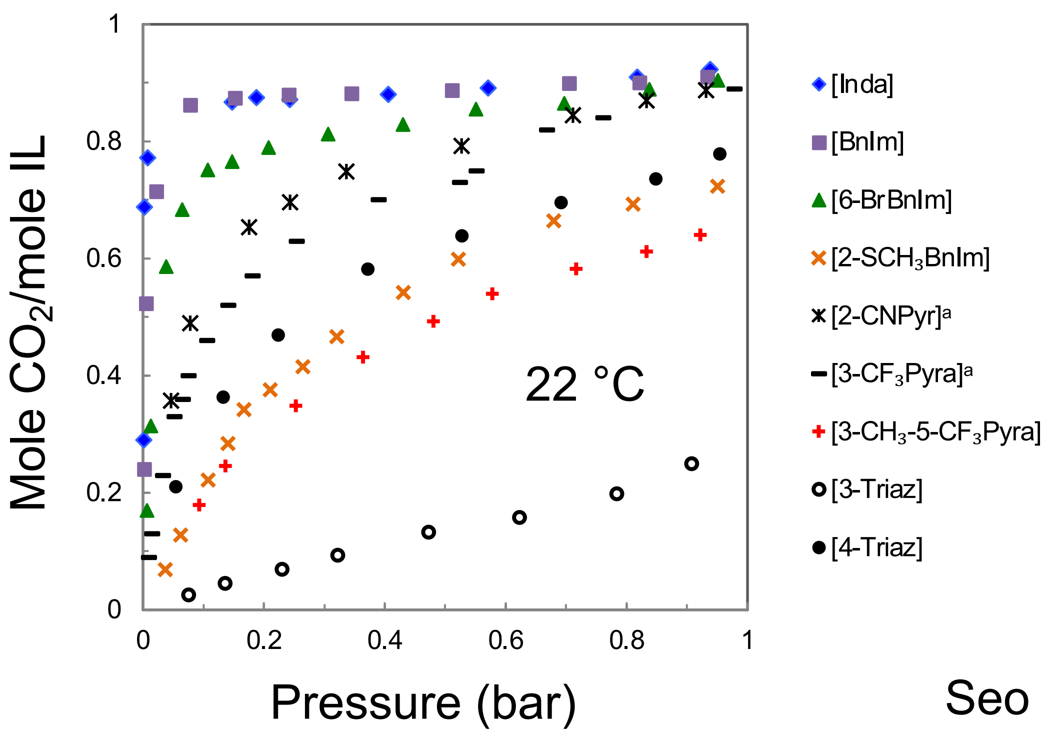
Gurkan et al., JPC Lett, 2010

Ionic Liquids for CO_2 Capture

- Equimolar capacity – 1 mol CO_2/mol IL
- No viscosity increase upon reaction with CO_2
- Tunable enthalpy of reaction

Tuning Reaction Enthalpy of AHA ILs





ΔH_{rxn} (kJ/mol)

-54

-52

-48

-41

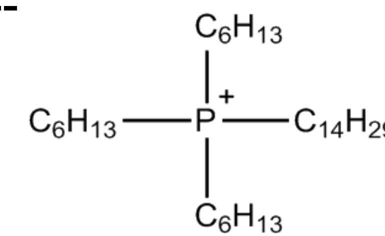
-45

-44

-41

-37

-42



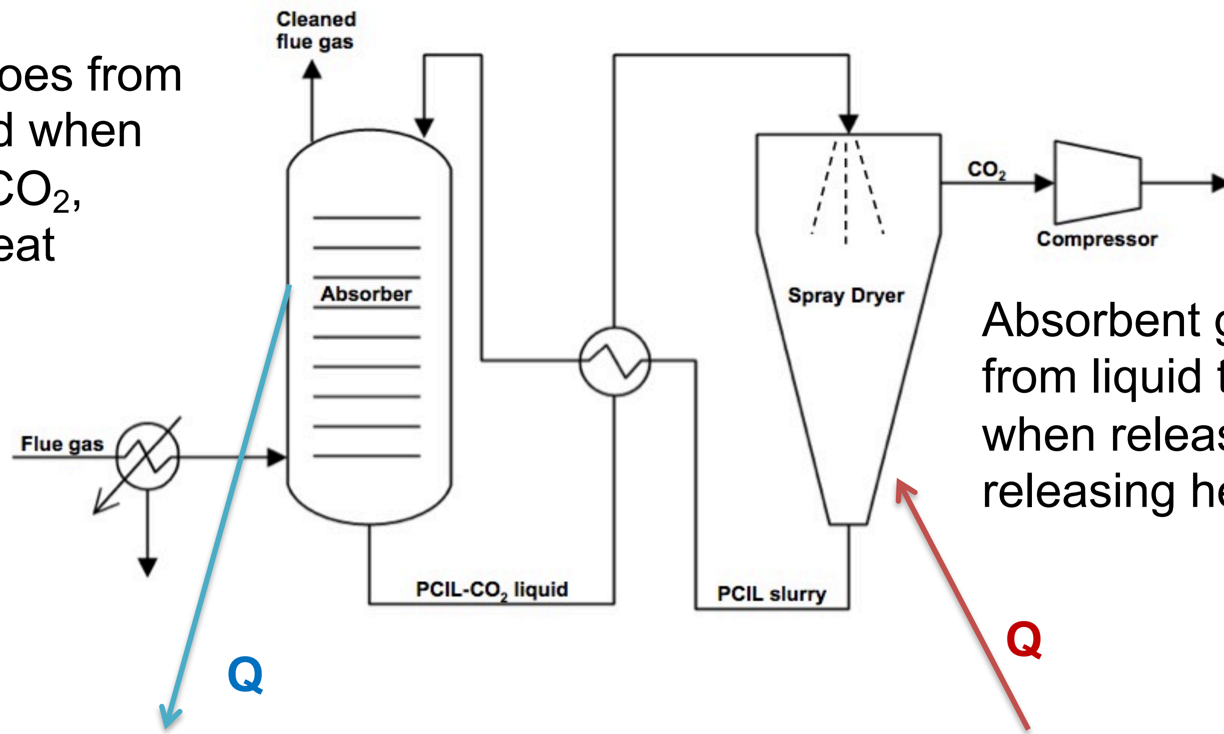
Seo et al., JPC B, 2014, 118, 5740

Ionic Liquids for CO_2 Capture

- Equimolar capacity – 1 mol CO_2/mol IL
- No viscosity increase upon reaction with CO_2
- Tunable enthalpy of reaction
- Phase change ionic liquids

CO_2 Capture with Phase Change Material

Absorbent goes from solid to liquid when reacts with CO_2, absorbing heat



Absorbent goes from liquid to solid when releases CO_2, releasing heat

‘Melting’ of absorbent reduces cooling duty

Heat duty in stripper reduced by the heat of fusion of the phase change material

CO_2 Capture with Phase Change Material

Absorber

Remove 50 kJ/mol

$[C^+][A^-]$ (s) + CO_2 ⟶ $[C^+][ACO_2^-]$ (s)
exothermic

$[C^+][ACO_2^-]$ (s) ⟶ $[C^+][ACO_2^-]$ (l)
endothermic

Add 20 kJ/mol

Q_{net} = Remove 30 kJ/mol

Regenerator

Add 50 kJ/mol

$[C^+][ACO_2^-]$ (l) ⟶ $[C^+][A^-]$ (l) + CO_2
endothermic

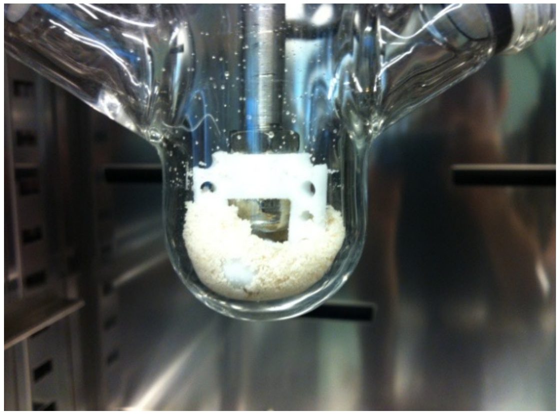
$[C^+][A^-]$ (l) ⟶ $[C^+][A^-]$ (s)
exothermic

Remove 20 kJ/mol

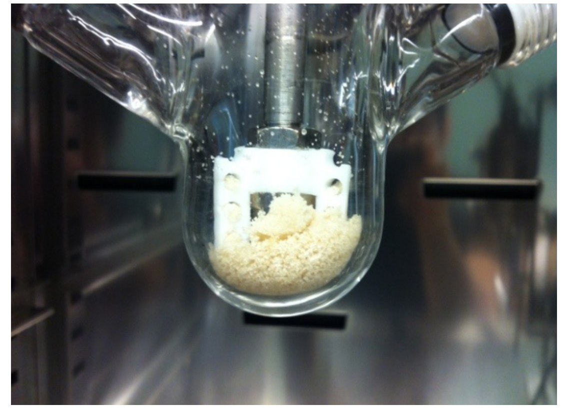
Q_{net} = Add 30 kJ/mol

Phase Change Ionic Material

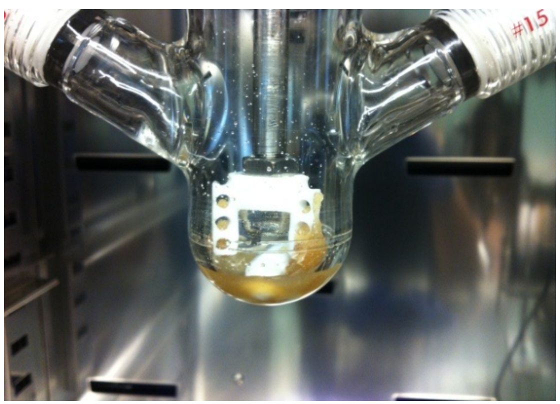
70 °C



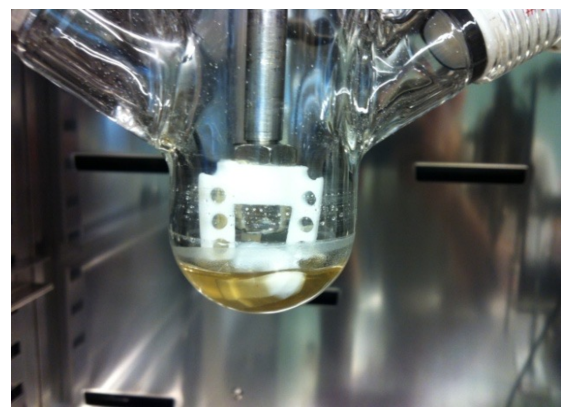
Pure material; T_m=166 °C; no CO_2



60 mbar CO_2

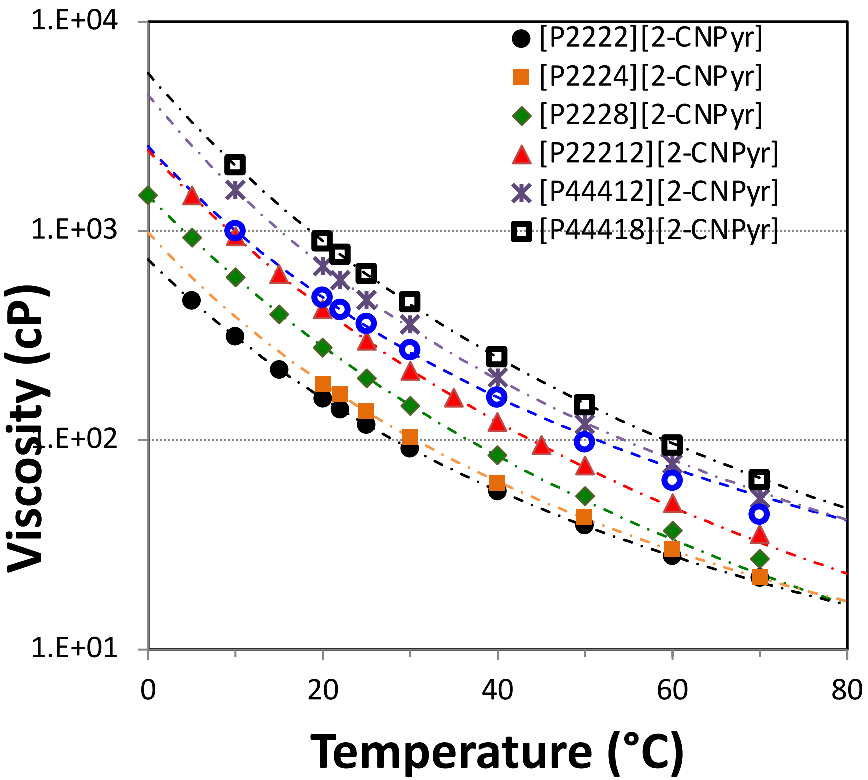


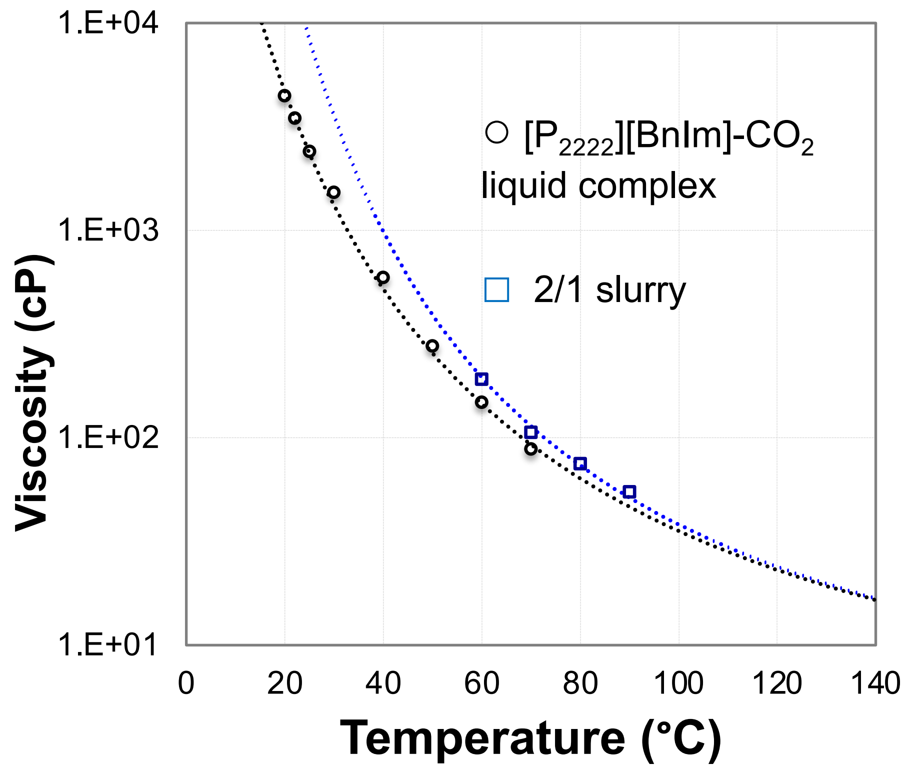
100 mbar CO_2



150 mbar CO_2

Challenge: High Viscosity/Poor Mass Transfer



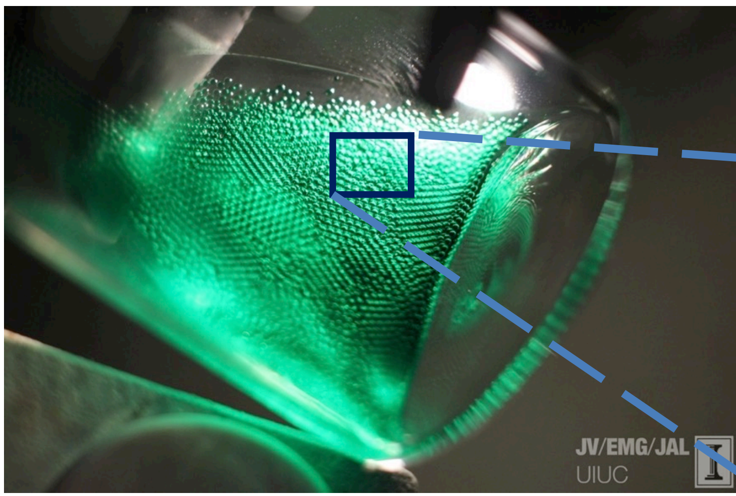


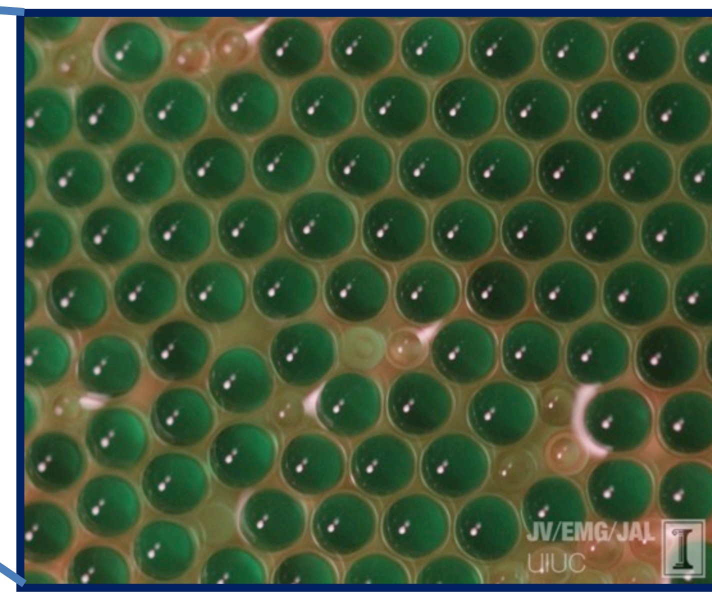
Seo et al., Energy & Fuels, 2014, 28, 5968-5977

Microencapsulation

- Idea: improve mass transfer by increasing mass transfer AREA

- Successfully encapsulated ILs and PCILs



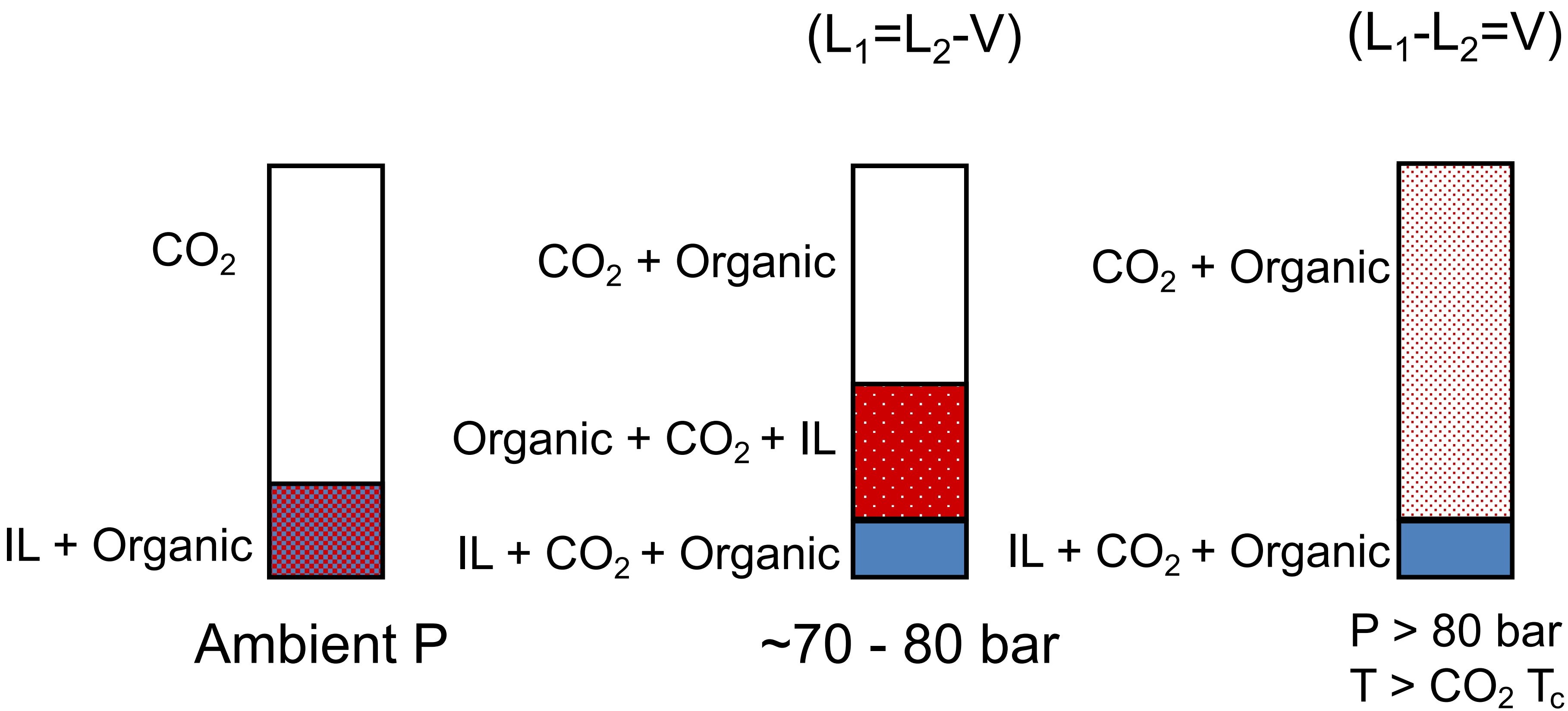


- Need shell materials with selectivity of CO_2 over water

Other Projects!

- Aromatic/aliphatic liquid-liquid separations
- Dissolution of biomass with protic ILs
- Recovery of organics (aromatics, sugars, etc.) using CO_2 as an antisolvent
- Hybrid polymer/IL membranes for gas separations
- Protic ILs for fuel cell applications
- Reversible electroplating of mirrors for space

Separation of **** from IL by VLLE



(Scurto et al., J. Am. Chem. Soc., 124, 2002, 10276)

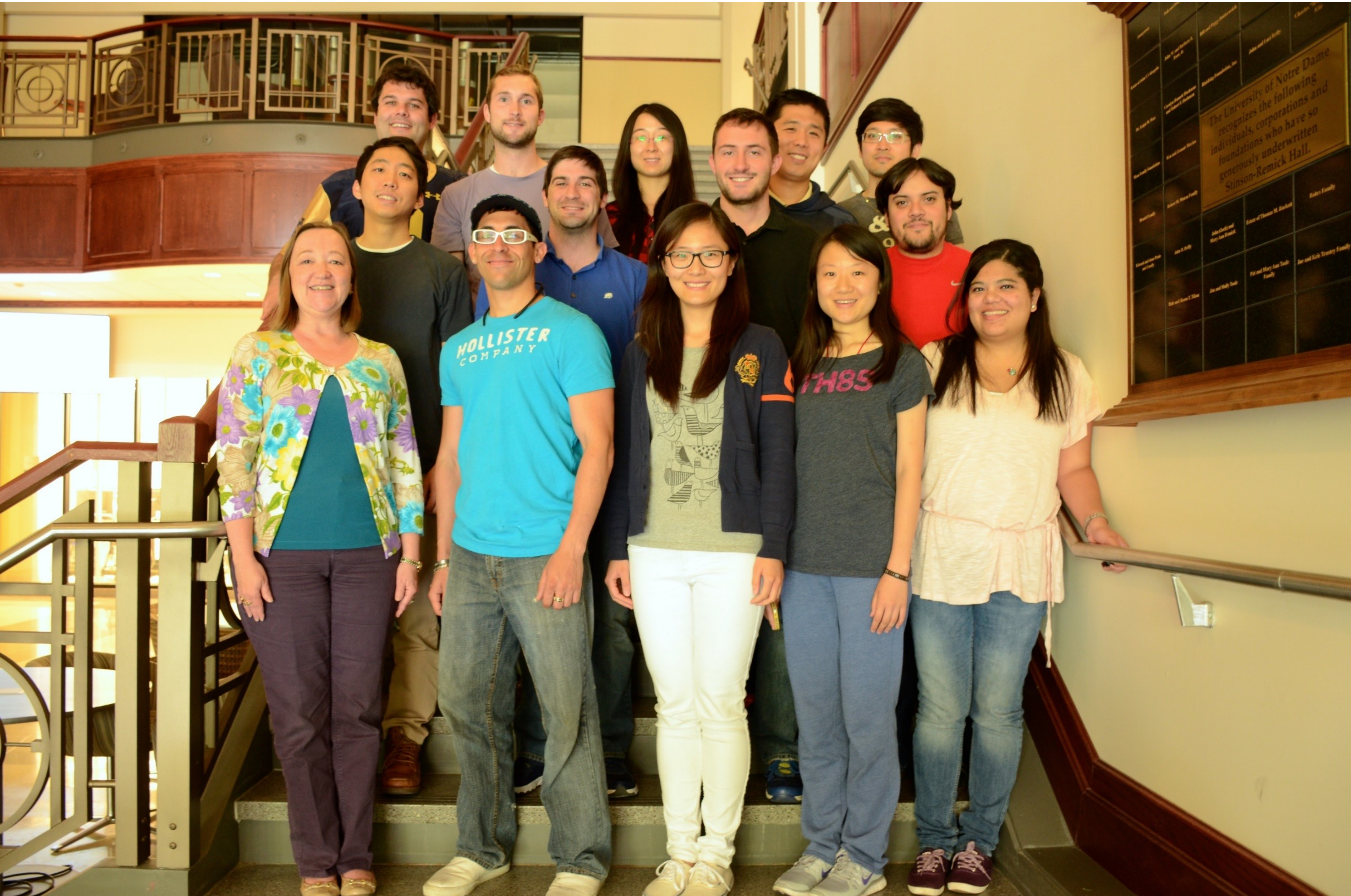
Addition of CO_2 will induce the homogeneous liquid phase (IL/organic) to form two liquid phases – leading to the separation of organics from ILs

Where are my former group members?

- Faculty - Auburn, Kstate, Kansas, Queens Univ. Belfast, Univ. Costa Rica, U.Mass Lowell, Creighton Univ., UI, Case Western
- Govt - EPA
- Industry - Dow, Chemours, Hyundai, Nissan, Praxair, Exxon-Mobil, P&G, Lyondell Basell, Bayer, SolidEnergy, Rohm&Haas, Eli Lilly, Goodyear, RTI, P2Science, SimSci, United Technologies, …

Brennecke Group

- Looking for 2 grad students to start this year
- Bringing 5 grad students and 2 postdocs from ND
- Ask Mike Lucas (Keitz group) about me
  - mlucas2@utexas.edu
  - CPE 4.470


The University of Notre Dame recognizes the following individuals, corporations and foundations who have so generously underwritten Stinson-Remick Hall.
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