Making an inorganic analogue of a cell for direct air capture of CO_2

Project Number 76830

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U.S. Department of Energy

National Energy Technology Laboratory

Direct Air Capture Kickoff Meeting

February 24-25, 2021

Program Overview

a. **Funding:** DOE-BES 1/3 CGBS and 2/3 MSE

b. **Overall Project Performance Dates:** FY2021-FY 2023

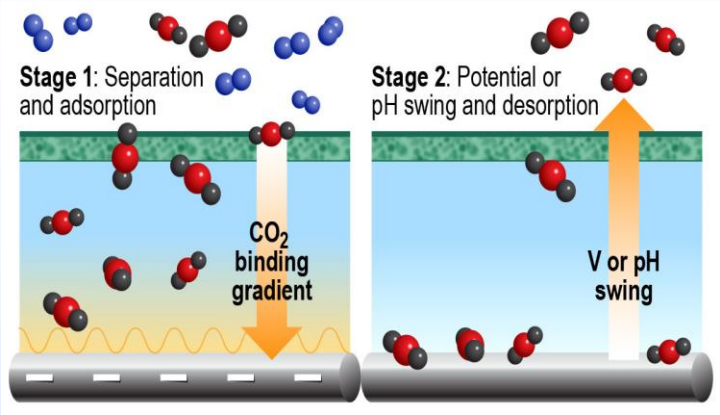
c. **Project Participants:** PNNL, MIT, U. Alabama

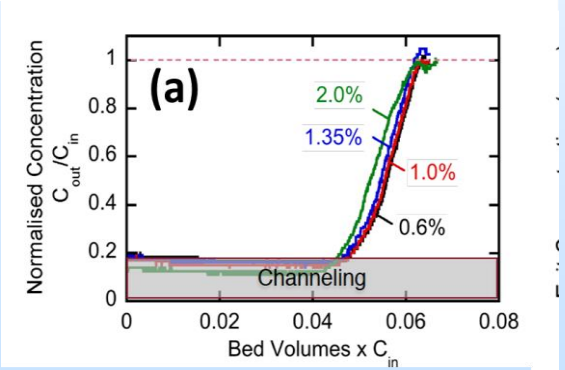
d. **Overall Project Objectives:** *We seek to elucidate the fundamental science that will drive CO_2 direct air capture (DAC) by mimicking crucial functions of single-cell organisms that enable selective and kinetically efficient uptake under the small thermodynamic driving force created by the low partial pressure of CO_2 in the atmosphere.*

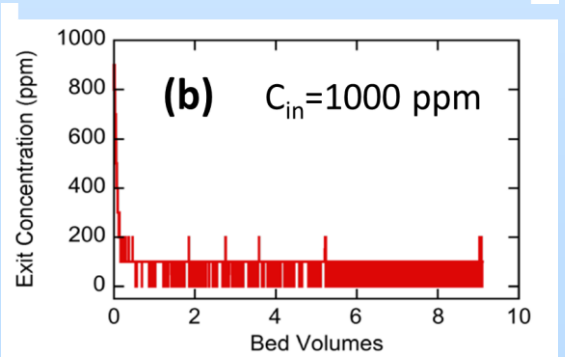
Technology Background

a. **Concept:** Set up a thermodynamic funnel to channel CO_2 towards a capture site which can be switched by electrochemical and/or pH swing. System consist of
   - CO_2-Ionene membranes (U Alabama)
   - Tunable CO_2 water lean capture solvent (PNNL)
   - Electrochemical Capture/release PNNL/MIT

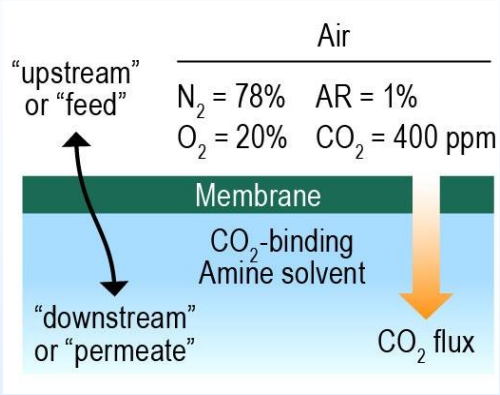
b. **Preliminary Data:** Electrochemical Capture demonstrated under near DAC conditions.



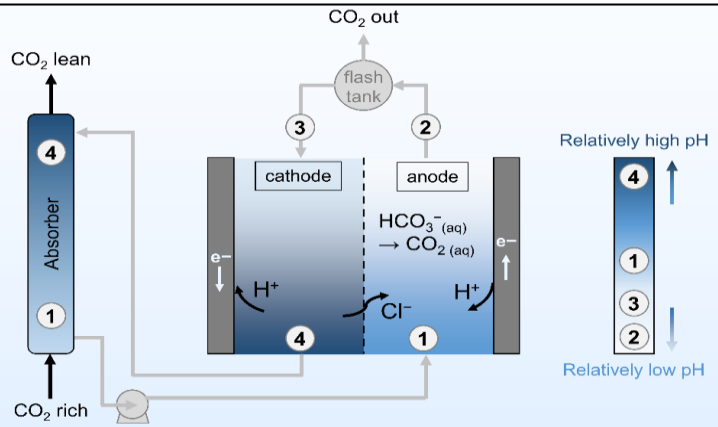




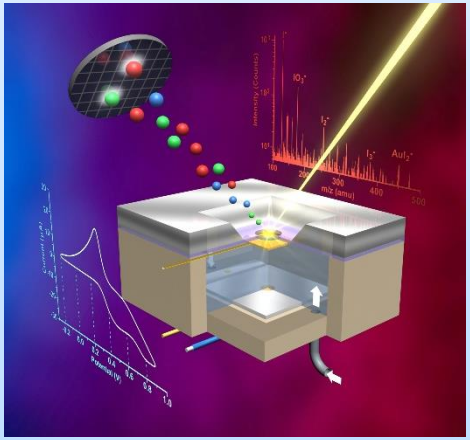
Technical Approach



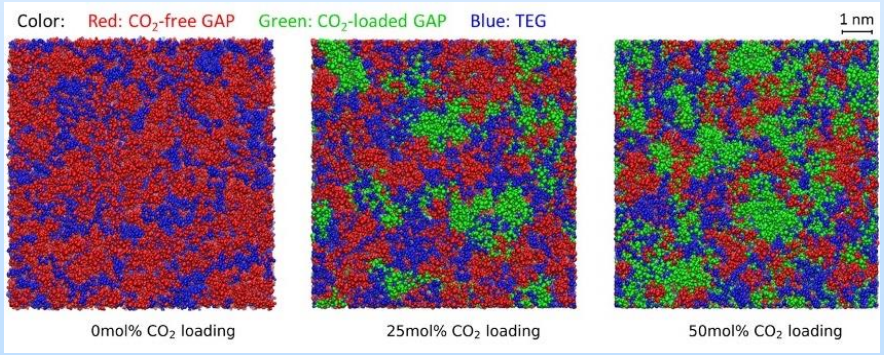
Task 1. Coupling Membranes to Capture Solvents



Task 2. Integrating Electrochemistry with Capture Solvents



Task 3: Interfacial Chemical Imaging, Spectroscopy, and Kinetics



Task 4. Theory and Computation

Technical Approach

a. Project schedule:

Year	Activity
1	Investigate individual components for DAC conditions, including membranes (ST1, ST3, ST4), solvent system (all STs), and electrochemistry (ST2, ST3)
2	Integrate membrane to solvent (ST1, ST3, ST4) and solvent to electrochemistry (ST2, ST3, ST4)
3	Fully integrate membranes, solvents, and electrochemistry (all STs)

b. Project success criteria: (i) Fully assemble a functioning DAC system; (ii) demonstrate a capture process with energy penalties lower than those of current commensal technology.

Team

Task 1 Membranes

J. Bara
(U. Alabama)

D. Heldebrant
(PNNL)

Task 2 Electrochemistry

T. A. Hatton
(MIT)

E. Wiedner
(PNNL)

A. Appel
(PNNL)

Task 3 Spectroscopy and Imaging

X.-Y. Yu
(PNNL)

E. Walter
(PNNL)

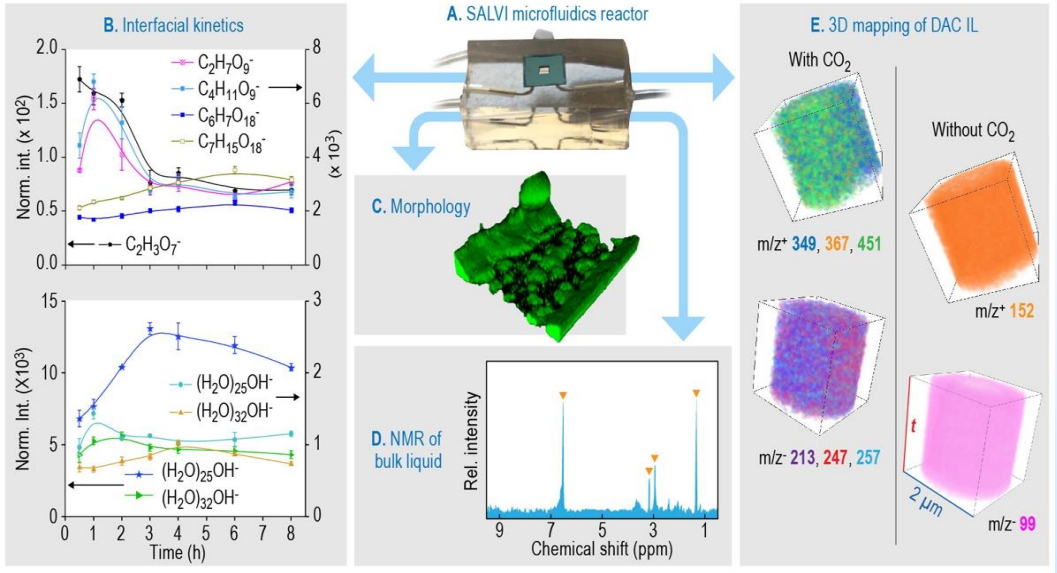
D. Hoyt
(PNNL)

Task 4 Theory and Simulation

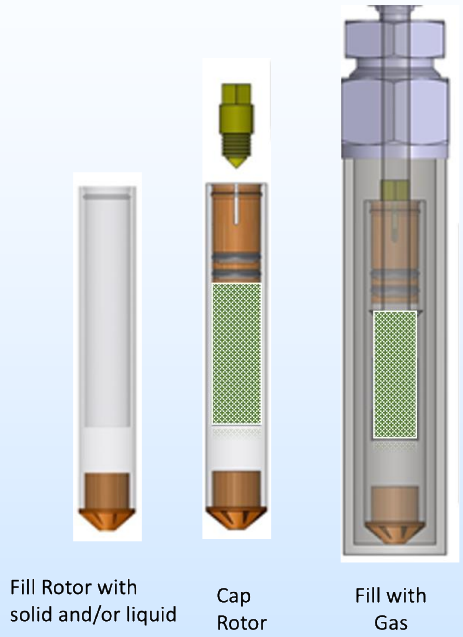
V. A. Glezakou
(PNNL)

R. Rousseau
(PNNL)

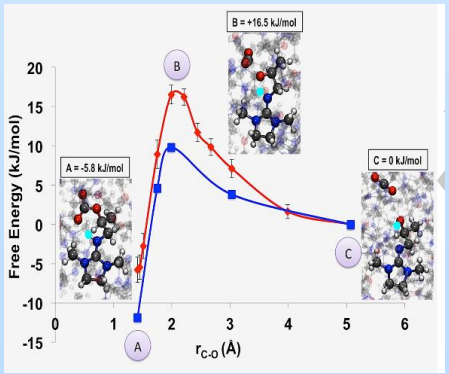
Unique Facilities

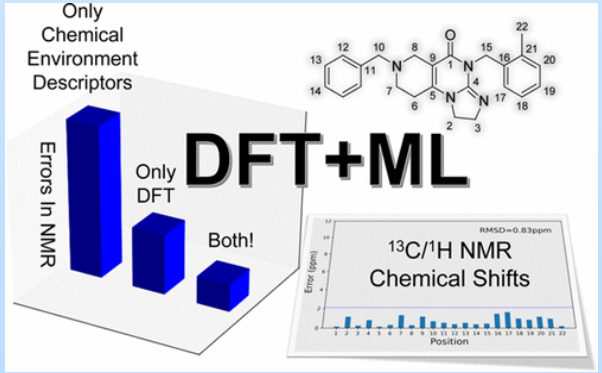


Advanced solid-liquid and liquid-liquid imaging



Advanced NRM and EPR





HPC based atomistic simulation and data science

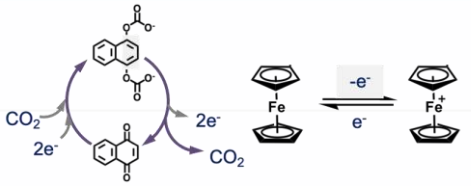
Progress and Current Status of Project

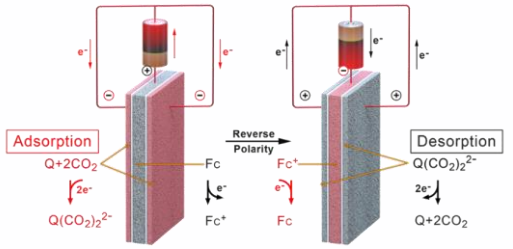
a. We set up basic electrochemical reactors.

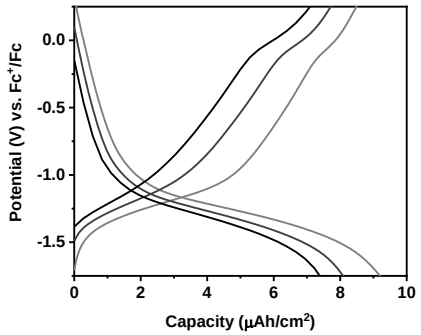
b. We demonstrated the stability of capture solvents in an electrochemical cell/interface: we need to raise the ionic strength.

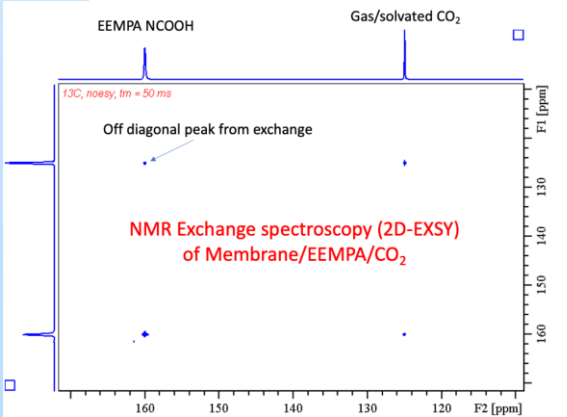
c. We demonstrated a 5X enhancement of CO_2 permeability for ionene/capture solvent interfaces.

d. NMR suggests the formation/presence of unanticipated anhydride species at the ionene/solvent interface.









Opportunities for Collaboration

a. **Collaboration Synergies:** our project is a prime example of inter-institutional and inter-disciplinary collaborations; it is specifically structured to take advantage of each team's unique expertise and relies on the synergies between the tasks and the teams.

b. **Potential for additional Collaborations:**
   - Alternate membrane and electrode materials
   - System level analysis
   - Engineering modeling (TEA, LCA etc)
   - Scale-up