Rational Development of Novel Metal-Organic Polyhedra-based Membranes for CO₂ Capture (FE0031736)

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Project Overview

Award number:	DE-FE0031736
Project period:	7/1/19 to 6/30/22
Program manager:	Isaac Aurelio
Project Objectives:	

Rationally develop solubility-selective mixed matrix materials comprising polar rubbery polymers and metal organic polyhedra (MOPs);

- Develop thin film composite membranes achieving high CO₂ permeance (3000 GPU) and high CO₂/N₂ selectivity (75) at 60°C;
- Demonstrate separation performance and stability with raw flue gas at NCCC; and
- > Perform **techno-economic analysis** on the membrane processes.

Membrane technology can be attractive



Productivity Selectivity $P_A = S_A \times D_A \qquad \alpha_{A/B} = \frac{P_A}{P_A} =$



Merkel, Lin, Wei and Baker, J. Membr. Sci., 359, 126 (2010) Merkel, et al., NETL CO₂ Capture Technology Review Meeting, 2015.



Membrane technology can be attractive



Merkel, et al., NETL CO_2 Capture Technology Review Meeting, 2015.

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Our Approach: Sorption-Enhanced Mixed-Matrix Membranes



$$\alpha_{A/B} = \frac{P_A}{P_B} = \left(\frac{S_A}{S_B}\right) \times \left(\frac{D_A}{D_B}\right)$$

Highly Polar Rubbery Polymers



Metal-Organic Polyhedra (MOPs)



MOPs

- 2 5 nm in size
- Soluble in solvents
- Permanent pores to increase gas diffusivity
- Open metal sites to interact with CO₂



High Throughput Simulations





Membrane Development and Field Test







- Develop industrial membranes and modules
- Test with real flue gas

Project Budget and Team Roles

	Govt Share	Cost Share	Role
UB	\$1,259,501	\$599,997 †	Materials development
Subcontracts:			
RPI	\$400,000	\$102,913	Polymer synthesis scale-up
Caltech	\$388,130	\$97,508	Computational simulation
MTR	\$599,468	\$174,987	Membranes development and field test
Trimeric	\$110,000	0	TEA analysis
NCCC	0	0	Host site
Total	\$2,857,577	\$975,405	

[†] UB cost-share is provided by Empire State Development's Division of Science, Technology and Innovation (NYSTAR)