New Materials Development for Carbon Capture Applications

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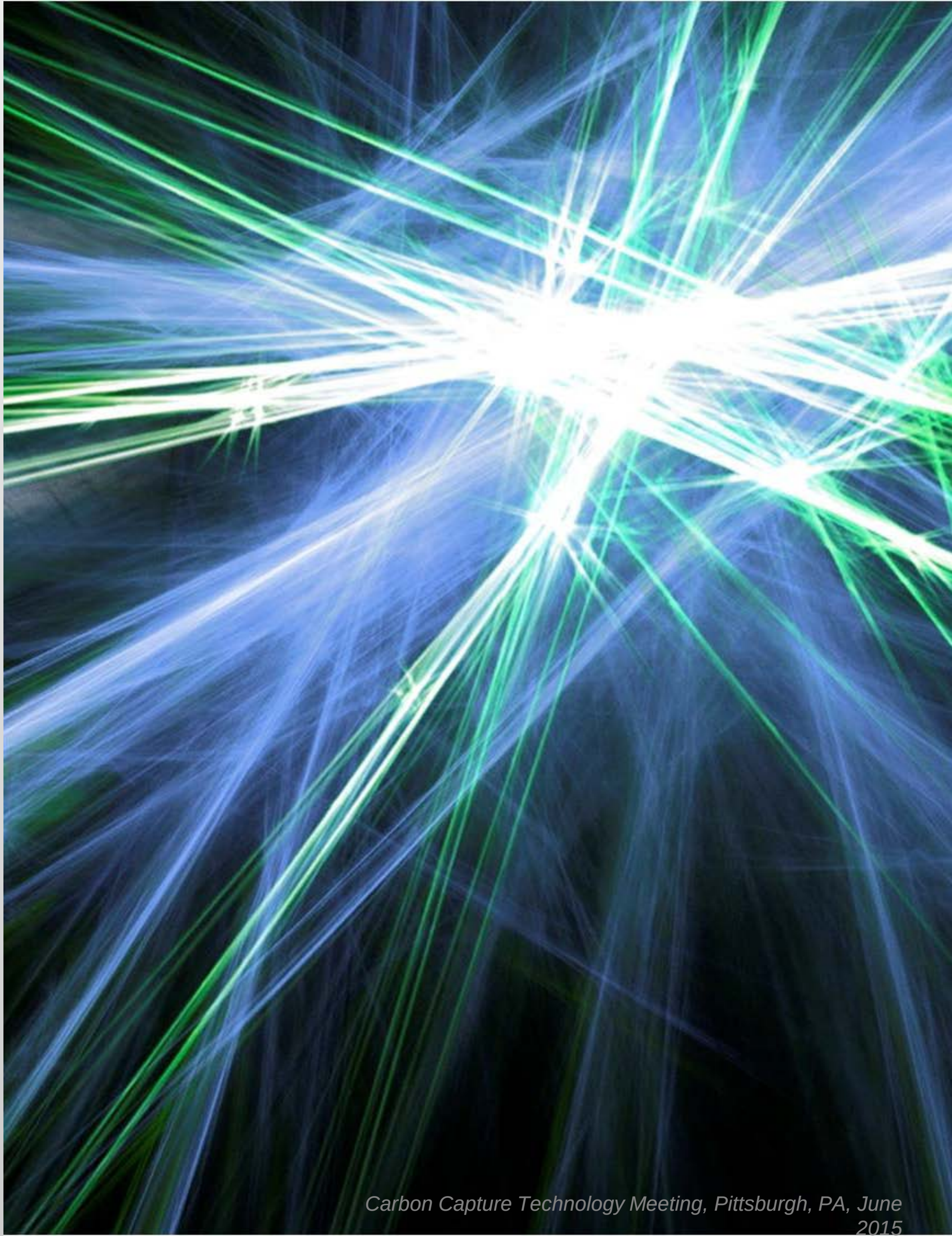

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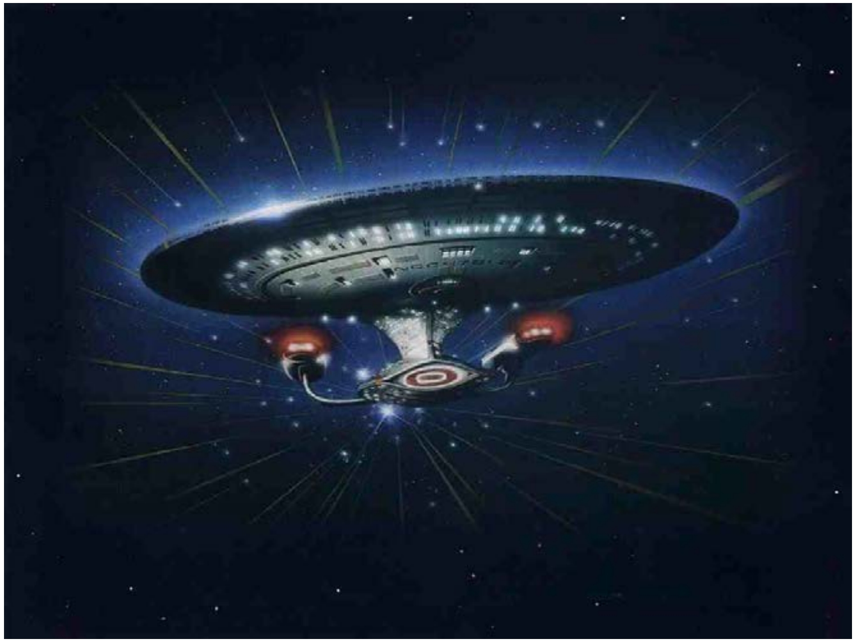
To boldly go where no one has gone before



- A future with no or little CO_2 emission
- Cheap and abundant electricity
- Reliable electricity

We explore new ideas

Project overview: Transformational technologies

- **In-house NETL-ORD Carbon Capture FWP**
- **Project performance dates: 10/1/2014 – 9/30/2015.**
- **Total cost for transformation program $1.065M**
  - No cost share
- **Project objectives: Evaluate new materials and characterize them to determine the potential for carbon capture.**
- **TR 2-3 level**

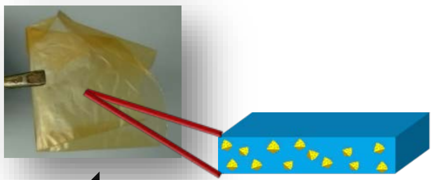
BOLDLY GO WHERE NO ONE HAS GONE BEFORE IN ***1- 2 YEARS***

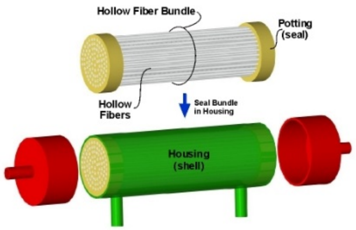
What is the NETL-ORD role in transformation technology development?

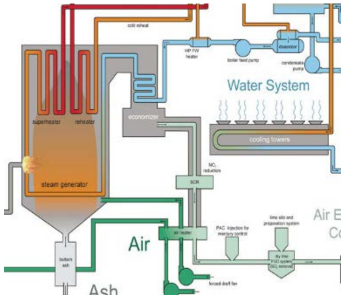
And what is it not?

- **It’s not:**
  - Basic science
  - New synthetic methodologies
  - Pilot-scale testing
  - Commercialization
- **It is:**
  - Examination of novel classes of materials for capture
  - Exploration of innovative process configurations
  - Development of advanced screening approaches

Integrated technology development







Materials Synthesis

Systems Fabrication

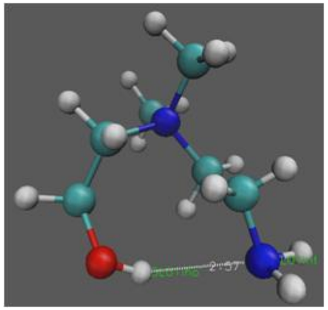
Systems Analysis

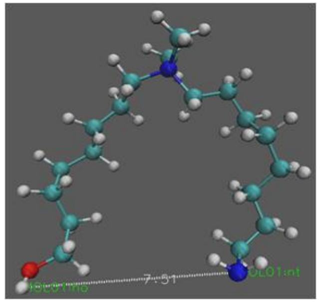
Materials properties

Performance Criteria

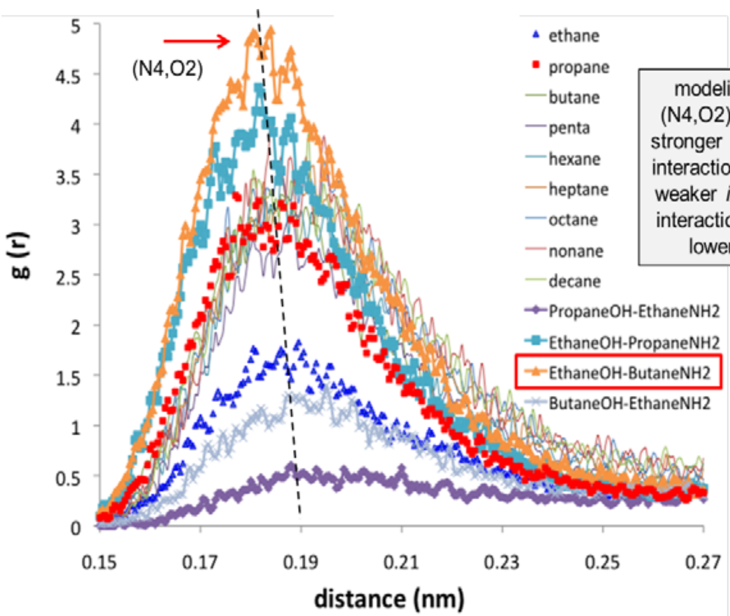
Advanced solvents

Choline-based ILs





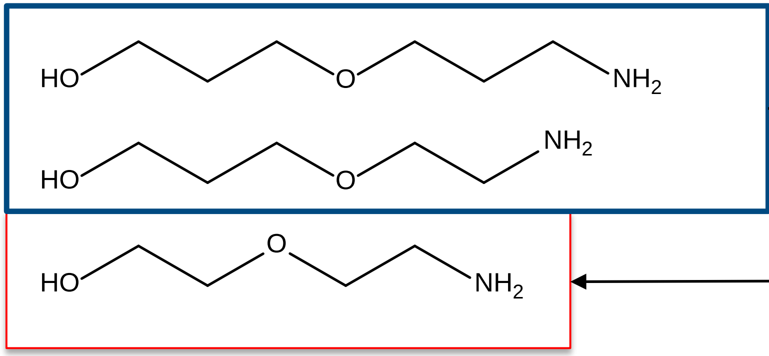
RFIL	viscosity cP	T_g °C	Setaram CO_2 uptake, mol CO_2 / mol IL
$[NH_2(CH_2)_2NMe_2(CH_2)_2OH]Tf_2N$ (**N2, O2**)	4530	-39.4	0.017
$[NH_2(CH_2)_2NMe_2(CH_2)_3OH]Tf_2N$ (**N2, O3**)	1146	-44.6	not determined
$[NH_2(CH_2)_3NMe_2(CH_2)_2OH]Tf_2N$ (**N3, O2**)	1303	-49.6	not determined
$[NH_2(CH_2)_3NMe_2(CH_2)_3OH]Tf_2N$ (**N3, O3**)	1424	-39.2	0.018
$[NH_2(CH_2)_3NMe_2(CH_2)_5CH_3]Tf_2N$ (**N3, hex**)	1084	-46.8	0.018
$[NH_2(CH_2)_4NMe_2(CH_2)_2OH]Tf_2N$ (**N4, O2**)	**280**	**-66.6**	**0.028**



modeling predicts (N4,O2) should have stronger *intra*molecular interactions, leading to weaker *inter*molecular interactions and thus lower viscosity

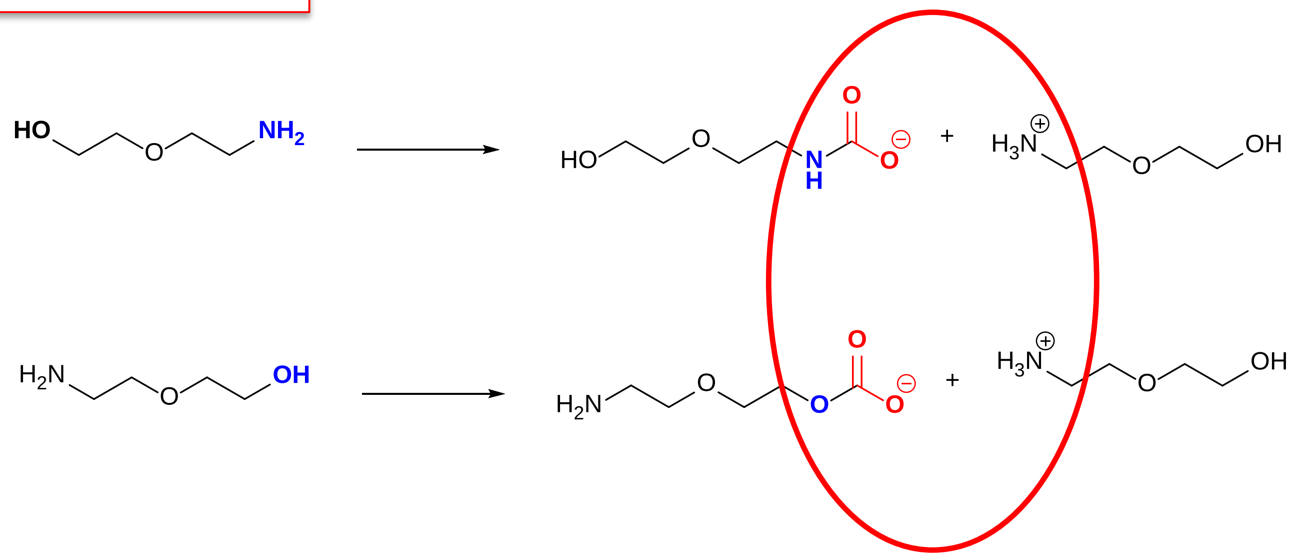
- **Focused on improve the CO_2 interactions.**
- **Intramolecular HB causes decrease in viscosity which is dictated by the spacers.**
- **Effect of anion and cation on CO_2 solubility was evaluated.**

Advanced solvents



No or little carbonate reaction

Carbamate Vs. Carbonate



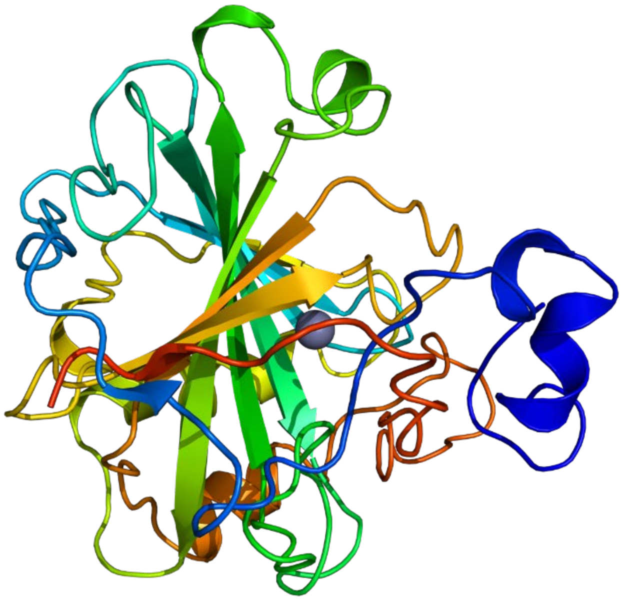
In the process of experimental verification

Simulations were performed by Hyung group in CMU (Fangyong Yan)

CO_2 catalyst for amine solvents

Thermodynamic aspects: 3) pK_a values of coordinated ligands

Reaction	Metal ion	water pK_a
$H_2O + M^{2+} \rightleftharpoons [M\text{-}OH]^+ + H^+$	none	14.0
	Ca^{2+}	13.4
	Mn^{2+}	11.1
	Cu^{2+}	10.7
	Zn^{2+}	**10.0**



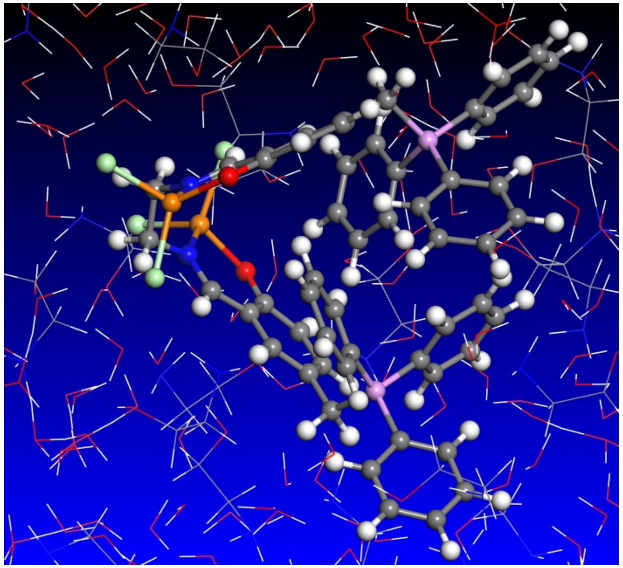
Zn coordinated water is 10000 more acidic

The catalyst is inspired by the function of carbonic anhydrase. (Uky)

$$\boxed{H_2O + CO_2} \rightleftharpoons \boxed{HCO_3^- + H^+}$$

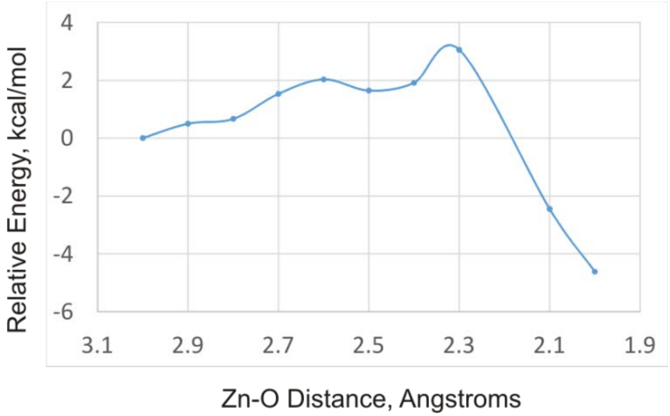
Carbonic acid formation is 10^7 faster in carbonic anhydrase

CO_2 catalyst for amine solvents



Condensed Phase Model

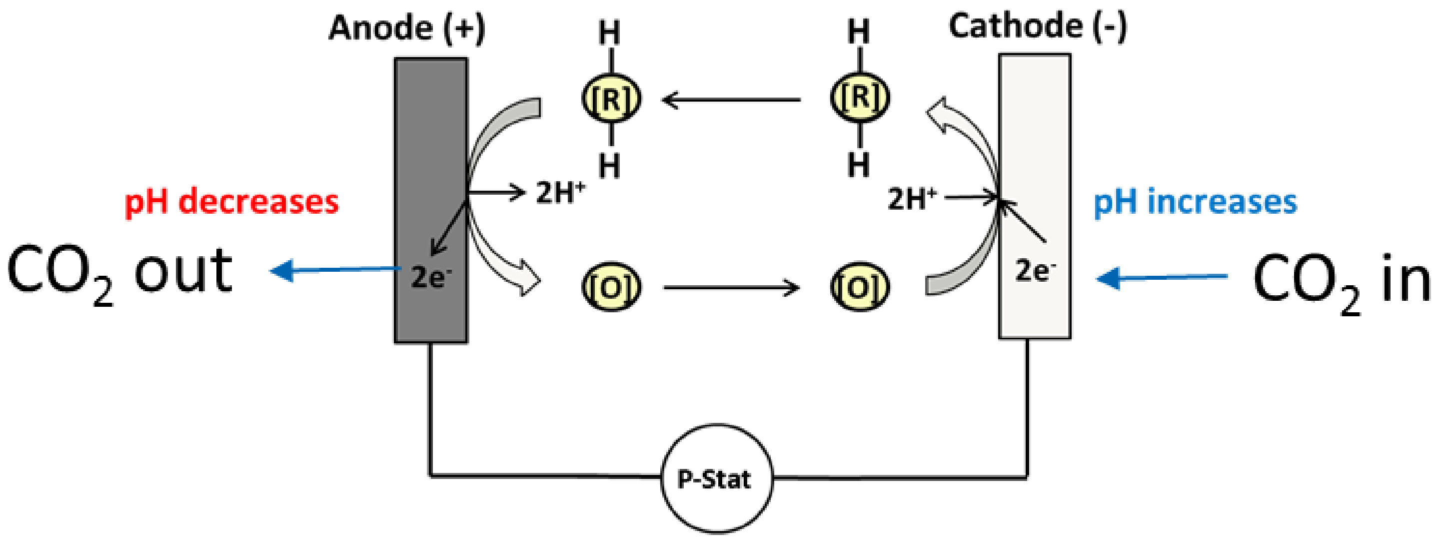
Reaction Profile – Cluster Model



- Collaborative work with University of Kentucky, Center for Applied Energy Research have developed catalysts that boost carbon capture in aqueous amine solutions.
- Developing fundamental understanding of these catalysis.
- Currently, Density Functional Theory Nudged Elastic Band calculations on a larger, condensed phase is being carried out.
- **Via simulation clear evidence is seen of hydrogen bonded networks as well as a hydrophobic region inside the catalyst, reminiscent of carbonic anhydrase.**

Energy efficient regeneration methodologies

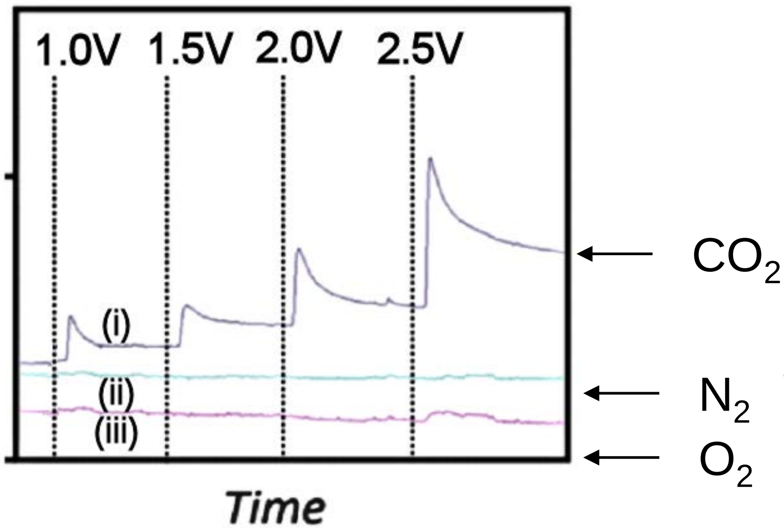
Redox-driven Regeneration of Amines: Material Development

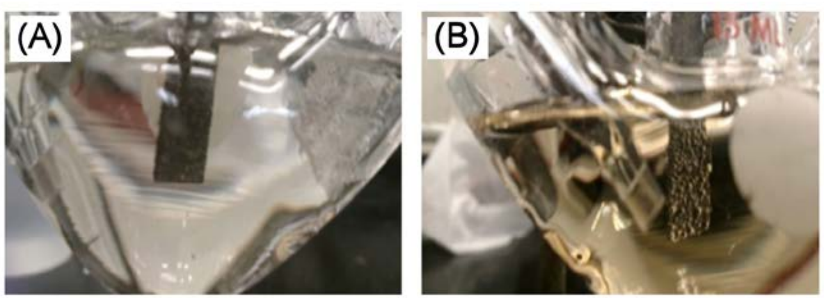


- Redox probe is able to bind protons in the reduced [R] form but NOT the oxidized form [O].
- Protons effectively pumped from Cathode to Anode.
- Lower potential than water splitting, no gaseous byproducts.
- pKa of [R] is critical!

Combination of innovative process and chemistry; voltage needs to be lower.

Energy efficient regeneration methodologies

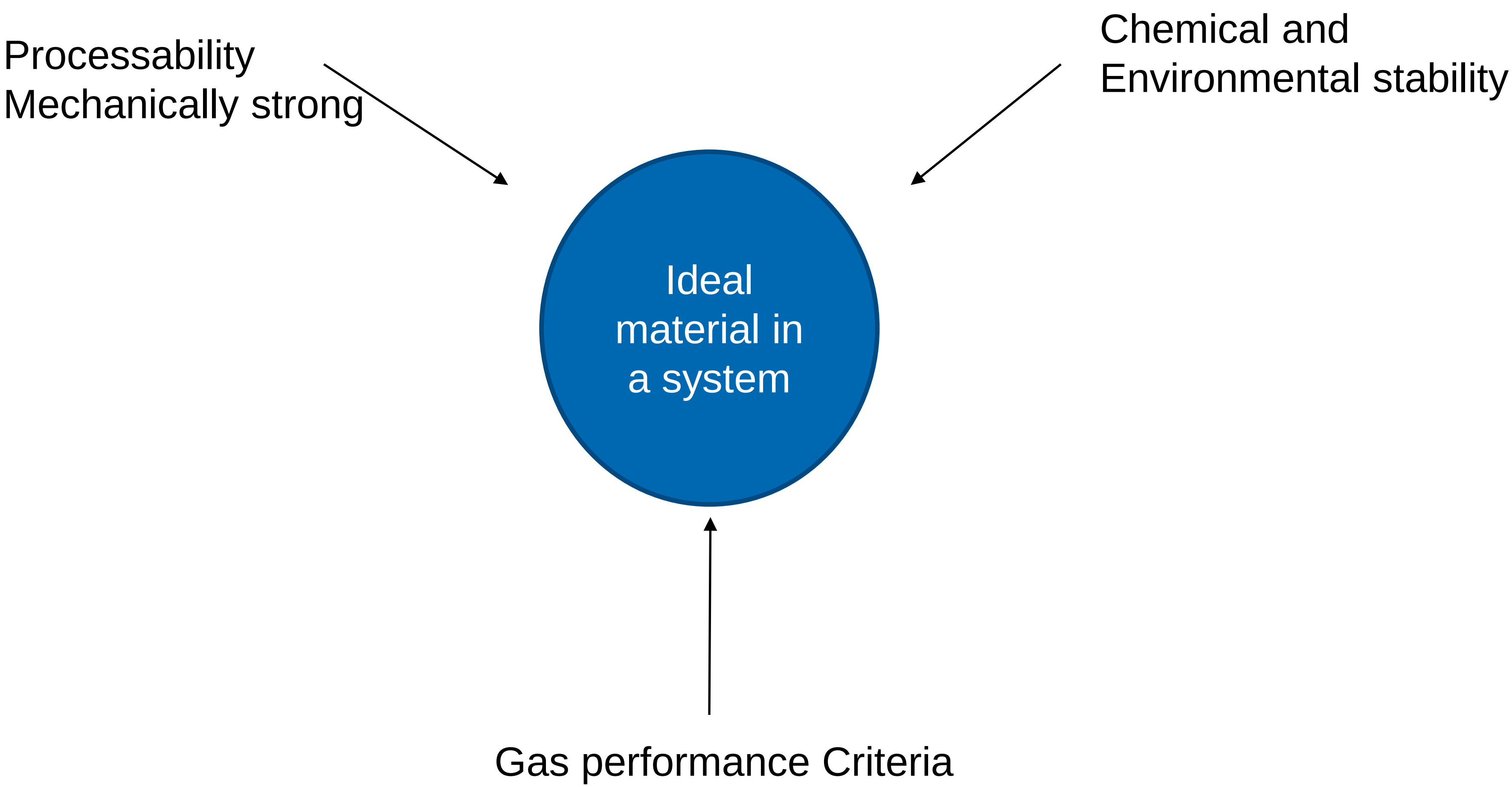




- **Voltage needs to be lowered**
- **Current state of the art is 0.5 V (needs to be lowered)**
- **Proof of concept completed**
- **Quantitative analysis is currently being performed.**

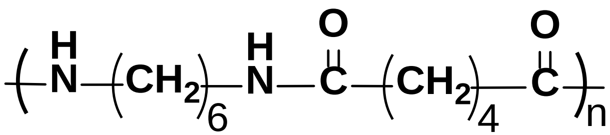
Provisional filed

Processing of materials

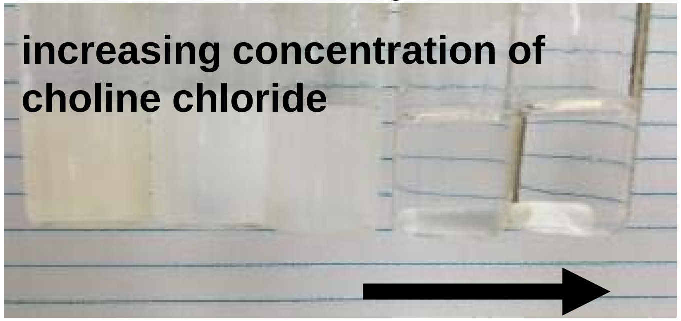


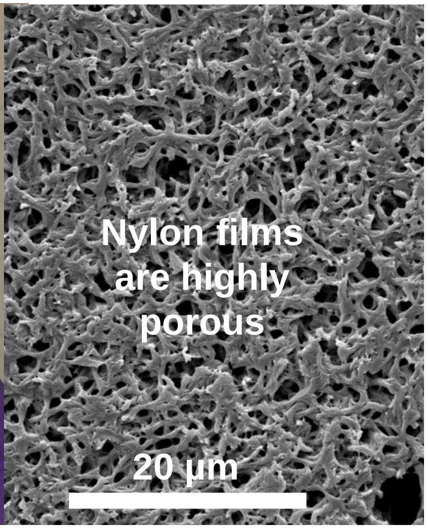
Innovative processing solutions

Polyamides (Nylon 6/6)



6 min after removing from heat

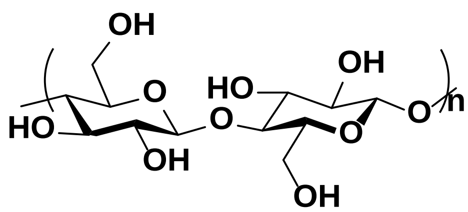


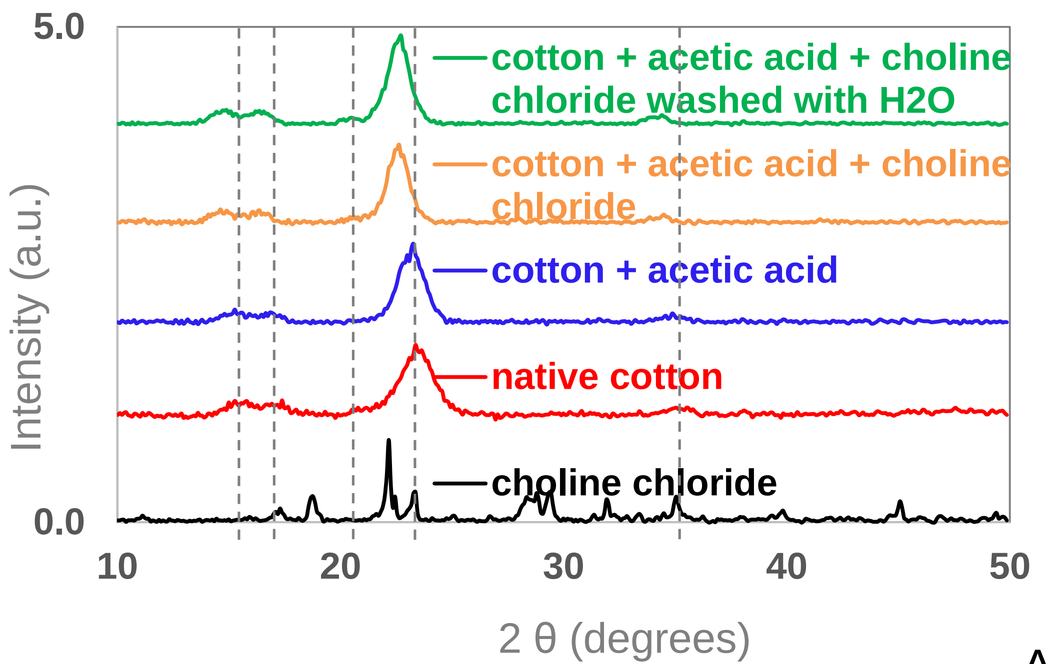


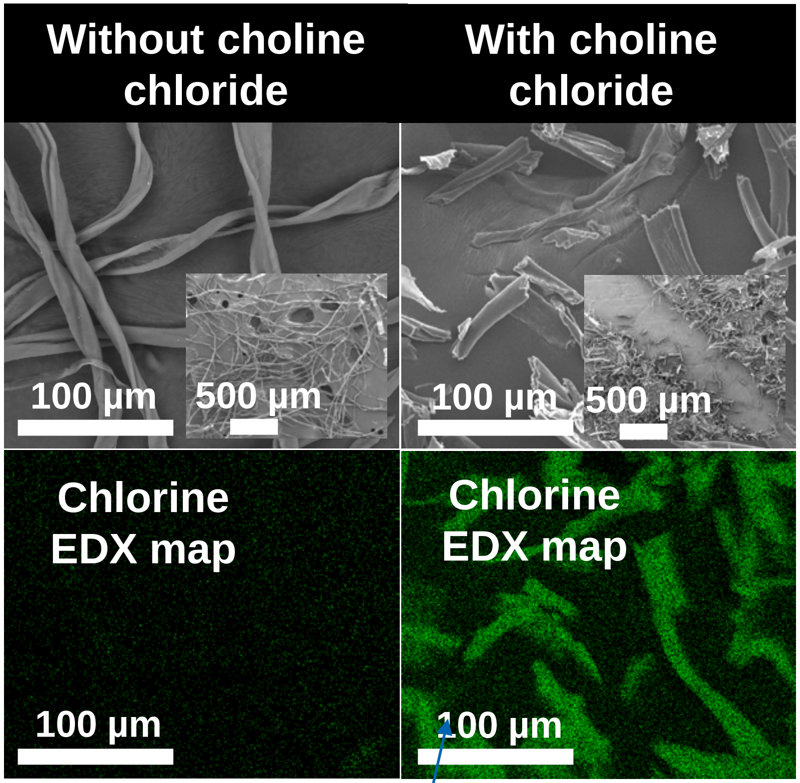
Process enables preparation of polymer dope for film casting

Innovative processing solutions

Cellulose Processing and modification





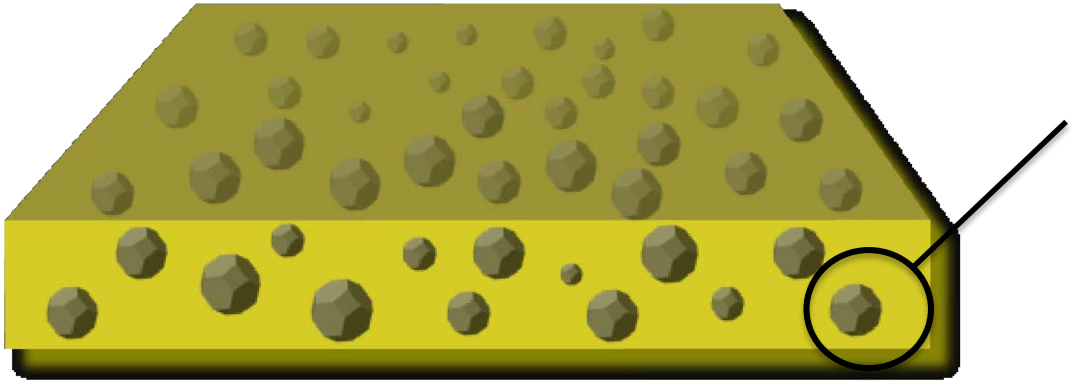


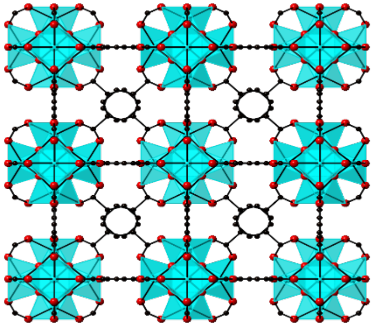
Able to add ionic content in the cellulose
To be evaluated for MMM

Using our insight in ionic liquids

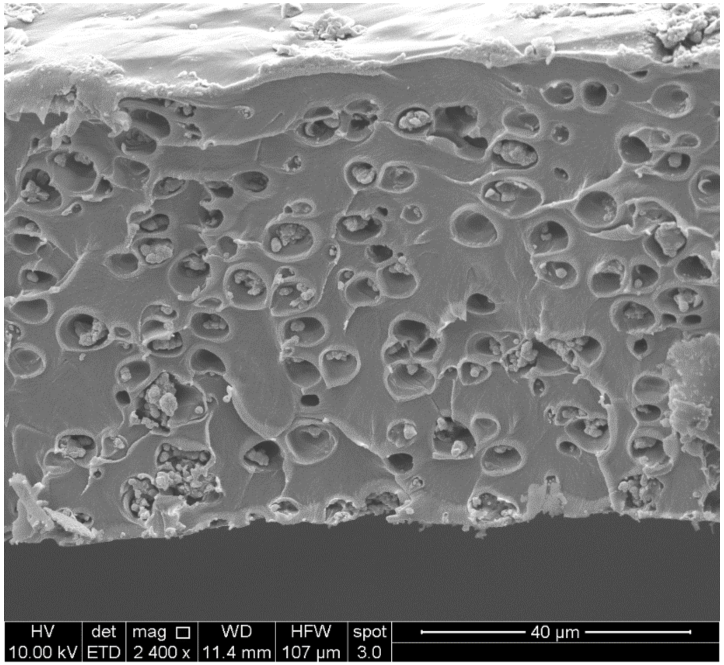
Provisional filed

In-situ MOF growth in polymers



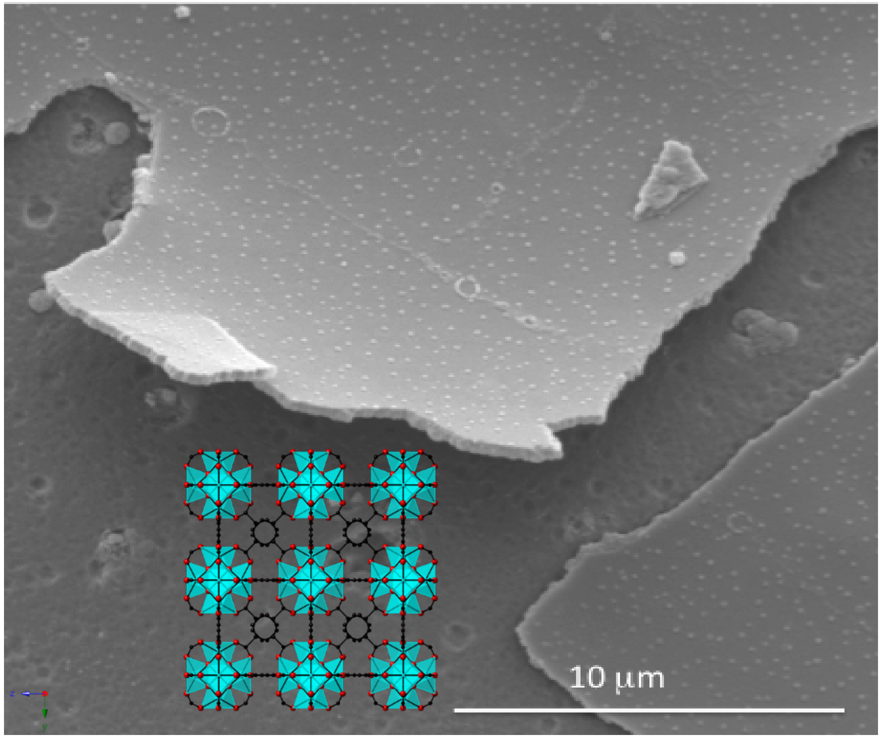


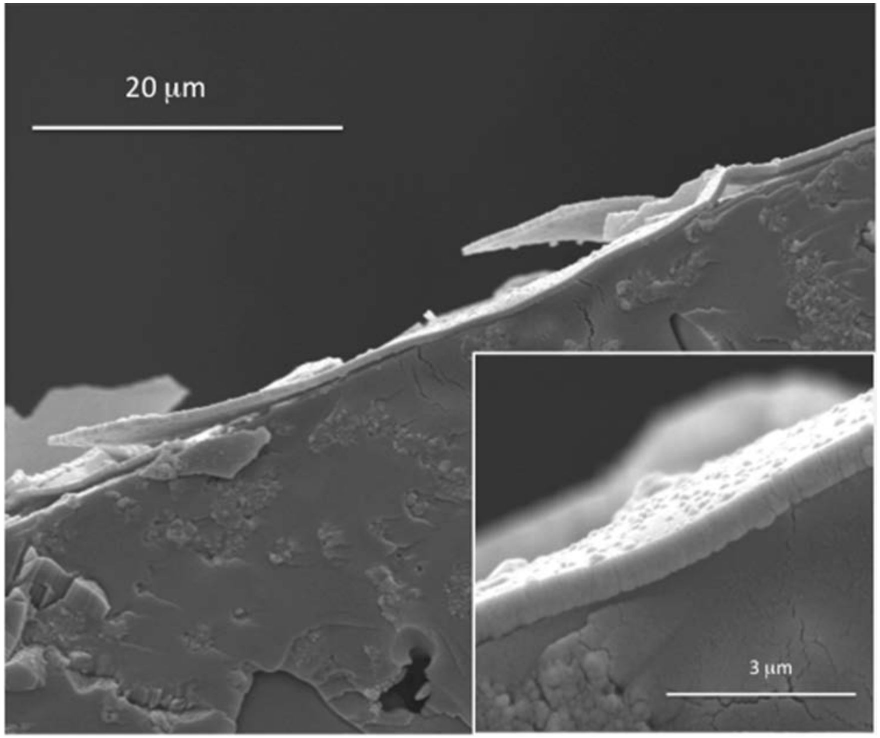
Zirconium MOF: UiO66



Formation of MOF thin films

New simple, surface-templating approach to fabricate pure MOF membranes that can be transferred to other surfaces





We have developed a novel templating technique to make sheets of MOF materials

Patent pending

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