**Stimuli-Responsive Metal-Organic Frameworks for Energy-Efficient Post-Combustion CO₂ Capture**

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**PROJECT GOAL**

The goal of this work is to develop innovative metal-organic framework-based molecular sieves whose adsorption and desorption properties can be finely tuned for energy-efficient post-combustion CO₂ capture from coal-fired power plants.

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**MOTIVATION**

- Coal-fired power plants are the single largest anthropogenic CO₂ emission sources domestically and globally.
- Post-combustion CO₂ capture can be retrofitted to existing plants (in contrast to oxy-combustion or pre-combustion capture technologies).
- DOE/NETL goal: 90% CO₂ capture at less than 35% increase in the cost of electricity.
- Finding novel sorbents for commercialization by partner, framergy™ (www.framergy.com) is paramount to this goal.

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**Why Stimuli-responsive Metal-Organic Frameworks?**

- **Metal-Organic Frameworks**: physisorbents with high surface area, tunable pore size, and physico-chemical functionalities.
- **High CO₂ / N₂ selectivity**: sorption properties can be tuned specifically for CO₂ (i.e., adjusting the size of its mesh by slightly changing temperature).
- **High CO₂ loading**: MOF materials are highly porous materials with high surface area, thereby exhibiting high CO₂ loading. Tuning the length of organic ligands can control the pore/cavity size thereby the CO₂ uptake.
- **Efficient regeneration**: slight increase in temperature (e.g., ΔT ~ 10°C) will release CO₂ by opening up the gates.

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**Single molecular traps (SMTs)**

1. SMT design and construction
2. MOF with built-in SMTs
3. Simulated locations for CO₂/N₂ (15:85) mixture

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**Stimuli-responsive MOF**

1. MOF structure and Structural Changes upon Activation and CO₂ Adsorption
2. In situ PXRD - CO₂ vs. N₂ Loading @ 296 K
3. Gas uptake, heat of adsorption, and selectivity

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**Amine-Tethered PPNs**

1. Synthesis of amine-tethered PPNs
2. Gas uptake of amine-tethered PPNs
3. TGA of amine-tethered PPNs in air
4. Cyclability of amine-tethered PPNs

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**Summaries**

- Innovative stimuli-responsive MOFs have a great potential for efficient post-combustion CO₂ capture.
- A new concept, the ‘SMT’ has been utilized in designing porous materials at the molecular level for CO₂ adsorption applications.
- PCN-200 is very promising with high CO₂/N₂ selectivity, low cost, high chemical (SO₂/NOₓ)/thermal stability, easy regeneration.
- Amine-tethered PPNs show comparable CO₂ working capacity to MEA with much lower energy consumption.