Engineering Accessible Active Sites in Metal Organic Frameworks for CO_2 Capture

Saki Golafale, Alexis McGill, Huayang Li, Dinadaylane Tandabany (co-PI), Conrad Ingram (PI)
Clark Atlanta University, 223 James P. Brawley Drive, Atlanta, GA 30314
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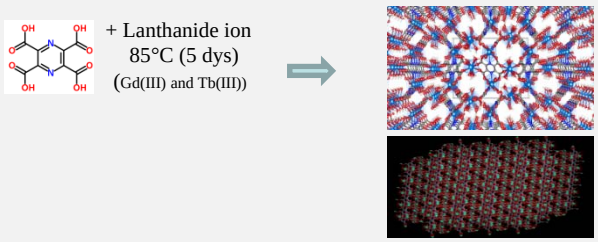
Introduction

Carbon dioxide, CO_2, capture and sequestration (CCS) from coal-derived power plant is a major drive by the United States towards mitigating CO_2 emissions. Post-combustion capture is the primary technological approach in the Department of Energy's Carbon Sequestration program [1].

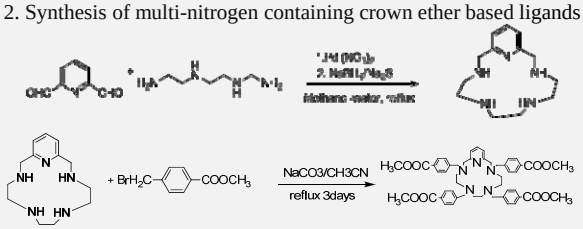
The research goal for this project is to synthesize metal organic framework (MOFs) with improved sites accessibility for enhanced carbon dioxide (CO_2) adsorption and selectivity properties. MOFs are a special class of ultra high surface area, porous multidimensional coordination polymers that shows impressive CO_2 adsorption characteristics. The three specific research objectives are as follows: **1)** Synthesize MOFs with metal ion adsorption sites in more accessible locations (toward the center of the organic linkers) to enhance their CO_2 adsorption characteristics; **2)** Synthesize MOFs with nitrogen-containing ligand as linker as a possible improved alternative to amine-functionalized MOFs; and **3)** Understand the nature of the adsorption sites and mechanism(s) by conducting computational studies.

Research Update

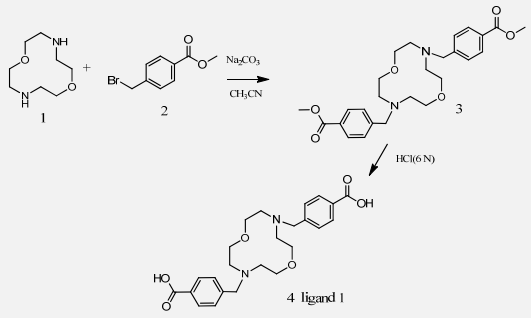
1. Synthesis of nitrogen containing pyrazine MOF with lanthanide ion and pyrazine-2,3,5,6-tetracarboxylate ligand.



2. Synthesis of multi-nitrogen containing crown ether based ligands

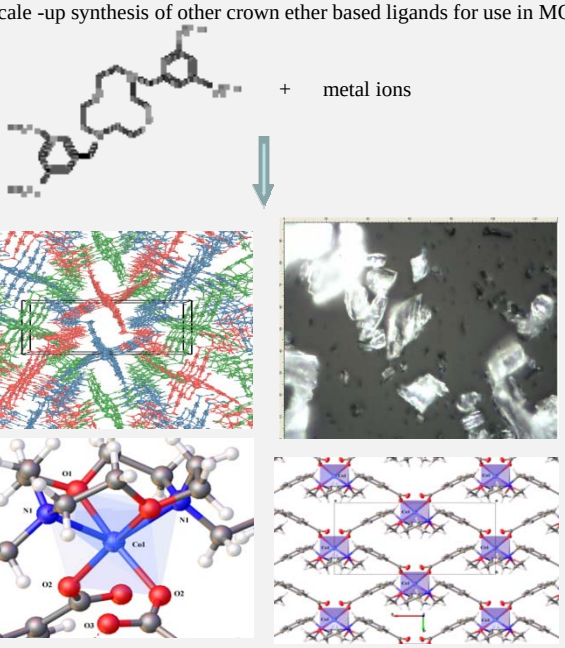


3. Scale -up synthesis of other crown ether based ligands for use in MOFs



Research Update cont'd

4. Scale -up synthesis of other crown ether based ligands for use in MOFs



Future work

1.Evaluate the CO_2 adsorption properties of recently synthesized MOFs.

2.Synthesize new MOFs based on an expanded series of diaza crown ethers and judicious choice of metal ions, and, evaluate their CO_2 adsorption properties.

3.Evaluate the CO_2 adsorption properties of MOFs synthesized with the nitrogen-containing pyrazine linker. These were also recently synthesized in our laboratory.

4.Investigate the nature of the sites and mechanism(s) of adsorption by conducting density functional theory

Students

Alexis McGill (graduate student), Stephan Mathis II (Ph. D. student), Huyang Li, (Post doc), Kimberli Hill (undergraduate)

References

1.http://energy.gov/fe/science-innovation/carbon-capture-and-storage-research/carbon-capture-rd