

# Biomimetic strategies for selective carbon dioxide capture with metal-organic frameworks

PI: Casey R. Wade  
Assistant Professor

Dept. of Chemistry and Biochemistry  
The Ohio State University

Email: [wade.521@osu.edu](mailto:wade.521@osu.edu)

Web: <http://u.osu.edu/wadelab>



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## Approach

Postsynthetic modification will be used to generate reactive metal hydroxide groups at the inorganic and organic building units of MOFs constructed from earth abundant metals.

Gas sorption analyses and breakthrough experiments will be used to investigate the CO<sub>2</sub> adsorption-desorption properties and adsorbent stability under simulated air conditions.

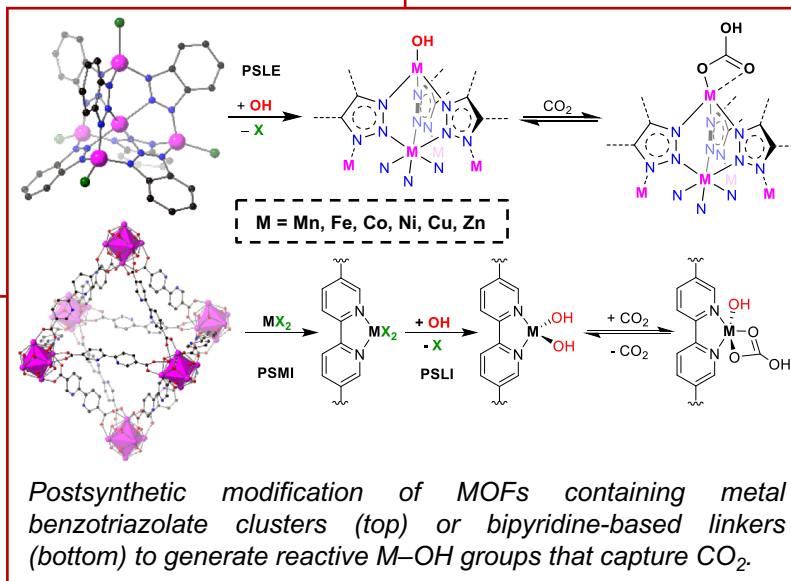
In situ FTIR and UV-Vis spectroscopic characterization techniques will be used to elucidate the mechanisms of CO<sub>2</sub> adsorption.

Computational studies will facilitate the design and optimization of new CO<sub>2</sub> adsorbents.

## Research Objectives

Develop porous metal-organic frameworks (MOFs) containing bio-inspired metal hydroxide functional groups as reliable and efficient solid adsorbents for CO<sub>2</sub> remediation from ambient air.

Investigate structure-function and composition-function relationships to optimize the selectivity, stability, and regeneration requirements of the MOF adsorbents.



The technology is currently at TRL 1. Fundamental research is needed to develop and evaluate the proposed adsorbents. Proof-of-concept testing will advance the technology to TRL 3.

## Potential Impacts

This research targets the design of new adsorbent materials for application in the Carbon Dioxide Removal Assembly (CDRA) of the Atmosphere Revitalization Systems (ARS).

A selective CO<sub>2</sub> → HCO<sub>3</sub><sup>-</sup> chemisorption process and the absence of volatile components will offer improved performance and reliability versus current state of the art adsorbents.

This research involves elucidating the structure and reactivity of organometallic species that are difficult or impossible to study in homogeneous solution, and will provide insight into reactive and/or transient intermediates that are implicated in catalytic processes.