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Entrapment of VOCs in Defective UiO-66 MOF: Ab Initio Molecular Dynamics Simulations at 300K

Authors: Brianne Boyd, Scott Bobbitt, Dr. Deep Choudhuri

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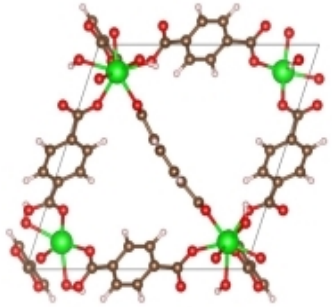
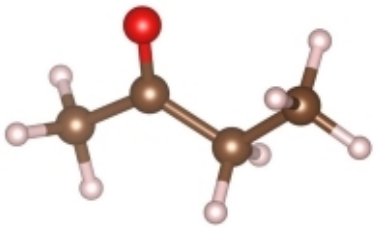
Introduction and Motivation

Metal Organic Frameworks (MOF) have been shown to be effective for Volatile Organic Compound (VOCs) absorption. 2-Butanone is one such VOC that is typically found in lung cancer patients. If a MOF could be shown to interact favorably with this VOC, it could be used as an indicator.

UiO-66 is well known for its use in gas capture due to its structural and thermal stability. It is composed of $Zr_6O_4(\mu_3\text{-}OH)_4$ nodes and BDC linkers. Frequently, defects in UiO-66 manifest as missing BDC linkers.





This project asks if UiO-66 could be effective in capturing 2-butanone molecules and how we can understand the influences of defects, temperature, and moisture on this interaction.

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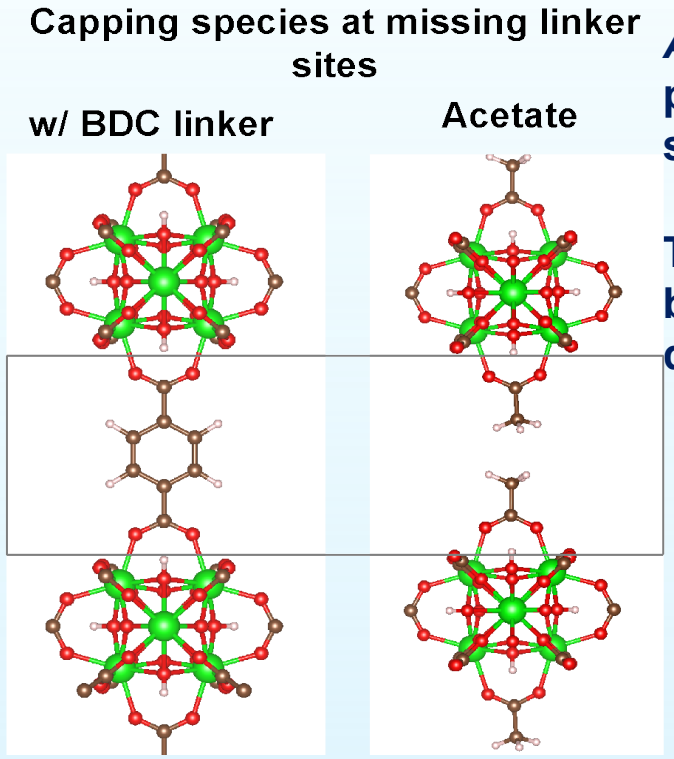
Approach

-Observation:UiO-66 has proven to be effective for certain VOC absorption

-Curiosity: Could UiO-66 be used to absorb 2-Butanone?

-Application: 2-Butanone is often found in lung cancer patients. If a MOF were to be found to interact favorably with the VOC, it could be used to determine if butanone is found in their breath.



***Ab initio* molecular dynamics (AIMD) was performed using the Vienna ab initio simulation package (VASP)**

The time-evolution of interaction energy between 2-butanone and MOF was quantified at 300K using the expression:

$$\Delta E^{Interaction}_{MOF+VOC+water}(t) = \Delta E^{t}_{Defective-MOF+VOC} - \Delta E^{Time\ Avg}_{defective-MOF} - n \times \Delta E^{Time\ Avg.}_{VOC},$$

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Current Status

Research has been completed and a paper is currently under review with Langmuir

Four molecule loading with preexisting H2O showed favorable energies.

Bonds were formed from a hydrogen bond tween 2-butanone and H2O, and then to the Hydroxyl Zr Nodes

At higher loadings, 2 butanone has been observed vacating the octahedral cage.

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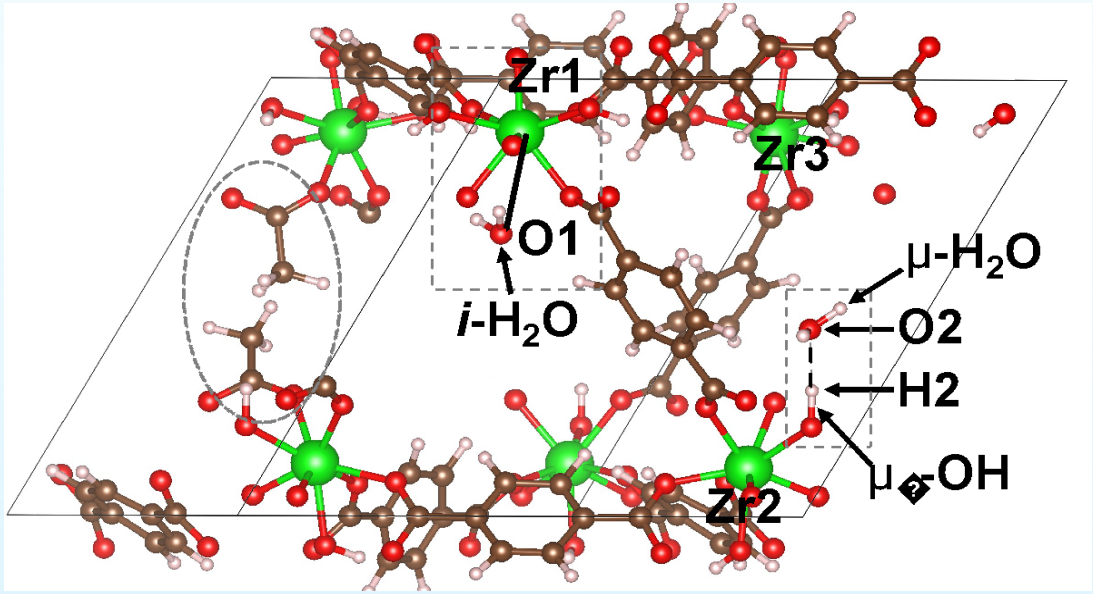
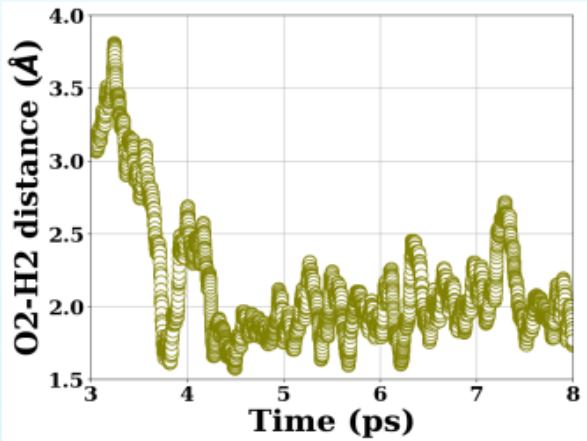
Results

AIMD snapshot of defective UiO-66 at 300K

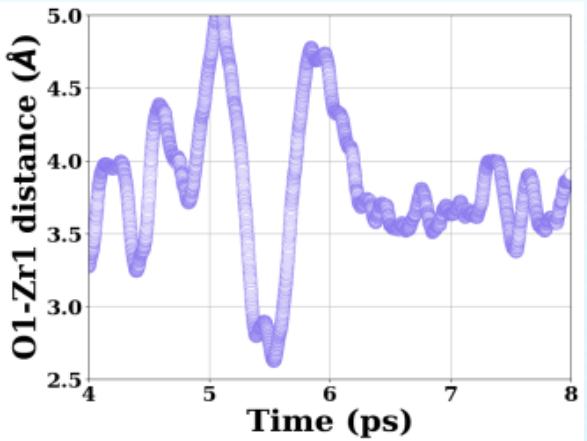


Energetically favorable structure at 300K: Missing BDC linker compensated by acetate groups and two neighboring water molecules (μ-H_2O & i-H_2O)

μ-H_2O (near μ_3-OH)



i-H_2O



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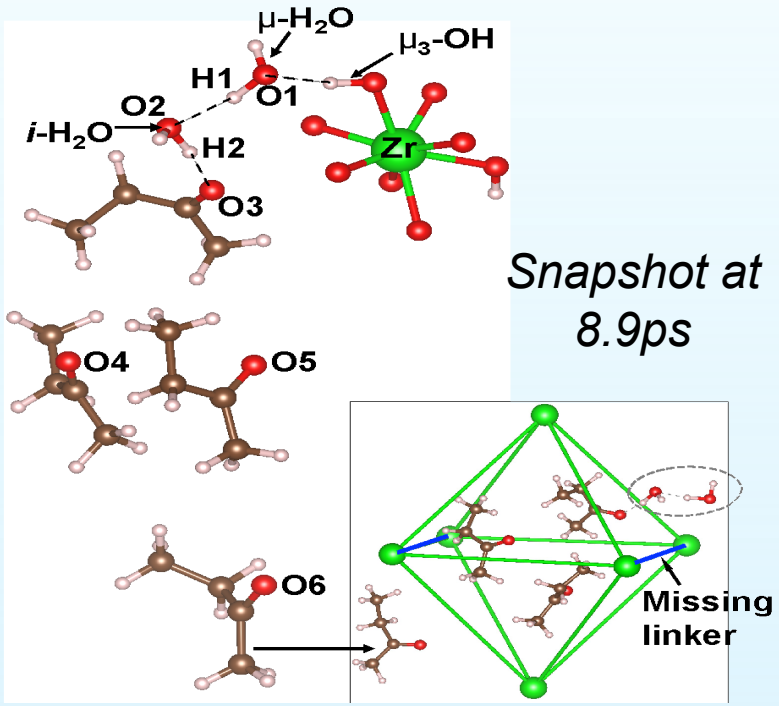
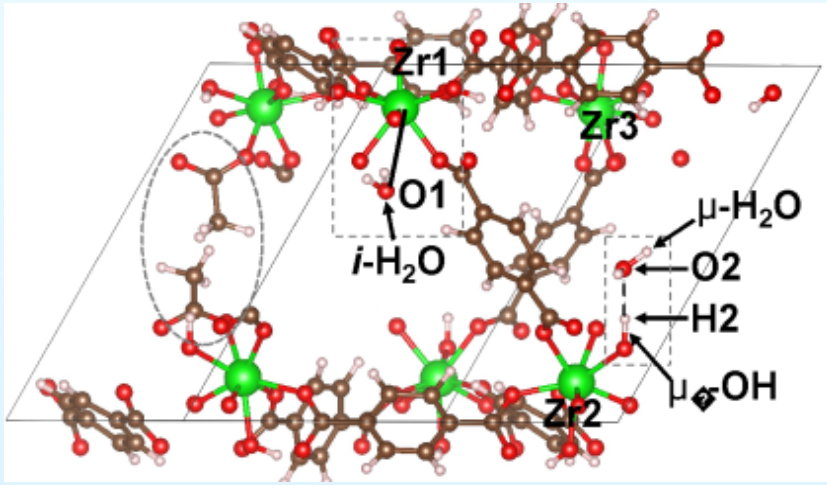
Results

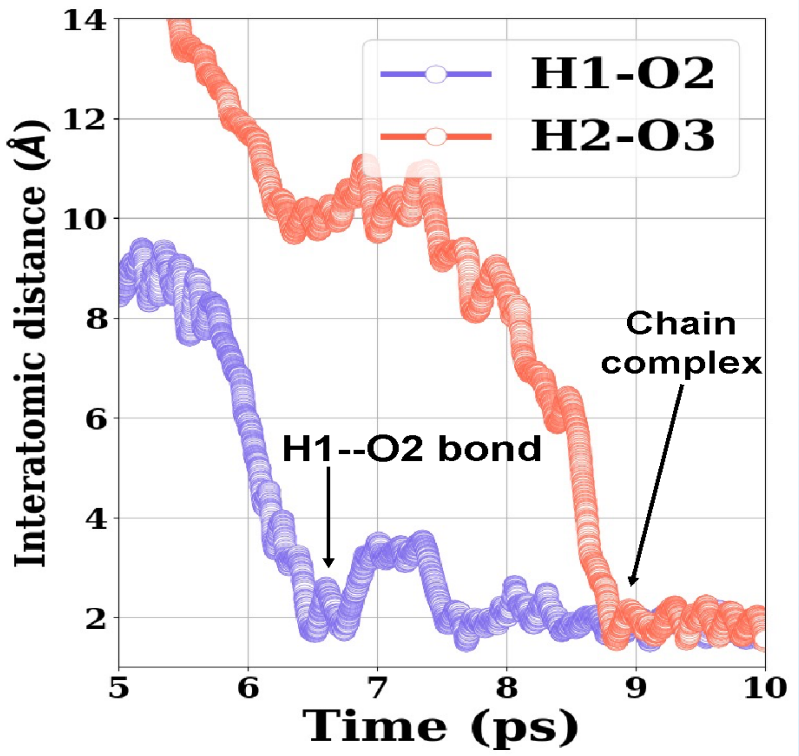
Trapping mechanism of 2-butanone VOC within defective UiO-66



Snapshot at 8.9ps

Formation of a stable chain complex between μ3-OH, μH2O, i-H2O, and 2-Butanone





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Impact of Work

This project will provide insights to the usage of 2-butanone as a biomarker by encapsulating the compound within the voids of UiO-66

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Challenges and Risks / Next Steps and Future Work

Next Steps:

Consider UiO-66 for absorption of CO2