
Contribution ID: **24** Type: **Oral Presentation**

# Ab Initio Molecular Dynamics Investigation of Water and Butanone Adsorption on UiO-66 with Defects

*Tuesday, 20 May 2025 09:35 (15 minutes)*

Volatile organic compounds (VOCs) are harmful chemicals that are found in minute quantities in the atmosphere and are emitted from a variety of industrial and biological processes [1-3]. They can be harmful to breathe or serve as biomarkers for disease detection [4,5]. Therefore, capture and detection of VOCs is important. Here, we have examined if the Zr-based UiO-66 metal–organic framework (MOF) can be used to capture butanone - a well-known VOC. Toward that end, we have performed Born–Oppenheimer ab initio molecular dynamics (AIMD) at 300 and 500 K to probe the energetics and molecular interactions between butanone [CH3C(O)CH2CH3] and open-cage Zr-UiO-66. Such interactions were systematically interrogated using three MOF structures: defective MOF with a missing 1,4-benzene-dicarboxylate linker and two H2O; pristine MOF with two H2O; and pristine dry MOF. These structures were loaded with one and four molecules of butanone to examine the effect of concentration as well. One-molecule loading interacted favorably with the defective structure at 300 K, only. In comparison, interactions with four-molecule loading were energetically favorable for all conditions. Persistent hydrogen bonds between the O atom of butanone, H2O, and μ3–OH hydroxyl attachments at Zr nodes substantially contributed to the intermolecular interactions. At higher loadings, butanone also showed a pronounced tendency to diffuse into the adjoining cages of Zr-UiO-66. The effect of such movement on interaction energies was rationalized using simple statistical mechanics-based models of interacting and noninteracting gases. Broadly, we learn that the presence of prior moisture within the interstitial cages of Zr-UiO-66 significantly impacts the adsorption behavior of butanone. Our findings are published in the journal Langmuir: https://doi.org/10.1021/acs.langmuir.4c02502.

References:
1. Ulanowska, A.; Kowalkowski, T.; Trawińska, E.; Buszewski, B. The application of statistical methods using VOCs to identify patients with lung cancer. J. Breath Res. 2011, 5, 046008 DOI: 10.1088/1752-7155/5/4/046008
2. Li, X.; Zhang, L.; Yang, Z.; Wang, P.; Yan, Y.; Ran, J. Adsorption materials for volatile organic compounds (VOCs) and the key factors for VOCs adsorption process: A review. Sep. Purif. Technol. 2020, 235, 116213
3. Bhattarai, D. P.; Pant, B.; Acharya, J.; Park, M.; Ojha, G. P. Recent progress in metal-organic framework-derived nanostructures in the removal of volatile organic compounds. Molecules 2021, 26, 4948 DOI: 10.3390/molecules26164948
4. Siu, B.; Chowdhury, A. R.; Yan, Z.; Humphrey, S. M.; Hutter, T. Selective adsorption of volatile organic compounds in metal-organic frameworks (MOFs). Coord. Chem. Rev. 2023, 485, 215119 DOI: 10.1016/j.ccr.2023.215119
5. Li, H.-Y.; Zhao, S.-N.; Zang, S.-Q.; Li, J. Functional metal-organic frameworks as effective sensors of gases and volatile compounds. Chem. Soc. Rev. 2020, 49, 6364–6401, DOI: 10.1039/C9CS00778D

## Country

USA

## Acceptance of the Terms & Conditions

Click here to agree

## Student Awards

## Water & Porous Media Focused Abstracts

This abstract is related to Water

## References


1. Ulanowska, A.; Kowalkowski, T.; Trawińska, E.; Buszewski, B. The application of statistical methods using VOCs to identify patients with lung cancer. J. Breath Res. 2011, 5, 046008 DOI: 10.1088/1752-7155/5/4/046008 2. Li, X.; Zhang, L.; Yang, Z.; Wang, P.; Yan, Y.; Ran, J. Adsorption materials for volatile organic compounds (VOCs) and the key factors for VOCs adsorption process: A review. Sep. Purif. Technol. 2020, 235, 116213 3. Bhattarai, D. P.; Pant, B.; Acharya, J.; Park, M.; Ojha, G. P. Recent progress in metal-organic framework-derived nanostructures in the removal of volatile organic compounds. Molecules 2021, 26, 4948 DOI: 10.3390/molecules26164948 4. Siu, B.; Chowdhury, A. R.; Yan, Z.; Humphrey, S. M.; Hutter, T. Selective adsorption of volatile organic compounds in metal-organic frameworks (MOFs). Coord. Chem. Rev. 2023, 485, 215119 DOI: 10.1016/j.ccr.2023.215119 5. Li, H.-Y.; Zhao, S.-N.; Zang, S.-Q.; Li, J. Functional metal-organic frameworks as effective sensors of gases and volatile compounds. Chem. Soc. Rev. 2020, 49, 6364–6401, DOI: 10.1039/C9CS00778D



**Primary author:** Ms BOYD, Brianne (New Mexico Tech)

**Co-authors:** CHOUDHURI, Deep (New Mexico Tech); Dr BOBBITT, Scott (Sandia)

**Presenter:** CHOUDHURI, Deep (New Mexico Tech)


**Session Classification:** MS24

**Track Classification:** (MS24) Molecular Modelling in Porous Media