University Of Warsaw
Faculty of Chemistry
Crystallochemistry Laboratory

Poster title: Modeling Solvent Inclusion in Metal Organic Frameworks Poreswith diverse topological landscapes by Molecular Dynamics with the Use of Large-scale Atomic/Molecular Massively Parallel Simulator

Patryk Skóra
Supervisor: dr hab. Mihails Arhangelskis

Abstract:

Background:
Metal Organic Frameworks (MOFs) have emerged as promising materials for various applications due to their unique structural properties. Understanding the behavior of solvents within MOFs is crucial for designing and optimizing their performance. However, the impact of solvent inclusion on the stability of MOF structures is not yet fully understood.
Aims/Purpose:
This study aims to investigate the effect of water inclusion as a solvent on the stability of MOF structures, specifically focusing on the pores within Zinc imidazolate polymorphs.The objective is to gain insights into the behavior of solvent molecules within these frameworks and determine their influence on structural stability.
Methods:
Molecular dynamics simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). The MOF structures were modeled, and water molecules were included as solvents. The simulations allowed for the study of solvent behavior and their interactions with the framework atoms over time.
Results:
Preliminary results demonstrate that water inclusion as a solvent negatively affects the stability of the MOF structures. The presence of solvent molecules introduces structural distortions, leading to reduced integrity of the frameworks. These findings suggest that water inclusion should be carefully considered in the design and optimization of MOFs for specific applications.
Conclusion:
The findings of this study highlight the importance of understanding the influence of solvents on the stability of MOF structures. The results indicate that water inclusion as a solvent is unfavorable and increases the energy of a structure. These insights have implications for the design and engineering of MOFs, providing valuable guidance for further research and development in the field of physical therapy.

Keywords: Metal Organic Frameworks, solvent inclusion, molecular dynamics, stability, water, LAMMPS.

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