

Investigating the Effects of Framework Flexibility on Water Adsorption in the Metal-Organic Framework NbOFFIVE-1-Ni via Molecular Modeling

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Many metal–organic frameworks (MOFs) exhibit complex structural flexibility, including breathing, swelling, and linker rotation. Understanding how these dynamic behaviors influence guest adsorption is crucial for designing MOFs for practical applications. In this study,¹ we employed a multiscale computational approach to gain molecular-level insight into the effect of flexibility on water adsorption in the MOF, NbOFFIVE-1-Ni. This material has narrow pores and good hydrothermal stability, which makes it attractive for CO₂ capture. We utilized density functional theory (DFT) calculations and grand canonical Monte Carlo (GCMC) simulations to study the impact of NbOFFIVE-1-Ni structural flexibility on its water adsorption at different humidity conditions. To mimic possible changes in the MOF structure during water adsorption, we generated 14 derivatives of NbOFFIVE-1-Ni by performing DFT optimization of the structure at different water loadings and by rotating the pyrazine linkers in the framework. Studying the water adsorption in different configurations of NbOFFIVE-1-Ni demonstrated that DFT optimization in the presence of adsorbed water molecules and rotating the linkers are useful strategies to mimic its structural flexibility. Our results illustrate the significance of taking structural flexibility into account when designing MOFs for water adsorption and other relevant applications.

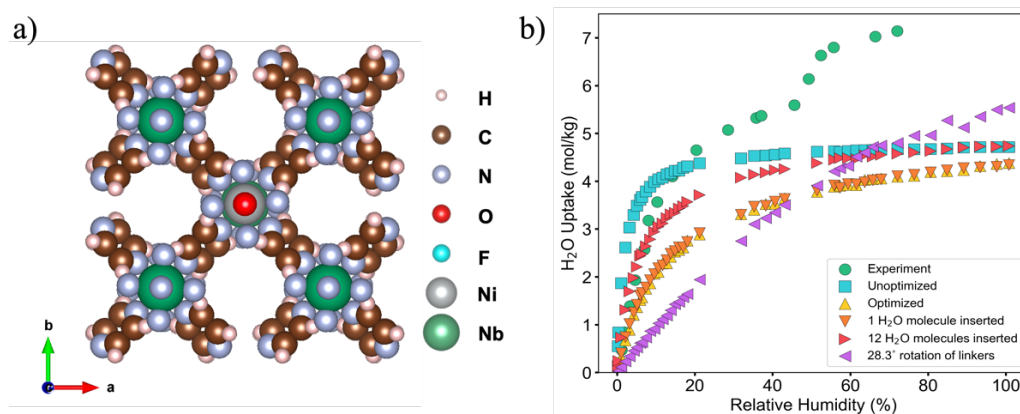


Fig. 1. a) NbOFFIVE-1-Ni shown from c direction. b) Comparison of the experimentally reported water adsorption isotherm² with the simulated isotherms of representative structures obtained from different computational methods.

References

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