

Abstract Submitted
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Using NMR to study small molecule adsorption in metal organic frameworks M.G. LOPEZ, P. CANEPA, T. THONHAUSER, Wake Forest University — We calculate the carbon nuclear magnetic resonance (NMR) chemical shift for the CO₂ molecule and the hydrogen shift for both H₂ and H₂O inside the metal organic framework structure Mg-MOF74 using *ab initio* calculations at the density functional theory level^{1,2} with the van der Waals density functional (vdW-DF).³ These shifts are obtained while placing the small molecules throughout the structure, including the calculated adsorption site for various loading scenarios. Our binding energy results agree well with previous experiments and calculation, and the NMR calculations show that it is reasonable to expect an experimentally observable change in the chemical shift depending on adsorbant, position, and loading. By providing this mapping of chemical shift to position and loading for these adsorbants, we argue that NMR probes could be used to provide information about the position at which these small molecules bind within the MOF and provide information about the loading of the adsorbed molecule.

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