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Probing Adsorption Interactions In Metal-Organic Frameworks Using X-ray Spectroscopy and Density Functional Theory[1] WALTER DRISDELL, Lawrence Berkeley National Laboratory, ROBERTA POLONI, SIMAP, laboratoire de Recherche sur les Matériaux, Grenoble, THOMAS MCDONALD, JEFFREY LONG, BEREND SMIT, University of California, Berkeley, JEFFREY NEATON, DAVID PRENDERGAST, JEFFREY KORTRIGHT, Lawrence Berkeley National Laboratory — Metal-organic frameworks (MOFs) are currently among the most promising materials for gas separation applications such as carbon capture. We explore the local electronic signatures of molecular adsorption at coordinatively unsaturated binding sites in the metal-organic framework Mg-MOF-74 using X-ray spectroscopy and first principles calculations. *In situ* measurements at the Mg K-edge reveal distinct pre-edge absorption features associated with the unique, open coordination of the Mg sites. These spectral features are suppressed upon adsorption of CO_2 and N,N'-dimethylformamide. Density functional theory shows that these spectral changes arise from modifications of local symmetry around the Mg sites upon gas uptake and are strongly dependent on the metal-adsorbate binding strength. Similar sensitivity to local symmetry is expected for any open metal site, making X-ray spectroscopy an ideal tool for examining adsorption in such MOFs.

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