In-situ visualization of loading-dependent water effects in a stable metal-organic framework

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Water adsorption can have a significant impact on metal-organic framework (MOF) performance properties, ranging from occupying active sites in catalytic reactions to co-adsorbing at the most favorable adsorption sites in gas separation and storage applications. The novel topic addressed in this presentation is understanding, for a MOF that is stable after moisture exposure, what are the reversible, loading-dependent structural changes that occur during water adsorption. Herein, a combination of *in situ* synchrotron diffraction along with complimentary molecular modelling analysis was used to understand the important role of loading-dependent water effects in a water stable MOF. Through this analysis, insights into changes in crystallographic lattice parameters, water siting information, and water-induced defect structure as a response to water loading was obtained. This work shows that, even in stable MOFs that maintain their porosity and crystallinity after moisture exposure, important molecular-level structural changes can still occur during water adsorption due to guest-host interactions such as water-induced bond rearrangements.