Novel CO$_2$ Binding Mechanism Determined Via in-situ X-ray Absorption Spectroscopy & Theory

**Scientific Achievement**

Distinguished between several proposed CO$_2$ adsorption mechanisms in amine-appended metal-organic frameworks using sensitive x-ray spectroscopy and *ab initio* theory.

**Significance and Impact**

Identified key chemical details of CO$_2$ adsorption mechanism and extended the applicability of combined x-ray absorption spectroscopy & 1st principles theory into new regimes.

**Research Details**

– Distinct spectral changes observed at the N and O K edges as CO$_2$ is adsorbed in two diamine-appended MOFs.

– Theoretical spectra for 3 distinct adsorption mechanisms reveal that only one is consistent with measurement.

– Spectra show particular sensitivity to subtle chemical changes in the appended amine species on CO$_2$ adsorption.

As CO$_2$ is adsorbed into amine appended Mg$_2$(dobpdc), spectral changes (red arrows) in element-specific x-ray absorption data are interpreted to uniquely identify bonding signatures in adsorption mechanism.


Work coordinated out of MSD, LBNL involved collaborators several institutions and use of DOE measurement and computational facilities.