Elucidating CO₂ Chemisorption in Diamine-Appended Metal–Organic Frameworks

Scientific Achievement
Determination of CO₂ chemisorption mechanisms in 13 diamine-appended metal–organic frameworks (MOFs), and discovery of a new mixed ammonium carbamate – carbamic acid adsorption mechanism.

Significance and Impact
Diamine-appended MOFs are promising materials for CO₂ capture, but elucidating adsorption mechanisms and designing new materials has remained challenging. Our new toolkit for assessing CO₂ chemisorption mechanisms can be applied broadly to CO₂ capture materials.

Research Details
- Hardware made to study CO₂-dosed samples by NMR.
- Combining solid state NMR spectra and DFT calculations enabled determination of CO₂ chemisorption mechanisms.


Work performed at UC Berkeley, Lawrence Berkeley National Lab, Advanced Light Source.