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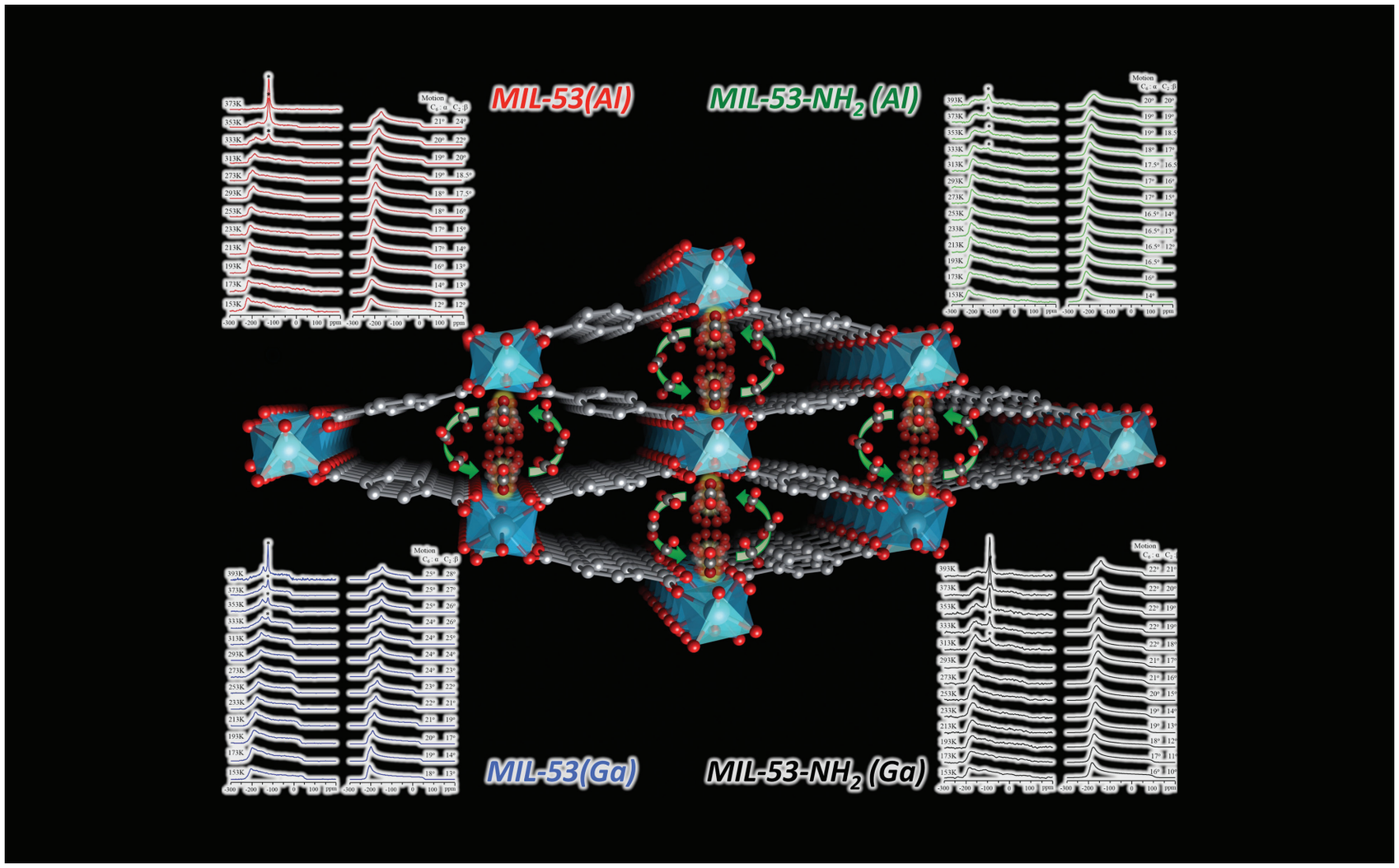
NMR is Science



Static variable-temperature 13C solid-state NMR of dynamic carbon dioxide trapped in the MIL-53 metal organic framework

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Field strength: 9.4 T

Why is this your favorite spectrum?

These may look like relatively simple ^{13}C powder patterns, but their appearances are deceiving: encoded within the apparent ^{13}C NMR parameters and spectral evolution with temperature are many details of CO_2 motion within MIL-53. Also, these spectra got us on the cover of Physical Chemistry Chemical Physics, so that's a pretty good reason these are my favorite spectra.

It was evident that CO_2 undergoes a localized "wobbling" on adsorption sites and a nonlocalized "hopping" between adsorption sites in MIL-53, as shown in the central illustration. We also explored the effect of the metal center on CO_2 motion, as well as amine functionalization of the aromatic linkers. For each set of spectra, the experimental spectra are shown in the left column, and the simulated spectra are shown in the right column. The angles of CO_2 motion (local C_6 wobbling (alpha) and nonlocalized C_2 hopping (beta)) are shown above each simulated spectrum; note their changes with temperature. All motions take place at a rate equal or greater than 10^7 Hz.