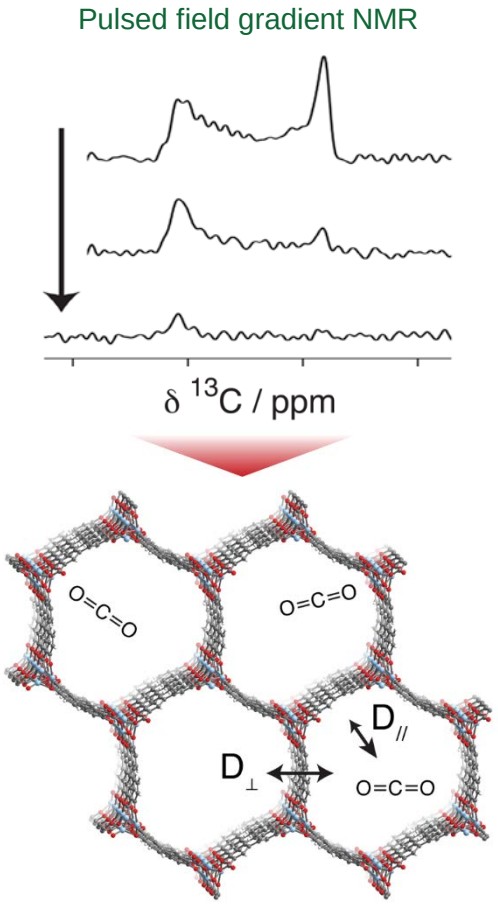
Unexpected Diffusion Anisotropy of Carbon Dioxide in the Metal–Organic Framework Zn_2(dobpdc)



Diffusion anisotropy from PFG NMR: (Top) Example PFG NMR spectra for CO_2 in Zn_2(dobpdc) **(Bottom)** Diffusion along ($D_{//}$) and between ($D_{\perp}$) channels is measured.

Scientific Achievement

NMR methods developed to measure the diffusion anisotropy of CO_2 in Zn_2(dobpdc) and reveal unexpected diffusion between the 1-D pores.

Significance and Impact

First measurement of diffusion anisotropy in a MOF with 1-D pores. Will aid design of materials with improved transport.

Research Details

- Pulsed field gradient (PFG) nuclear magnetic resonance (NMR) measurements used to measure the diffusion anisotropy of gas-dosed Zn_2(dobpdc) crystals.
- Single-crystal diffraction and molecular dynamics simulations showed that structural defects are most likely explanation for unexpected diffusion between pores.

Forse, A. C.; Gonzalez, M. I.; Siegelman, R. L.; Witherspoon, V. J.; Jawahery, S.; Mercado, R.; Milner, P. J.; Martell, J. D.; Smit, B.; Blümich, B.; Long, J. R.; Reimer, J. A. *J. Am. Chem. Soc.* **2018**, *140*, 1663-1673.

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