Unexpected Diffusion Anisotropy of Carbon Dioxide in the Metal–Organic Framework Zn$_2$(dobpdc)

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.


Work was performed at UC Berkeley, RWTH Aachen (Germany), and the Advanced Photon Source at Argonne National Laboratory.