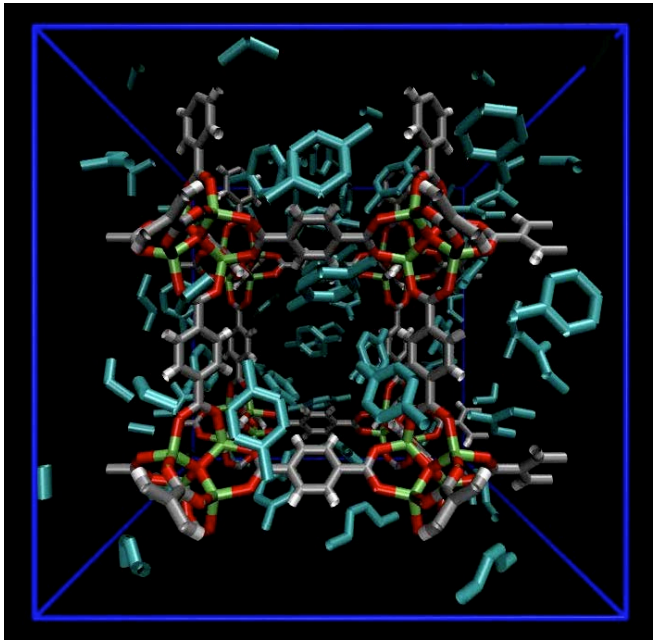
Relaxometry and Diffusometry of Small Molecules in MOFs

Scientific Achievement

The effects of subtle geometric differences between the para, meta, and ortho isomers of xylene were manifest in their restricted translational and rotational motions when confined to a metal–organic framework.



MD simulations of paraxylene in IRMOF-1.

V. J. Witherspoon, L. M. Yu, S. Jawahery, E. Braun, S. M. Moosavi, S. K. Schnell, B. Smit, and J. A. Reimer *J. Phys. Chem. C*, **2017**, *121*, 15456.

Work was performed at UC Berkeley.

Significance and Impact

A combined NMR and MD study of xylene motion in confined media were found to have qualitative and semi quantitative agreement, showing that molecular shape and interactions with framework walls dictate their motion.

Research Details

- *p*-Xylene is shown by NMR to have the fastest self-diffusion coefficient, consistent with MD simulations which show that *p*-xylene's probability distribution is least localized.
- *p*-Xylene has the highest activation energy for rotational motion, which is is informed by MD simulations showing that *p*-xylene's rotation is limited by confined geometry.