

Cooperative Adsorption of Carbon Disulfide in Diamine-Appended Metal–Organic Frameworks

Scientific Achievement

Demonstration of reversible, step-shaped uptake of CS₂ in the framework mm-2–Mg₂(dobpdc) (mm-2 = *N,N*-dimethylethylenediamine) via a cooperative chemisorption mechanism previously known only for CO₂

Significance and Impact

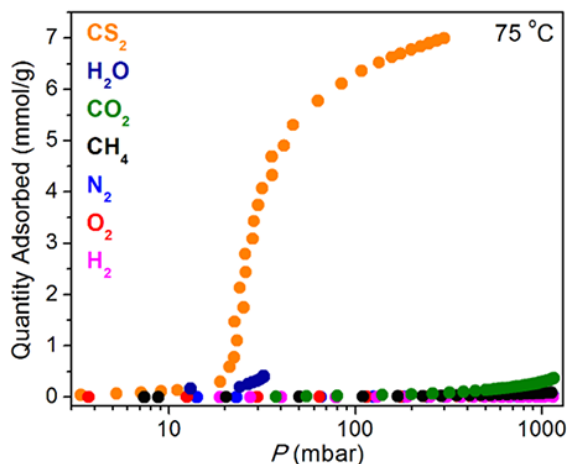
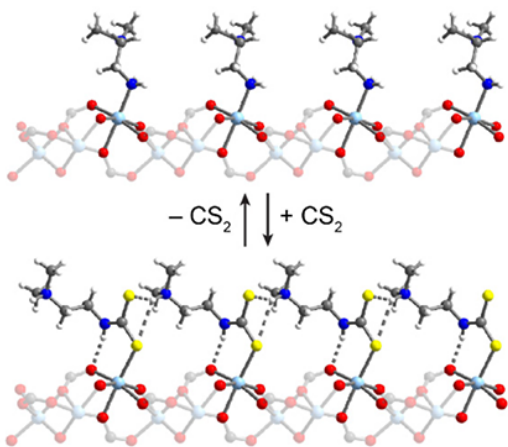
Low-energy capture of the volatile, flammable, and toxic commodity chemical CS₂ is of relevance to industry and an important proof-of-concept that this mechanism can be extended to other target small molecules

Research Details

– Gas adsorption, crystallography, and spectroscopy were used to characterize the mechanism of CS₂ uptake, which occurs via formation of electrostatically paired ammonium-dithiocarbamate chains

McGuirk, C. M.; Siegelman, R. L.; Drisdell, W. S.; Runcevski, T.; Milner, P. J.; Oktawiec, J.; Wan, L. F.; Su, G. M.; Jiang, H. Z. H.; Reed, D. A.; Gonzalez, M. I.; Predergast, D.; Long, J. R. *Nat. Commun.* **2018**, *9*, 5133.

Work was performed at UC Berkeley, the Molecular Foundry, and the Advanced Light Source.



(Top) Single-crystal X-ray diffraction structures illustrating CS₂ insertion into the metal–amine bonds in mm-2–Zn₂(dobpdc). (Bottom) Comparison of adsorption isotherms for CS₂ and other gases in mm-2–Mg₂(dobpdc).



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