

New Material Overcomes a Long- Standing Challenge for Efficient, Onboard Storage of Hydrogen using Adsorbents

The quest to develop a low cost material that efficiently stores hydrogen onboard fuel cell electric vehicles at low pressures and near room-temperature has been pursued by U.S. Department of Energy since the early 2000's. Researchers recently made an early stage scientific breakthrough, that could open the door to achieving a material that offers a 300+ mile driving range with 5 minute refuels, while still only emitting water vapor at the tail pipe.

For the first time, the simultaneous binding of two hydrogen gas molecules to a single metal site was demonstrated in a metal-organic framework (MOF), opening the door to significantly enhanced hydrogen adsorption capacity and increased fuel cell electric vehicle driving range at a lower cost. These metal sites are referred to as coordinatively-unsaturated metal centers, and are known to be among the strongest binding sites for hydrogen molecules in adsorbents such as MOFs. Stronger affinity for hydrogen molecules is highly desirable as it enables higher capacity hydrogen storage systems that can operate under more realistic operating conditions (lower pressure and higher temperatures). Consequently, a major goal of adsorption-based hydrogen storage material research has been to increase both the density of these metal sites and the number of hydrogen molecules adsorbed per site.

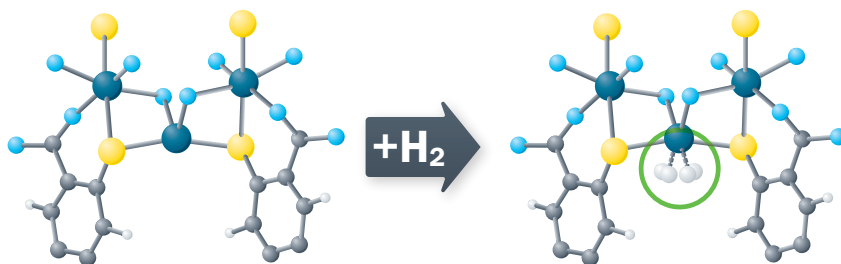


Illustration of multiple hydrogen (H_2) molecules bound to a single metal site. A portion of the $Mn_2(dsdbc)$ MOF crystal structure shown on the left with two hydrogen molecules bound to metal site on the right. Blue, yellow, light blue, gray and small white spheres represent Mn, S, O, C, and H atoms respectively. The hydrogen molecules bound at the open metal site are shown as larger white spheres inside the green circle.

This breakthrough, achieved by researchers at Lawrence Berkeley National Laboratory, was observed using a MOF material, which is a compound consisting of metal clusters coordinated to organic ligands to form highly porous structures with tunable pore sizes. The specific MOF synthesized, $Mn_2(dsdbc)$, contains manganese (Mn) cations in two separate coordination environments connected through 2,5-disulfido-1,4-benzenedicarboxylate (dsdbc) linkers to form an extended porous network. One of the Mn cations is attached to two solvent molecules which can be thermally removed, leaving behind space for two hydrogen molecules (H_2) to bind simultaneously (see figure).

Confirmation that multiple hydrogen molecules were adsorbing to the Mn sites was provided by in-situ neutron powder diffraction, carried out at the National Institute of Standards and Technology's Center for Neutron Research. Loadings of deuterium molecules were used as a proxy for

hydrogen to exploit the higher scattering cross section of deuterium compared to hydrogen. As shown in the figure, the interaction of two deuterium molecules with a single Mn site is clearly observed at adjacent locations on the four-coordinate Mn cation. While the binding strength of hydrogen in this material is modest compared to other MOFs, this result provides an important proof of concept for designing adsorption-based hydrogen storage materials with significantly enhanced hydrogen capacity. Current work is aimed at extending this chemistry to materials which can bind more than two molecules per metal site, which modeling has predicted to have the potential to yield materials that could meet the 2025 DOE hydrogen storage system targets of 5.5 wt.% and 40 g/L hydrogen.

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INVESTMENT:

\$2.4M

Total DOE Share

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