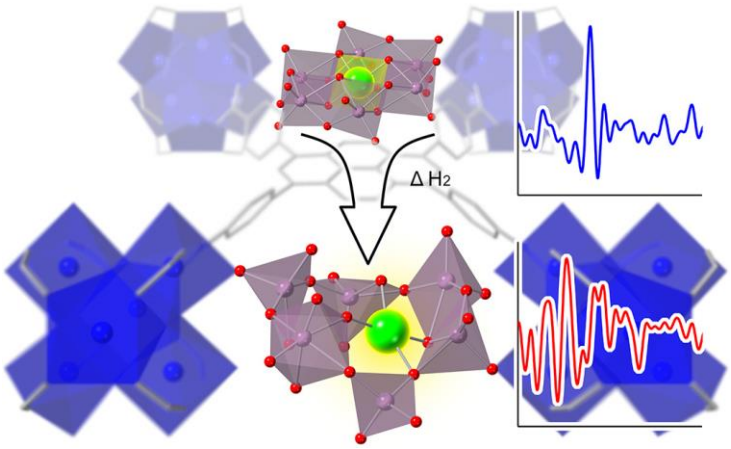
SCIENCE AT THE ADVANCED PHOTON SOURCE

ISOLATING ACTIVE SITES FOR MORE EFFICIENT CATALYSTS

Scientists are always searching for new catalysts to enable fast, energy-efficient chemical reactions to transform wastes into useful chemical fuels. Single-site catalysts are a promising new class of catalyst. The challenge with such materials is that the active catalytic sites, which can be as small as a single atom, tend to aggregate, degrading their efficiency and selectivity.

Now researchers using the Advanced Photon Source have demonstrated a design for such single-site catalysts that resist aggregating and retain their high efficiency. The design starts with polyoxometalate clusters, discrete polyatomic anions in which three or more metals, including molybdenum, share oxygen atoms. Catalytic atoms, often noble metals such as platinum or rhodium, can be embedded with the POM.

The team used pair distribution function analysis (PDF) a technique that is a specialty of beamline 11-ID-B at the APS. The team also performed X-ray absorption spectroscopy (XAS) at beamline 5-BM-D, the Dupont-Northwestern-Dow Collaborative Access Team (DND-CAT) beamline. This technique provides element-specific information, allowing them to isolate the platinum and the rhodium environments. Combining the PDF and XAS measurements allowed the researchers to figure out the local geometry of the catalyst's active site during the catalytic reaction. They found that the distance between the rhodium or platinum and the molybdenum in the active catalyst was shorter than the metal-to-metal bond lengths in bulk metals.



Z. Chen, et. al., "Atomically precise single-site catalysts via exsolution in a polyoxometalate-metal-organic framework architecture," *Journal of the American Chemical Society* 2024, 146, 12, 7950-7955 (March 2024)

A POM consisting of ring of molybdenum (purple)-oxygen (red) octahedra that surrounds a catalytically active rhodium (green) site, all supported on Zr-MOF. When the pristine catalyst (top) is activated under hydrogen at high temperature, its structure changes (bottom) and the Rh protrudes from the Mo-oxo ring.

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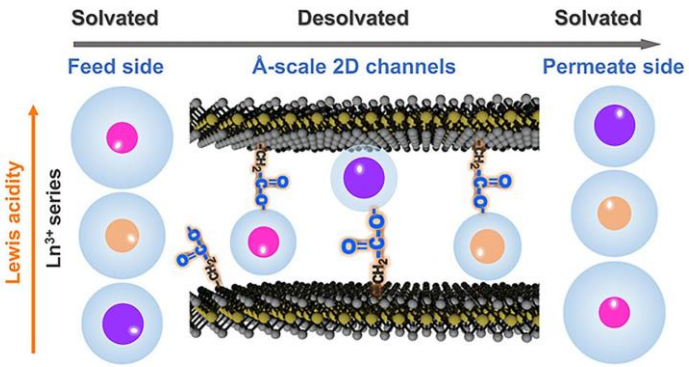

M. Wang, et. al., "Lanthanide transport in angstrom-scale MoS2-based two-dimensional channels," *Sci Adv* 10, eadh1330 (March 2024)

Schematic of transport of lanthanides through Angstrom-scale inorganic membranes composed of stacked sheets of MoS_2 that have been functionalized by acetate (COOH).

A GREENER POSSIBILITY USING LANTHANIDE SEPARATION IN 2D

Lanthanides and other rare earth elements (REEs) are quite difficult to separate and purify from the other materials with which they're usually found. Because of the great value and utility of these metals for many purposes, including electronics, computing, and various industrial processes that rely on their unique electronic and chemical properties, that difficulty is a major problem.

Most current processes for REE separation and purification involve organic and acidic materials, making them both energy-intensive and environmentally unfriendly. Researchers from the University of Chicago, Northwestern University, and Argonne National Laboratory took inspiration from nature to examine a new possibility for lanthanide separation. They constructed two-dimensional angstrom-scale artificial ion channels using MoS_2 nanosheets that were covalently functionalized with acetic acid to generate MoS_2-COOH membranes for lanthanide ion separation.

The ion transport process was studied using a variety of tools, including electron microscopy, infrared spectroscopy, molecular dynamics simulations and X-ray absorption spectroscopy and X-ray diffraction studies. Data were collected at the DuPont-Northwestern-Dow Collaborative Access Team 5-BM-D beamline at the Advanced Photon Source.

Read more about the upgraded APS at aps.anl.gov

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