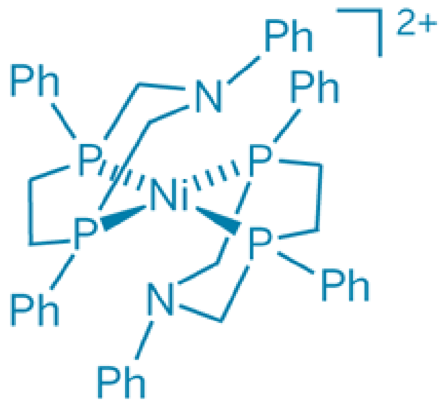

PNNL catalyst

Ph = phenyl

A synthetic nickel complex can catalyze the electrochemical combination of protons to produce hydrogen at rates more than 10 times faster than the fastest hydrogen-producing enzymes can, according to a study published in *Science* (DOI: 10.1126/science.1205864). The investigation highlights the role of molecular features that endow low-cost catalysts with record-setting kinetic properties.

Catalysts that use electrical energy to mediate production of fuels such as hydrogen—and those that facilitate the reverse reaction, oxidation—are widely expected to play a central role in future energy platforms. Such catalysts may be incorporated into future water-splitting systems for solar energy conversion to mediate the step in which two protons taken from water are joined to form a hydrogen molecule.

Platinum readily catalyzes hydrogen production and/or oxidation. Yet the metal's high cost and relative scarcity have motivated researchers to study hydrogenase enzymes, which do both jobs via complexes based on iron and nickel—inexpensive, abundant metals. Natural enzymes are not easily produced in bulk quantities and may not stand up to industrial conditions. But they exhibit molecular features that researchers can mimic in designing more durable catalysts.

In the new study, scientists at Pacific Northwest National Laboratory (PNNL) incorporated an amine-based proton relay similar to the one found in [FeFe]-hydrogenase enzymes into their nickel catalyst. The synthetic complex contains two seven-membered cyclic diphosphine ligands each with a pendant amine group.

On the basis of catalysis tests using protonated dimethylformamide as the proton source, the team, which includes Monte L. Helm, R. Morris Bullock, Daniel L. DuBois, and coworkers, finds that the new catalyst acts more than 10 times faster than the fastest natural enzyme and 100 times faster than the group's previous best catalyst.

The team notes that the fast-acting catalyst is nearly 100% efficient in terms of electrons in and hydrogen molecules out but still not "perfect" catalyst. They're addressing that issue now.

"This paper unveils a major catalyst design breakthrough," remarks Thomas B. Rauchfuss of the University of Illinois, Urbana-Champaign. Several years ago, he adds, the PNNL team seized on the proton-relay concept and has been using it to develop catalysts that are faster and more efficient ever since.

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