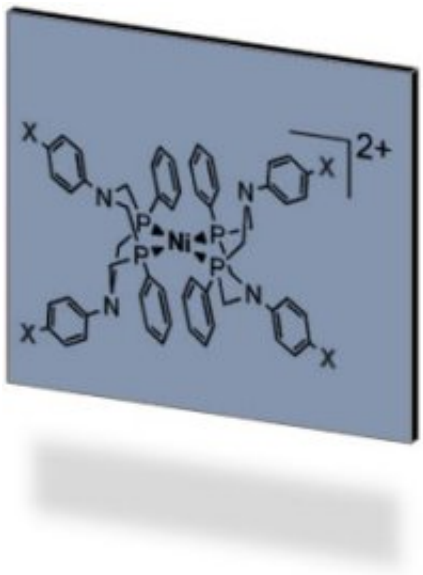
# World's fastest nickel-based complex

July 25 2011




(PhysOrg.com) -- Scientists at Pacific Northwest National Laboratory's Center for Molecular Electrocatalysis and Villanova University designed a nickel-based complex that more than doubled previously reported hydrogen gas production rates and increased the energy efficiency of the reaction. Additionally, the team found that adding water to the reaction significantly increased the reaction speed. As a result of the discoveries, researchers are closer to finding energy storage solutions for surplus energy generated from green technologies.

"These catalysts are, to the best of our knowledge, the fastest reported

molecular electrocatalysts for hydrogen production," said PNNL postdoctoral associate Dr. Uriah Kilgore, first author of the study's findings. "Small changes in their structure and small amounts of water led to significant increases in catalyst turnover frequencies."

Retooling America's energy industry requires storing surplus energy generated from renewable technologies. Storage of energy is needed due to the intermittent nature of renewable energy sources such as solar and wind power. One answer, storing energy in the creation of hydrogen gas, requires efficiencies that seem to be contradictory. To avoid losing energy generated by wind turbines, for example, hydrogen gas must be generated quickly. Generation of hydrogen gas must also be energy efficient to convert all of the electricity to chemical energy in hydrogen.

Storing energy in hydrogen gas requires an energy source to power a catalytic chemical reaction that results in the creation of hydrogen gas. This catalytic reaction is limited by the cost of the key catalyst. Platinum catalysts excel at two key energy-storage factors: turnover frequency and overpotential, but platinum is an expensive precious metal of low abundance. Turnover frequency describes the number of hydrogen gas molecules created by a catalyst over a period of time. Overpotential, the difference between the theoretical energy and the actual energy required to produce the hydrogen gas, often works against turnover frequency—typically, the faster hydrogen gas is created, the more energy it requires. Likewise, lower overpotentials usually translate to inefficiencies from slower turnover frequencies. The key for energy storage via the creation of hydrogen gas lies in finding a low-cost catalyst whose turnover frequency and overpotential matches or exceeds that of platinum.

The study completed by Pacific Northwest National Laboratory and Villanova University researchers led to important discoveries in the advancement of catalysis for production of hydrogen gas. First, small

changes in the catalyst have a significant effect on hydrogen gas production rates. Additionally, the team found that adding small volumes of water to the conversion led, in some cases, to an increase in turnover frequency of more than a factor of ten. The combined effect of the discoveries led to catalysts with higher rates of hydrogen gas production, lowered the overpotential, and provided insight for further research for hydrogen gas as an energy storage solution.

The research team synthesized nickel-based complexes and mixed the complexes with acids with a range of pH values. Electrochemical reduction of the acid produced hydrogen. The catalysts (in solution) were studied by cyclic voltammetry, in which an electrical current repeatedly sweeps between two set voltages, leading to the determination of the turnover frequencies.

The research team will continue to develop the nickel-based complexes to increase the turnover frequency and decrease the overpotential. Additionally, the effects of water on catalytic rates will continue to be evaluated.

**More information:** Kilgore UJ, et al. 2011. "[Ni(PPh2NC6H4X2)2]2+ Complexes as Electrocatalysts for H2 Production: Effect of Substituents, Acids, and Water on Catalytic Rates." *Journal of the American Chemical Society* 133(15):5861-5872.

Provided by Pacific Northwest National Laboratory