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NATIONAL RENEWABLE ENERGY LABORATORY

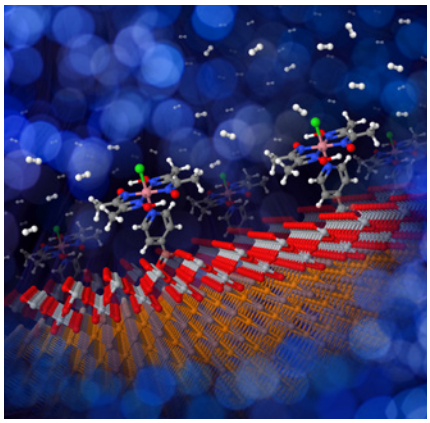
NREL Photoelectrode Research Advances Hydrogen Production Efforts

Highlights in Research & Development

Scientists have created a high-performing photoelectrode that boosts the ability of solar water-splitting to produce hydrogen.

Scientists at the National Renewable Energy Laboratory (NREL) have taken an innovative approach to solving a drawback in the photoelectrochemical (PEC) process, which uses solar energy to split water into hydrogen and oxygen. The standard approach uses precious metals such as platinum, ruthenium, and iridium as catalysts attached to a semiconductor. The downside of this approach is that the cost of precious metals hinders large-scale commercial efforts.

The use of less expensive molecular catalysts to replace precious metals has been suggested as a proposed solution to this conundrum. Yet, other challenges arise with using molecular catalysts, specifically poor stability and a shorter lifespan compared to photoelectrodes using metal-based catalysts.



Representation of a photocathode where the $GaInP_2$ semiconductor (orange) has been coated with TiO_2 (red/white layer). This surface modification allows the cobaloxime molecular catalyst (two large molecules shown) to bond to the semiconductor. Hydrogen (numerous white double-spheres) is generated when sunlight illuminates this electrode immersed in a basic aqueous solution. Illustration by Alfred Hicks, NREL

NREL explored a different approach to the solution and began examining molecular catalysts to see if they could be attached to the surface of the electrode semiconductor. Using atomic layer deposition, NREL scientists first laid down 35 nm of titanium dioxide (TiO_2) on the surface of the gallium indium phosphide ($GaInP_2$) semiconductor. Cobaloxime—a hydrogen-evolution molecular catalyst—was then attached to the TiO_2 surface. Finally, 0.4 nm of TiO_2 was deposited on top of the molecular catalyst to protect it from desorption of the TiO_2 surface.

This photoelectrode arrangement of cobaloxime/TiO_2/$GaInP_2$ has yielded the desired results—namely, molecular catalysts that can be as highly active as precious metal catalysts, but at a much lower cost. Furthermore, the TiO_2 protects the semiconductor from corrosion, thus increasing the photoelectrode's life span.

It is known that molecular catalysts are not as stable as the metal-based catalysts. However, PEC systems do not operate after sunset, and this down-time provides the opportunity to regenerate the molecular catalyst.

This new innovative structure—using these lower-stability, but highly active and lower-cost molecular catalysts—opens up the potential for a long-term scalable solution for developing large-scale commercial PEC water-splitting systems, circumventing the scalability issue of platinum-based catalysts.

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Reference: Gu, J.; Y. Yan; J.L. Young; K. Steirer; N.R. Neale; J.A. Turner. "Water reduction by a p-$GaInP_2$ photoelectrode stabilized by an amorphous TiO_2 coating and a molecular cobalt catalyst," *Nature Materials* 15 (2015). DOI: 10.1038/nmat4511.

Key Research Results

Achievement

NREL scientists were able to attach a highly active molecular catalyst through a TiO_2 layer to a high-efficiency III-V semiconductor and show hydrogen evolution activity commensurate with a platinum-metal-catalyzed semiconductor.

Key Result

Molecular catalysts that have relatively low stability but are highly active, such as cobaloxime, may potentially be a long-term solution to the scalability issue for photoelectrochemical water-splitting systems.

Potential Impact

This molecular catalyst/TiO_2/semiconductor architecture allows the decoupling of the electrocatalytic reactions from the underlying photovoltaic materials. This permits further improvements in activity by independent optimization of device parameters and offers the possibility of adaptations to other reactions of interest (besides hydrogen) and schemes that can be easily applied to other semiconductor surfaces.

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