Developing a catalyst that purifies herbicide-tainted water and produces hydrogen

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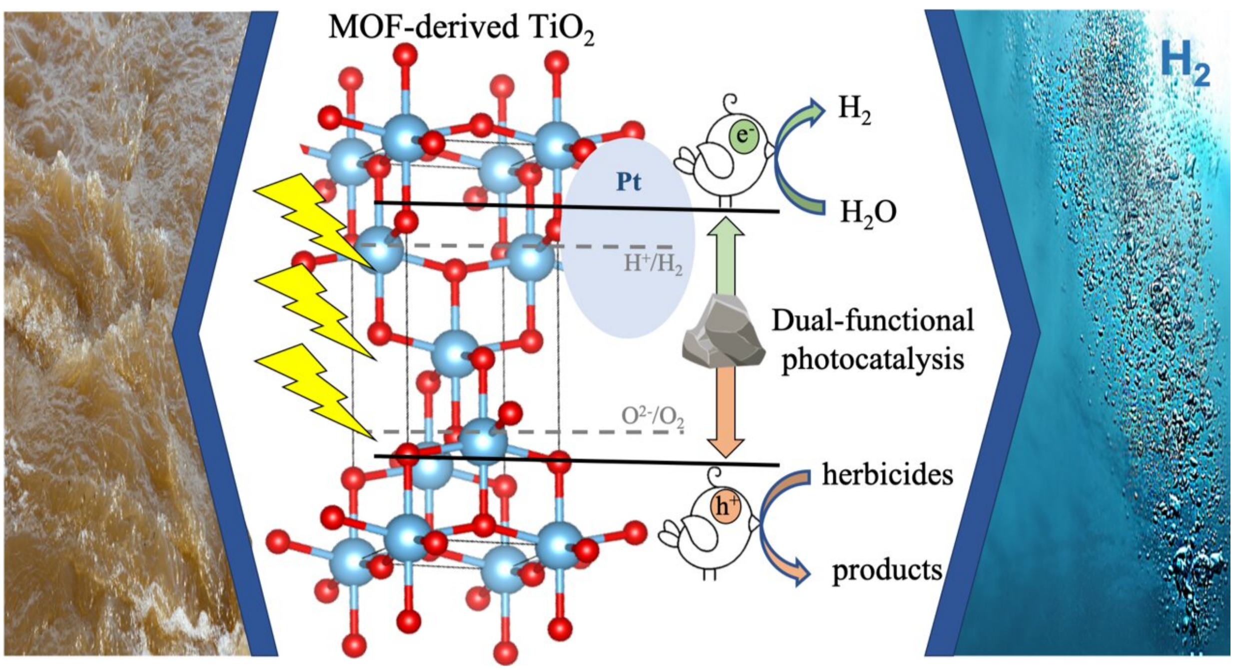

Graphic depicting how new photocatalyst works. Credit: *ACS Catalysis* (2023). DOI: 10.1021/acscatal.3c00265

Researchers in the Oregon State University College of Science have developed a dual-purpose catalyst that purifies herbicide-tainted water while also producing hydrogen.

The project, which included researchers from the OSU College of

Engineering and HP Inc. is important because water pollution is a major global challenge, and hydrogen is a clean, renewable fuel.

Findings of the study, which explored photoactive catalysts, were published today in the journal *ACS Catalysis*.

"We can combine oxidation and reduction into a single process to achieve an efficient photocatalytic system," OSU's Kyriakos Stylianou said. "Oxidation happens via a photodegradation reaction, and reduction through a hydrogen evolution reaction."

A catalyst is a substance that increases the rate of a chemical reaction without itself undergoing any permanent chemical change.

Photocatalysts are materials that absorb light to reach a higher energy level and can use that energy to break down organic contaminants through oxidation. Among photocatalysts' many applications are self-cleaning coatings for stain- and odor-resistant walls, floors, ceilings and furniture.

Stylianou, assistant professor of chemistry, led the study, which involved titanium dioxide photocatalysts derived from a metal-organic framework, or MOF.

Made up of positively charged metal ions surrounded by organic "linker" molecules, MOFs are crystalline, porous materials with tunable structural properties and nanosized pores. They can be designed with a variety of components that determine the MOF's properties.

Upon MOFs' calcination—high heating without melting—semiconducting materials like titanium dioxide can be generated. Titanium dioxide is the most commonly used photocatalyst, and it's found in the minerals anatase, rutile and brookite.

Stylianou and collaborators including Líney Árnadóttir of the OSU College of Engineering and William Stickle of HP discovered that anatase doped with nitrogen and sulfur was the best "two birds, one stone" photocatalyst for simultaneously producing hydrogen and degrading the heavily used herbicide glyphosate.

Glyphosate, also known as N-phosphonomethyl glycine or PMG, has been widely sprayed on agricultural fields over the last 50 years since first appearing on the market under the trade name Roundup.

"Only a small percentage of the total amount of PMG applied is taken up by crops, and the rest reaches the environment," Stylianou said. "That causes concerns regarding the leaching of PMG into soil and groundwater, as well it should—contaminated water can be detrimental to the health of every living thing on the planet. And herbicides leaching into water channels are a primary cause of water pollution."

Among an array of compounds in which hydrogen is found, water is the most common, and producing hydrogen by splitting water via photocatalysis is cleaner and more sustainable than the conventional method of deriving hydrogen—from natural gas via a carbon-dioxide-producing process known as methane-steam reforming.

Hydrogen serves many scientific and industrial purposes in addition to its energy-related roles. It's used in fuel cells for cars, in the manufacture of many chemicals including ammonia, in the refining of metals and in the production of plastics.

"Water is a rich hydrogen source, and photocatalysis is a way of tapping into the Earth's abundant solar energy for hydrogen production and environmental remediation," Stylianou said. "We are showing that through photocatalysis, it is possible to produce a renewable fuel while removing organic pollutants, or converting them into useful products."

The collaboration that included graduate student Emmanuel Musa, postdoctoral researcher Sumandeep Kaur and students Trenton Gallagher and Thao Mi Anthony also tested its photocatalyst against water tainted by two other often-used herbicides, glufosinate ammonium and 2,4-dichlorophenoxyacetic acid. It worked on water containing them as well—even water with those two compounds plus PMG.

More information: Emmanuel N. Musa et al, Two Birds, One Stone: Coupling Hydrogen Production with Herbicide Degradation over Metal–Organic Framework-Derived Titanium Dioxide, *ACS Catalysis* (2023). DOI: 10.1021/acscatal.3c00265

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