Metal-organic framework research makes key advance toward removing pesticide from groundwater

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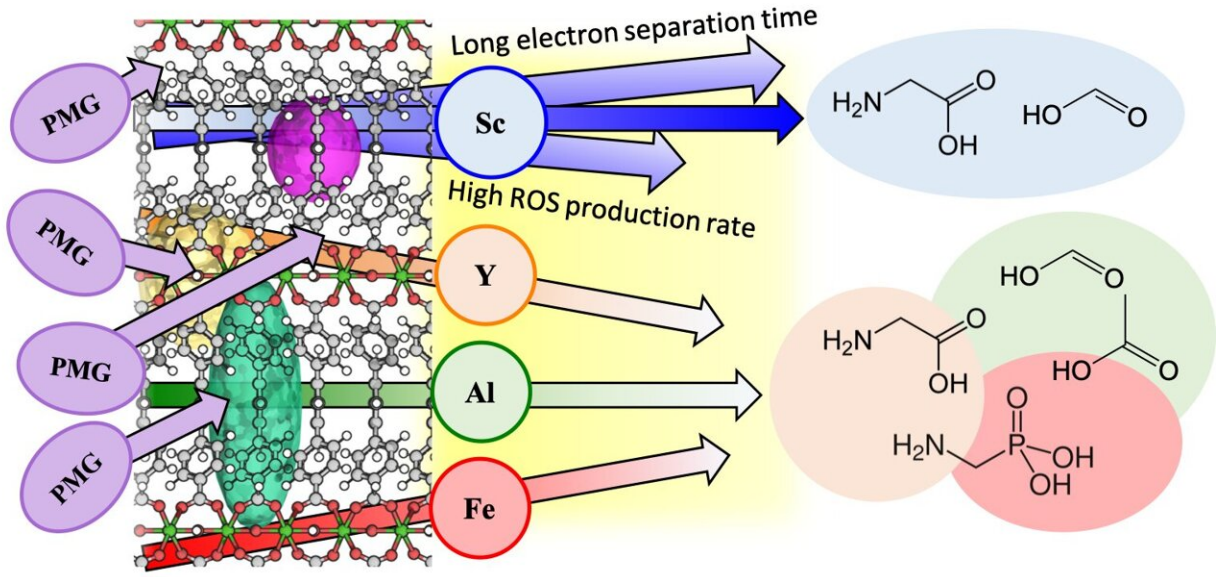

Synthesis of photoactive MOFs for the degradation of glyphosate. Combination of scandium and TBAPy ligand produces a MOF that photodegrades glyphosate into non-hazardous products. Credit: Oregon State University

Scientists led by an Oregon State University chemistry researcher are closing in on a new tool for tackling the global problem of weedkiller-tainted groundwater.

Kyriakos Stylianou of the OSU College of Science led an international team that identified a material known as a metal-organic framework, or MOF, that showed an ability to completely remove, and also break down, the oft-used herbicide glyphosate.

The MOF, one of four tested in a collaboration among scientists from Oregon State and Tiangong University in China, is based on scandium, chemical symbol Sc, and a carboxylate linker, TBAPy.

"When exposed to light for just five minutes, Sc-TBAPy eliminated 100% of glyphosate in water," Stylianou said. "In addition to its quicker adsorption and more efficient photodegradation of glyphosate compared to the other three TBAPy MOFs we looked at, it also degraded the glyphosate without producing a toxic acid, unlike the other three."

Findings were published in Nature Communications.

The MOFs in this experiment rely on photocatalysis. A catalyst is a substance that increases the rate of a chemical reaction without itself undergoing any permanent chemical change, and 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.

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.

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.

"Glyphosate and other herbicides are commonly used to safeguard farms from weed infestations, but the persistence of glyphosate in the environment has been associated with potential health effects on various living organisms including humans," Stylianou said.

"Only a small percentage of the total amount of PMG applied is taken up by crops, and herbicides leaching into water channels are a primary cause of water pollution. That means it's crucial to come up with innovative technologies and materials to combat this problem."

To uncover the PMG remediation abilities of Sc-TBAPy, Stylianou's lab collaborated with groups led by Chong Fang, Paul Ha Yeon Cheong and Hongliang Huang at Tiangong University. Stylianou said his collaborators provided key insights into the MOF's adsorption properties and photocatalytic activity.

A number of Oregon State graduate students also played important roles in the study, Stylianou said. Nan Chieh Chiu, Jacob Lessard and Emmanuel Musa led all the experiments and catalysis testing, Logan Lancaster investigated the optical properties of the materials being researched, and Clara Wheeler computationally examined their electronic properties.

OSU postdoctoral researcher Taylor Krueger, research associate Cheng Chen and graduate students Trenton Gallagher and Makenzie Nord also took part in the study.

More information: Chiu, N.C., et al. Elucidation of the role of metals in the adsorption and photodegradation of herbicides by metal-organic frameworks. *Nature Communications* (2024). DOI: 10.1038/s41467-024-45546-y

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