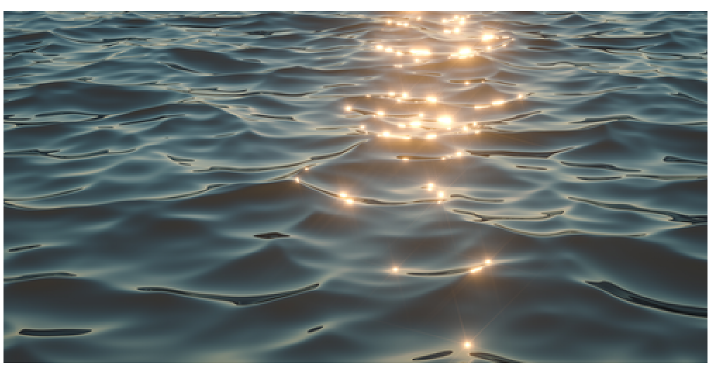
A Sunny Path to Green Hydrogen

A theoretical study of metal oxides identifies potential candidate materials for generating hydrogen fuel from water and sunlight.

By Michael Schirber

The dream of a green hydrogen economy rests on finding materials that can efficiently use sunlight to split water into hydrogen and oxygen. Ismaila Dabo from Pennsylvania State University and his colleagues have now performed a new theoretical search for these so-called photocatalysts, targeting a special type of metal oxide [**1**]. They found nine promising candidates, three of which have never previously been considered for water-splitting applications. The results highlight a material properties trade-off that might guide future photocatalyst development.

Hydrogen-powered cars and other vehicles could produce zero greenhouse-gas emissions. However, current hydrogen production relies on fossil fuels. Eco-friendly alternatives exist, but they must achieve water-splitting efficiencies of more than 10% to be cost competitive, Dabo says. To find those options, Dabo and his colleagues screened a database of metal oxides. The team targeted 109 oxides that contained both *p*-block (for example, indium and lead) and *s*-block (for example, cesium and calcium) elements, as previous work had found that this combination exhibits good water-splitting properties [**2**].



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The researchers performed band-structure calculations to identify target oxides with strong solar absorption. They then selected oxides on the basis of the materials' predicted electron-transfer properties, which are relevant to water-splitting reactions. They also looked at the materials' water stabilities, as an ideal material shouldn't degrade in water. Applying all these criteria, they found nine potential candidates, but the estimated efficiencies were all below 10%. Dabo and colleagues find that higher efficiency materials tend to be less stable in water. Considering this trade-off, they suggest structuring metal oxides with a highly efficient molecular core surrounded by a protective water-stable shell.

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REFERENCES

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