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Translating laboratory success into the large-scale implementation of photocatalytic overall water splitting

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A Viewpoint on the Frontiers in Science Lead Article

[Photocatalytic water splitting for large-scale solar-to-chemical energy conversion and storage](#)

Key points

- Sunlight-driven water splitting using particulate photocatalysts represents a promising and sustainable approach for the large-scale production of green hydrogen.
- Realizing higher solar-to-energy conversion efficiencies remains the primary focus to achieve the practical implementation of photocatalytic overall water splitting (OWS).
- Governments will play a crucial role in setting safety and environmental standards for the secure production, storage, and potential transport of surplus hydrogen, while investments in key infrastructure will further accelerate the adoption of photocatalytic OWS.

Introduction

As global energy consumption continues to rise, mitigating anthropogenic climate change demands the search for carbon-neutral energy sources to reduce our reliance on fossil fuels. Sunlight-driven water splitting using particulate photocatalysts represents a promising and sustainable approach for the large-scale production of green hydrogen. In their *Frontiers in Science* lead article, Hisatomi et al. (1) provide comprehensive yet succinct insights that lay a crucial foundation for the development of future hydrogen generation systems through particulate photocatalysis. They focus on key aspects such as photocatalyst stability, efficient hydrogen recovery, the safe design of reactor systems, and advancement in technologies for the separate production of hydrogen and oxygen from water. The authors have developed heterogeneous photocatalysts capable of efficiently splitting water

into hydrogen and oxygen in the near-ultraviolet region, highlighting the ideal structure and properties of cocatalyst/photocatalyst hybrid systems for overall water splitting (OWS) (2). Photocatalyst materials that split water with longer wavelengths of visible light have also been identified, but their apparent quantum yield (AQY) values remain low, mainly due to difficulties in fine-tuning their material properties (3). New techniques have been introduced to harness visible light for Z-scheme OWS by combining distinct photocatalysts. In addition, efforts are under way to develop reactors for large-scale applications and routes to extract pure hydrogen from oxyhydrogen mixture saturated with water vapor (4). Finally, the authors emphasize the importance of creating standardized methods for measuring solar-to-hydrogen (STH) efficiency, stressing that, given its current low technology-readiness level, leading researchers in photocatalysis should drive this initiative. The notable progress highlighted largely stems from over four decades of research in the field of OWS, with much of this work spearheaded by the authors themselves. At this pivotal juncture, where there is an unprecedented demand for scalable solar fuel production technologies, the influence of their research is anticipated to extend far beyond the scope of solar-driven catalysis and engineering, impacting a broad spectrum of industries. This viewpoint endeavors to spark a critical discussion on the challenges associated with translating laboratory success into the large-scale implementation of photocatalytic OWS.

Challenges of large-scale application of solar-driven OWS

Current maximum STH efficiencies for photocatalytic OWS systems are close to 1%; however, these are attained under laboratory conditions with constrained testing durations and remain considerably distant from real-world settings. In 2021, Domen et al. conducted a large-scale experiment (on a 100 m² scale) in which aluminum-doped strontium titanate (SrTiO₃) photocatalysts were immobilized on panels; this generated 600 L of hydrogen on a sunny day using a commercial separation membrane, reaching an optimal STH efficiency of 0.76%. This work highlights the potential for safely generating hydrogen on a large scale as well as the significant challenges facing its real-world application (4). At this stage, while the reported system can continuously produce hydrogen, the current efficiency levels are still insufficient to make this technology viable for large-scale hydrogen production. Thus, realizing higher solar-to-energy conversion efficiencies remains the primary focus to achieve practical implementation of photocatalytic OWS. In the search for suitable photocatalysts, an absorption limit over 600 nm coupled with an AQY value exceeding 60% are the necessary benchmarks to reach the goal of 10% STH efficiency (5). Conversely, band gap (E_g) reduction diminishes the ability of photocatalysts to facilitate redox reactions. Hence, it is crucial to strike a balance between lowering the E_g to extend light absorption and increasing it to generate stronger driving potential to promote

water splitting. Metal (oxy)nitrides and oxysulfides have been shown to be effective for photocatalytic OWS under light with wavelengths up to 600 nm. However, these photocatalysts generally display low efficiencies and limited chemical stability. Recent progress on metal-free carbon nitride photocatalysts for water splitting presents a promising alternative to these inorganic semiconductors (6, 7).

Enhancing solar energy conversion efficiency typically involves hybridizing photocatalysts with cocatalysts. These cocatalyst materials assist in carrier separation and transport while providing active sites and speeding up water-splitting reactions (8). However, most photocatalysts for OWS rely on rare or expensive materials, such as platinum-group metals and other toxic inorganic components, as cocatalysts. This dependence on scarce resources limits scalability and increases costs, thereby creating sustainability issues. For instance, Rh@CrO_x (or Rh-Cr mixed oxide) and ruthenium/iridium-based oxides, which both involve rare metals, serve as cocatalysts for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in these systems. Another concern is that the CrO_x shell could potentially leach Cr⁶⁺ ions during prolonged photo-irradiation, leading not only to catalyst deactivation but also environmental harm and health risks (9). Although these rare and hazardous materials are used in minimal amounts, their inclusion still presents economic and environmental challenges. Given the limited production capacities of noble metals, widespread adoption of photocatalytic OWS technology could cause substantial market price increases due to rising demand and expectations. As highlighted in the lead article, precious cocatalyst materials can be recycled using standard metal recovery processes once the photocatalyst's lifecycle is complete. Nonetheless, there is a pressing need to develop cost-effective, earth-abundant cocatalysts that offer performance similar to noble metals to eliminate the need for additional recycling steps. If using noble metals is necessary, one possible solution is to alloy at least one platinum-group metal with another or with a more widely available metal. Bimetallic systems can alter their electronic structure, resulting in a catalytic performance that surpasses that of their individual parent metals (10).

Similar to the previous concerns with cocatalysts, although immobilizing photocatalysts on substrates or sheets has demonstrated scalability and effectiveness in advancing OWS, attention must also be directed toward the disposal problems related to future water-splitting systems. Although the scalability and efficiency of photocatalysts are well established, it is of equal importance to address their environmental impact. Again, the key question is whether photocatalysts and other essential components in these systems can be restored or regenerated. More specifically, the photocatalysts need to endure multiple operational cycles with only minor losses in efficiency. Developing recycling protocols that do not involve dismantling the entire system could be an excellent solution to minimize operating and maintenance costs. Materials approaching the end of their service life must be disposed of correctly to mitigate environmental and health risks.

Lastly, one of the biggest challenges in the practical implementation of photocatalytic OWS systems is integrating them with existing energy infrastructure, especially when it comes

to safely storing and transporting generated hydrogen to avoid contamination and operational risks. Hisatomi et al. emphasize that, after hydrogen is separated and recovered, it can be used in various catalytic reactions to create other value-added chemicals and fuels. This approach is more practical for safe handling and transportation than managing hydrogen as the final product (1). In this context, governments will play a crucial role in setting safety and environmental standards for the secure production, storage, and potential transport of surplus hydrogen. Investments in key infrastructure by governments will further accelerate the adoption of photocatalytic OWS. Strong political commitment is crucial for implementing regulations and policies, such as setting hydrogen production standards and providing tax incentives, to make green hydrogen more competitive—similar to the approach taken with other emerging technologies. For example, Germany's National Hydrogen Strategy envisions a comprehensive hydrogen infrastructure by 2030. This involves plans to build over 1,800 km of new and repurposed pipelines dedicated to hydrogen transport, constructing an extensive network to support the country's transition to green hydrogen. This infrastructure development is part of Germany's initiative to spearhead hydrogen innovation and meet its climate targets (11). Similarly, in 2020, the Japanese government introduced the Green Growth Strategy through Achieving Carbon Neutrality in 2050. The strategy positions hydrogen as a key technology for reducing carbon emissions in various sectors such as energy, transportation, and manufacturing. To accelerate hydrogen technology development, the government provides subsidies, tax incentives, and research funding. It also encourages collaboration with private companies to bring innovative hydrogen technologies to market and scale up their production (12, 13).

Conclusion

In summary, although significant progress has been made in photocatalytic OWS technology, challenges remain, particularly in achieving higher STH efficiencies and addressing both economic and environmental sustainability concerns. The development of cost-effective, earth-abundant photocatalysts and cocatalysts, alongside standardized methods for efficiency measurement, will be crucial for the future scalability of these systems. Furthermore, the environmental impact of the future water-splitting systems must be thoroughly investigated in order to ensure their sustainability, minimize potential ecological risks, and create efficient recycling and disposal protocols that comply with

environmental safety regulations. With continued research, political support, and partnerships between industries, the shift from laboratory breakthroughs to scalable photocatalytic hydrogen production systems holds promise for contributing to global decarbonization efforts.

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