Rare-Earth Doped Transition Metal–Organic Frameworks for Photocatalytic Hydrogen Evolution: Applications and Integration in the Global Hydrogen Economy

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Abstract

Global decarbonization efforts have intensified interest in hydrogen (H_2) as a clean energy carrier, yet the practical value of any hydrogen-splitting technology depends on how the hydrogen produced is ultimately deployed across power, transport, and industrial sectors. Building on our previously reported rare-earth doped transition metal–organic framework (RE–TM–MOF) system for photocatalytic hydrogen evolution, this perspective examines in detail the downstream application landscape for hydrogen generated via photocatalytic and electrocatalytic water-splitting routes. We describe six major application domains — power generation, transportation, industrial decarbonization, chemical feedstock, energy storage, and decentralized solar-to-hydrogen generation — and compare photocatalytic MOF-based routes against established electrolysis technologies in terms of efficiency, cost, and infrastructure readiness. We argue that while electrolysis remains the nearer-term scalable pathway, RE–TM–MOF and related photocatalytic architectures are positioned to fill a complementary niche in low-infrastructure, high-insolation deployment scenarios, pending further pilot-scale validation.

Keywords

Hydrogen Evolution; Water Splitting; RE–TM–MOF; Green Hydrogen Applications; Photocatalysis; Hydrogen Economy

1. Introduction

Hydrogen has re-emerged as a cornerstone candidate for global decarbonization, with 147 countries having adopted net-zero targets as of December 2024 [1]. Despite this policy momentum, current global hydrogen demand, standing at approximately 100 million tonnes per year, remains overwhelmingly fossil-derived: roughly 62% from natural gas, 28% from coal, and the remainder as a by-product of refining, while low-emission hydrogen accounts for under 1% of total output [2]. This demand is itself heavily concentrated in two legacy industrial uses — ammonia synthesis (approximately 45%) and oil refining (approximately 40%) — rather than the emerging sectors, such as steelmaking, long-haul transport, and power generation, that are frequently cited as hydrogen's future growth markets [3].

Photocatalytic water splitting, the subject of our previous mechanistic study on RE–TM–MOF systems [4], offers a route to hydrogen production that bypasses the electricity-generation step entirely, using solar photons to drive proton reduction directly. This is mechanistically distinct from, and potentially complementary to, the electrolysis-based routes (alkaline, PEM, and solid oxide) that currently dominate green hydrogen deployment. However, a material system is only as valuable as the application it ultimately serves. This paper extends our earlier mechanistic work by examining, in detail, where hydrogen produced by photocatalytic and

electrocatalytic splitting routes is actually used today, where demand is growing, and where a decentralized, MOF-based photocatalytic system may offer genuine advantages over grid-dependent electrolysis.

2. Recap of the RE–TM–MOF Photocatalytic System

As detailed in our companion study [6], the RE–TM–MOF architecture combines a $Ru(phen)_3^{2+}$ photosensitizer, silver-based transition metal nodes acting as electron mediators, and rare-earth dopants (Nd^{3+} or Ce^{3+}) that trap charge carriers and suppress electron–hole recombination. Upon visible-light irradiation, electrons generated at the Ru-phenanthroline core are transferred through the Ag nodes and stabilized by the rare-earth centers before participating in proton reduction to hydrogen. The defining practical feature of this design, for the purposes of the application analysis that follows, is that it requires no external electrical input: light is the sole energy source. This distinguishes it fundamentally from electrolysis-based hydrogen production, where renewable or grid electricity must first be generated, transmitted, and converted before splitting occurs.

3. Applications of Hydrogen Evolution and Splitting Technologies

3.1 Power Generation and Fuel Cells

Hydrogen's role in power generation centers on fuel cells, which convert stored hydrogen back into electricity. Proton exchange membrane fuel cells (PEMFCs), the most common type for distributed and mobile power, typically operate at electrical efficiencies of 40–60%, while solid oxide fuel cells (SOFCs) reach 50–60% and, when integrated into combined heat and power (CHP) configurations that recover waste heat, total system efficiencies can exceed 80% [7]. Reversible fuel cell systems, which can both consume and regenerate hydrogen, are increasingly deployed alongside electrolyzers at wind and solar installations to buffer intermittent renewable output, storing surplus generation as hydrogen and reconverting it to electricity during low-output periods.

3.2 Transportation Sector

Fuel cell electric vehicles (FCEVs) extend beyond passenger cars to buses, trains, and increasingly heavy-duty trucks and maritime vessels, all of which emit only water vapor at the point of use. However, global refueling infrastructure remains limited to a few hundred stations concentrated mainly in Europe and Japan, with each new station costing an estimated USD 1–2 million depending on capacity [8]. Because passenger-vehicle hydrogen adoption faces direct competition from battery-electric vehicles, current market analysis suggests a substantial share of hydrogen demand growth in transport will instead be directed toward heavy-duty and long-haul applications, where hydrogen's higher energy density and rapid refueling times offer a more defensible advantage over batteries [9].

Maritime and aviation applications represent a further, more nascent frontier. Decarbonizing maritime shipping is closely tied to International Maritime Organization emissions targets, and hydrogen-derived fuels (including ammonia, discussed further in Section 3.5) are among the leading candidates for deep-sea vessels where battery-electric propulsion remains impractical at present energy densities. In aviation, hydrogen's potential role is still primarily at the demand-modeling and feasibility stage: recent simulation studies of hydrogen-fueled aviation project meaningful CO_2 emission reduction potential but also highlight substantial uncertainty in future demand and price dynamics, underscoring that this application remains considerably further from commercial deployment than road transport or shipping.

3.3 Industrial Decarbonization: Steel and Ammonia

Ammonia synthesis alone accounts for roughly 45% of existing global hydrogen demand, making the conversion of ammonia production from fossil-derived to green hydrogen one of the single largest decarbonization levers available [3]. Steelmaking represents a newer but rapidly watched application: Sweden's HYBRIT (Hydrogen Breakthrough Ironmaking Technology) initiative has demonstrated hydrogen-based direct reduction of iron ore at pilot scale, though as of 2024 hydrogen-based steel production still accounts for less

than 0.2% of global output, with only a handful of countries — Sweden, Germany, Japan, South Korea, China, the United States, and Australia — having progressed beyond laboratory trials to pilot demonstration facilities.

3.4 Chemical Feedstock and Refining

Oil refining consumes approximately 40% of current global hydrogen output, primarily for hydrocracking and hydrodesulfurization processes that upgrade crude fractions and remove sulfur contaminants [10]. As refineries face pressure to lower the carbon intensity of these processes, green hydrogen substitution for feedstock use represents a comparatively low-risk decarbonization pathway, since it requires no change to downstream refining chemistry — only to the hydrogen source itself.

3.5 Energy Storage and Grid Balancing (Power-to-X)

The "power-to-X" (P2X) concept converts surplus renewable electricity into hydrogen for later use as fuel, chemical feedstock, or synthetic fuel precursor, absorbing excess generation during peak renewable output and releasing stored energy during periods of high demand. However, the round-trip efficiency of a full hydrogen storage cycle — electrolysis, storage, and reconversion via fuel cell — is estimated at only 30–40%, compared to 70–90% for battery storage, positioning hydrogen as better suited to long-duration and seasonal storage rather than short-term grid balancing. Ammonia, containing 17.8 wt% hydrogen by mass, is gaining particular attention as a hydrogen carrier for this purpose, since it can be liquefied and transported using existing global maritime infrastructure and later "cracked" back to hydrogen near the point of use, though the endothermic cracking process (300–500°C) and the need for selective catalysts remain active areas of research.

3.6 Decentralized Solar-to-Hydrogen Generation — The RE–TM–MOF Niche

Photoelectrochemical (PEC) water splitting, which like RE–TM–MOF systems converts sunlight directly to hydrogen using semiconductor photoelectrodes, remains at an early technology readiness level (TRL 4–5). State-of-the-art laboratory PEC systems have reached 19.3% solar-to-hydrogen (STH) efficiency, though most operate in the 4–12% range, with levelized costs estimated at USD 5.78–23.27 per kilogram of hydrogen [3, 6]. RE–TM–MOF-type systems occupy a related but distinct position: because they require no electrolyzer stack, grid connection, or high-pressure balance-of-plant equipment, they are structurally suited to small-footprint, capital-light deployment in remote or off-grid locations, in contrast to the large centralized hubs favored by electrolysis. This positions the technology as a potential complement — rather than a competitor — to gigawatt-scale electrolyzer projects such as Saudi Arabia's NEOM Green Hydrogen Project, which targets production costs as low as USD 1.50 per kilogram using abundant regional solar resources at industrial scale [11]. High-insolation, infrastructure-sparse regions of the Middle East, North Africa, and South Asia represent plausible early deployment contexts for MOF-based photocatalytic hydrogen microgrids, though this application case remains conceptual pending pilot-scale efficiency and durability data.

4. Comparative Analysis of Hydrogen Production Routes

Table 1 summarizes the principal hydrogen-splitting routes discussed above, situating the RE–TM–MOF system relative to established electrolysis technologies and photoelectrochemical alternatives. It should be emphasized that efficiency and cost figures for the RE–TM–MOF route are not yet established at pilot or commercial scale; the comparison is included to frame the technology's intended niche rather than to claim performance parity with mature routes.

Route	Energy Input	Efficiency	Approx. Cost (USD/kg H_2)	Infrastructure Need	Best-Fit Application
Alkaline Electrolysis (AWE)	Grid / renewable electricity	50–80%	~3.9–12.8 (wind); 4.0–12.0 (solar)	High — electrolyzer stack + grid tie-in	Large industrial hydrogen hubs

PEM Electrolysis	Renewable electricity	60–70%	Comparable to AWE, higher CAPEX	High but dynamically flexible	Transport-linked, variable-load sites
Solid Oxide Electrolysis (SOEC)	Electricity + waste heat	>90% (stack, lab-scale)	Higher CAPEX, lower OPEX at scale	Requires industrial waste-heat source	Steelmaking, ammonia co-location
Photoelectrochemical (PEC)	Direct sunlight	4–12% typical; 19.3% lab record	~5.78–23.27	Low external infrastructure; low TRL (4–5)	Research / pilot demonstration
RE–TM–MOF Photocatalysis (this work)	Direct sunlight	Not yet quantified at scale — early-stage	Not yet established	Minimal — no electrolyzer stack required	Decentralized, off-grid, remote microgrids

5. Challenges for RE–TM–MOF-Based Applications at Scale

Several challenges must be resolved before RE–TM–MOF systems can move from mechanistic demonstration toward the application contexts described above. Stability in aqueous and prolonged-irradiation environments remains a central concern for MOF architectures generally, as noted in our earlier structural analysis. The cost and supply-chain availability of rare-earth dopants such as neodymium and cerium also constrain large-area deployment, particularly relative to the earth-abundant nickel- and iron-based catalysts now favored in alkaline electrolyzers. Notably, this is not a challenge unique to photocatalytic systems: PEM electrolyzers face an analogous constraint through their reliance on platinum-group metals such as iridium and platinum, whose scarcity and cost are widely cited as a barrier to gigawatt-scale PEM deployment. This suggests that noble- and rare-metal dependency is a shared frontier for next-generation hydrogen catalysts generally, rather than a liability specific to MOF-based approaches.

6. Future Outlook

Building on the design strategies outlined in our earlier work, integration of RE–TM–MOF architectures with two-dimensional conductive materials such as graphene or MoS_2 may help address the low electrical conductivity that limits pristine MOF systems, while machine-learning-guided screening of dopant and linker combinations could accelerate the search for stable, cost-effective compositions. On the application side, coupling decentralized photocatalytic hydrogen generation with ammonia-based carrier infrastructure could allow hydrogen produced at remote, high-insolation sites to be transported using existing global shipping networks, extending the reach of off-grid photocatalytic systems well beyond their point of generation. Realizing this outlook will also depend on broader policy progress: the current absence of a harmonized, internationally recognized green hydrogen certification framework continues to create uncertainty for investors and adopters across all production routes, not only photocatalytic ones.

7. Conclusion

Hydrogen's application landscape spans power generation, transportation, heavy industrial decarbonization, chemical feedstock use, and grid-scale energy storage, with legacy industrial demand (ammonia and refining) still dominating current consumption. RE–TM–MOF-type photocatalytic systems are not, at present, a drop-in replacement for electrolysis at the gigawatt scale needed to serve these established markets. Rather, they represent a promising complementary pathway for decentralized, infrastructure-light hydrogen generation in high-insolation, off-grid, or remote industrial-cluster settings. Realizing this potential will require dedicated pilot-scale studies establishing solar-to-hydrogen efficiency and long-term stability data directly comparable to the electrolysis and PEC benchmarks reviewed here.

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