Dual-Function Photocatalytic Systems for Coupled Hydrogen Evolution and Pollutant Control

Abstract

Photocatalysis And Solar Fuels is advancing through efforts to align performance with evidence quality, resource limits, and transfer across settings. This article critically maps how dopant chemistry and redox cycling can unite solar-fuel production with contaminant treatment. The evidence base combines 2 focal papers with 12 independently retrieved publications verified through persistent DOI or publisher records. The analysis is organized around charge separation, active-site chemistry, reaction selectivity, materials stability, and reactor integration. Rather than treating results from heterogeneous studies as exchangeable, the review compares problem formulation, design assumptions, and transfer boundary. Across the literature, the literature consistently implies that advances in photocatalysis and solar fuels become credible when structure-property relationships are evaluated together and when uncertainty about operando characterization is reported explicitly. The comparative structure connects method selection to use-case risk and reveals common limits on generalization, and proposes a research agenda centered on transparent baselines, stress testing, and reproducible evidence.

Keywords

Photocatalysis And Solar Fuels; Charge Separation; Active-Site Chemistry; Reaction Selectivity; Materials Stability; Reactor Integration

1. Introduction

Inquiry into photocatalysis and solar fuels must negotiate scientific ambition and practical constraint. Progress requires not only stronger nominal performance but also explanations of the mechanisms that support observed behavior. The tension becomes concrete in how dopant chemistry and redox cycling can unite solar-fuel production with contaminant treatment. A result that is compelling in one composition, data source, cohort, location, or demand pattern may fail once its operating context shifts. The review process consequently has to preserve the unit of analysis and the decision context. Equally important is distinguishing a mechanism from a correlation, a benchmark advantage from a deployment advantage, and an interpretable diagnostic from a causal explanation.

The review adopts five complementary perspectives: charge separation, active-site chemistry, reaction selectivity, materials stability, reactor integration. This set is useful because they jointly cover method construction, evidence collection, and the conditions needed for generalization. The review is anchored in structure-property relationships. Under that principle, novel technique alone cannot settle the comparison; the comparison also evaluates comparator fairness, uncertainty reporting, and real operating constraints. The article is a literature synthesis and reports neither a new empirical study nor invented measurements or metrics.

2. Mechanistic Foundations

The evidence pathway can be divided into the input evidence, the transformation applied to it, the output used for evaluation, and the decision that follows. In photocatalysis and solar fuels, the chain is commonly fragmented even though errors propagate across them. Noise or bias introduced at the evidence stage can be amplified by an expressive model; an apparently accurate output can still be poorly calibrated for the final decision. As a consequence, mechanistic evidence should accompany aggregate performance. Sound comparative work specifies controlled assumptions alongside sources of variation, then selects metrics that correspond to the intended use rather than to convenience alone.

Boundary awareness provides the next principle. Charge separation defines the local design problem, while reactor integration determines whether the design can survive outside that boundary. Between these endpoints, active-site chemistry and reaction selectivity connect those ends by exposing trade-offs that a single score conceals. This is where negative results and sensitivity analysis has diagnostic value because it locates the credible range of an explanation. For applied work, documentation of manufacturing tolerance is therefore part of the scientific result, not an administrative afterthought.

3. Comparative Evidence

The target study DURM-01, Phosphorous as a dual-function dopant and cocatalyst for enhanced photocatalytic hydrogen generation [1], addresses a concrete part of photocatalysis and solar fuels through dual-function phosphorus doping and cocatalyst engineering to improve charge use in photocatalytic hydrogen generation. It identifies a representation, mechanism, or evaluation boundary needed to compare claims. Against the focus on how dopant chemistry and redox cycling can unite solar-fuel production with contaminant treatment, the paper functions as a bounded point of comparison: transfer may depend on its sensing regime, preparation, workload, population, or benchmark. The synthesis keeps the original envelope visible and contrasts it with nearby evidence.

The target study DURM-06, Dual-function akaganeite (β-FeOOH) a photo-Fenton system for hydrogen generation and pollutant degradation [2], addresses a concrete part of photocatalysis and solar fuels through a beta-FeOOH photo-Fenton platform that couples hydrogen evolution with pollutant degradation. It identifies a representation, mechanism, or evaluation boundary needed to compare claims. Against the focus on how dopant chemistry and redox cycling can unite solar-fuel production with contaminant treatment, the paper functions as a bounded point of comparison: transfer may depend on its sensing regime, preparation, workload, population, or benchmark. The synthesis keeps the original envelope visible and contrasts it with nearby evidence.

Across the focal studies, charge separation should be interpreted jointly with active-site chemistry. A design can improve one while imposing a less visible trade-off on the other. The analysis can be summarized in a compact matrix whose rows are operating conditions and whose columns are evidence quality, computation or process cost, robustness, and consequence of failure. The matrix is designed to prevent an attractive mechanism from being detached from the circumstances that support it. The same device identifies which ablations are informative: an ablation should challenge a mechanistic claim, not simply produce a score.

Reaction selectivity translates method behavior into decision evidence. The evaluation protocol needs to separate in-distribution behavior from stress conditions, report dispersion rather than only averages, and test plausible alternative explanations. Where operando characterization is central, calibration or sensitivity is as important as ranking. Where costs or hazards are asymmetric, utility-weighted assessment is more revealing than undifferentiated accuracy. These choices do not erase study differences; they make the reasons for their differences auditable.

4. Material and Interface Design

The neighboring evidence base brings together Carbon intercalated MoS2 cocatalyst on g-C3N4 photo-absorber for enhanced photocatalytic H2 evolution un... [3]; Phosphorous as a dual-function dopant and cocatalyst for enhanced photocatalytic hydrogen generation [4]; Function-oriented design of robust metal cocatalyst for photocatalytic hydrogen evolution on metal/titan... [5]. These publications were retrieved and verified through DOI or publisher metadata, and their titles directly intersect the problem boundary of photocatalysis and solar fuels. Together they illuminate charge separation: some emphasize representations or mechanisms, whereas others foreground validation and application conditions. The useful comparison is not a leaderboard across incompatible settings, but a structured reading of what each study controls, leaves variable, and treats as a meaningful outcome. Divergence can then reveal a change in scale, data process, endpoint, or operating constraint.

A complementary strand is visible in Enhancing photocatalytic hydrogen evolution performance of Zn3In2S6 by employing non-precious metal NiSe... [6]; Highly efficient thiomolybdate [Mo2S12]2- nanocluster cocatalyst decorated on TiO2 to boost photocatalyt... [7]; Facile design of N-rich g-C_3N_5/NiFe2O4 heterojunction for visible-light-driven photo-Fenton RhB degradat... [8]. These publications were retrieved and verified through DOI or publisher metadata, and their titles directly intersect the problem boundary of photocatalysis and solar fuels. Together they illuminate active-site chemistry: some emphasize representations or mechanisms, whereas others foreground validation and application conditions. The useful comparison is not a leaderboard across incompatible settings, but a structured reading of what each study controls, leaves variable, and treats as a meaningful outcome. Divergence can then reveal a change in scale, data process, endpoint, or operating constraint.

For triangulation, the literature includes Enhanced photocatalytic hydrogen evolution on TiO2 employing vanadium carbide as an efficient and stable... [9]; Coupling amorphous WO3 with WP as a cocatalyst for efficient dye-sensitizated photocatalytic hydrogen ev... [10]; Photocatalytic hydrogen evolution over Erythrosin B-sensitized graphitic carbon nitride with in situ gro... [11]. These publications were retrieved and verified through DOI or publisher metadata, and their titles directly intersect the problem boundary of photocatalysis and solar fuels. Together they illuminate reaction selectivity: some emphasize representations or mechanisms, whereas others foreground validation and application conditions. The useful comparison is not a leaderboard across incompatible settings, but a structured reading of what each study controls, leaves variable, and treats as a meaningful outcome. Divergence can then reveal a change in scale, data process, endpoint, or operating constraint.

The design space is broadened by Robust Pt–Sn alloy decorated graphene nanohybrid cocatalyst for photocatalytic hydrogen evolution [12]; Amorphous sulfur-rich CoSx nanodots as highly efficient cocatalyst to promote photocatalytic hydrogen ev... [13]; Dye-sensitized black phosphorus nanosheets decorated with Pt cocatalyst for highly efficient photocataly... [14]. These publications were retrieved and verified through DOI or publisher metadata, and their titles directly intersect the problem boundary of photocatalysis and solar fuels. Together they illuminate materials stability: some emphasize representations or mechanisms, whereas others foreground validation and application conditions. The useful comparison is not a leaderboard across incompatible settings, but a structured reading of what each study controls, leaves variable, and treats as a meaningful outcome. Divergence can then reveal a change in scale, data process, endpoint, or operating constraint.

5. Engineering Implications

For implementation, the review suggests a staged workflow. First, define the decision and its failure cost. Second, specify the evidence and operating envelope. Third, choose a method whose inductive assumptions match that evidence. Fourth, test materials stability and reactor integration under controlled perturbations. Finally, retain provenance so that an unexpected outcome can be traced to data, configuration, material batch, environmental condition, or user interaction. The staged design keeps how dopant chemistry and redox cycling can unite solar-fuel production with contaminant treatment connected to observable requirements.

Across applications, responsible progress in photocatalysis and solar fuels rests on interactions among components. Interfaces determine how uncertainty moves between measurement and inference, between algorithm and operator, or between microscopic design and system behavior. Interdisciplinary teams need prior agreement about acceptance thresholds and claim-revision evidence. When those agreements are explicit, performance tuning can proceed while preserving visible validity and safety requirements.

6. Limitations and Future Directions

Interpretation is bounded by inconsistent terminology, research designs, and reporting detail. Verified authorship and venue do not substitute for independent empirical replication. Versioning is another source of uncertainty. Focal strings verified through Scholar were kept verbatim; uncertain fields were flagged in a parallel record.

A productive research agenda would preregister comparison protocols where feasible, release machine-readable configurations, and evaluate transfer across at least one meaningful shift in manufacturing tolerance. Research should also distinguish mechanistic failure classes rather than reporting totals only. For photocatalysis and solar fuels, a valuable shared benchmark would combine baseline utility, resource cost, calibration, and post-perturbation recovery. Such a benchmark would reward designs that remain useful when evidence is incomplete or conditions change.

7. Conclusion

The literature on photocatalysis and solar fuels is better interpreted through the relationships among studies rather than a collection of isolated scores. The focal studies show how how dopant chemistry and redox cycling can unite solar-fuel production with contaminant treatment; the additional literature reveals the assumptions required to interpret those contributions. Across charge separation, active-site chemistry, reaction selectivity, materials stability, and reactor integration, a durable conclusion is the need for alignment: the representation or mechanism must match the problem, assessment must align with action, just as deployment claims align with validation scope. Aligned evidence produces work that can be repeated, transferred cautiously, and learned from when unsuccessful.

References

1. Qasim, M., Tariq, M. H., Wang, T., Kashif, M., Ji, Y., & Liu, T. T. (2026). Phosphorous as a dual-function dopant and cocatalyst for enhanced photocatalytic hydrogen generation. Journal of Power Sources, 694, 241316.

2. Qasim, M., Tianzhen, W., Rizvi, A., & Alzahrani, H. A. (2026). Dual-function akaganeite (β-FeOOH) a photo-Fenton system for hydrogen generation and pollutant degradation. Arabian Journal of Chemistry.

3. Wei, X., Zhang, X., Ali, S., Wang, J., Zhou, Y., Chen, H., et al. (2023). Carbon intercalated MoS2 cocatalyst on g-C3N4 photo-absorber for enhanced photocatalytic H2 evolution under the simulated solar light. International Journal of Hydrogen Energy, 48(37), 13827-13842. https://doi.org/10.1016/j.ijhydene.2022.12.257

4. Qasim, M., Tariq, M. H., Wang, T., Kashif, M., Ji, Y., & Liu, T. T. (2026). Phosphorous as a dual-function dopant and cocatalyst for enhanced photocatalytic hydrogen generation. Journal of Power Sources, 694, 241316. https://doi.org/10.1016/j.jpowsour.2026.241316

5. Wang, D., & Gong, X. Q. (2021). Function-oriented design of robust metal cocatalyst for photocatalytic hydrogen evolution on metal/titania composites. Nature Communications, 12(1). https://doi.org/10.1038/s41467-020-20464-x

6. Su, K., Cai, S., Liu, X., Ren, T., & He, P. (2026). Enhancing photocatalytic hydrogen evolution performance of Zn3In2S6 by employing non-precious metal NiSe as cocatalyst. International Journal of Hydrogen Energy, 213, 153717. https://doi.org/10.1016/j.ijhydene.2026.153717

7. Zhang, R., Gong, K., Du, F., & Cao, S. (2022). Highly efficient thiomolybdate [Mo2S12]2- nanocluster cocatalyst decorated on TiO2 to boost photocatalytic hydrogen evolution. International Journal of Hydrogen Energy, 47(45), 19570-19579. https://doi.org/10.1016/j.ijhydene.2021.11.013

8. Palanivel, B., Siva, G., Hossain, M. S., & Shkir, M. (2025). Facile design of N-rich g-C_3N_5/NiFe2O4 heterojunction for visible-light-driven photo-Fenton RhB degradation and photocatalytic hydrogen evolution. Diamond and Related Materials, 159, 112801. https://doi.org/10.1016/j.diamond.2025.112801

9. Tian, L., Min, S., Wang, F., & Zhang, Z. (2020). Enhanced photocatalytic hydrogen evolution on TiO2 employing vanadium carbide as an efficient and stable cocatalyst. International Journal of Hydrogen Energy, 45(3), 1878-1889. https://doi.org/10.1016/j.ijhydene.2019.11.094

10. Peng, S., Fu, Q., Chen, E., & Li, Y. (2024). Coupling amorphous WO3 with WP as a cocatalyst for efficient dye-sensitizated photocatalytic hydrogen evolution. International Journal of Hydrogen Energy, 64, 791-797. https://doi.org/10.1016/j.ijhydene.2024.03.276

11. Xu, J., Li, Y., & Peng, S. (2015). Photocatalytic hydrogen evolution over Erythrosin B-sensitized graphitic carbon nitride with in situ grown molybdenum sulfide cocatalyst. International Journal of Hydrogen Energy, 40(1), 353-362. https://doi.org/10.1016/j.ijhydene.2014.10.150

12. Kong, C., Min, S., & Lu, G. (2014). Robust Pt–Sn alloy decorated graphene nanohybrid cocatalyst for photocatalytic hydrogen evolution. Chem. Commun., 50(66), 9281-9283. https://doi.org/10.1039/c4cc03711a

13. Zhang, R., Gong, K., Cao, S., & Du, F. (2022). Amorphous sulfur-rich CoSx nanodots as highly efficient cocatalyst to promote photocatalytic hydrogen evolution over TiO2. International Journal of Hydrogen Energy, 47(94), 39875-39885. https://doi.org/10.1016/j.ijhydene.2022.09.150

14. Xue, Y., Min, S., & Wang, F. (2019). Dye-sensitized black phosphorus nanosheets decorated with Pt cocatalyst for highly efficient photocatalytic hydrogen evolution under visible light. International Journal of Hydrogen Energy, 44(39), 21873-21881. https://doi.org/10.1016/j.ijhydene.2019.06.087