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Molecular and materials design for efficient solar energy conversion: a review of photochemical technologies

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The inexorable rise in global energy demand, coupled with the pressing imperative to mitigate anthropogenic climate change, has catalyzed unprecedented research effort into renewable energy sources. Photochemistry, the study of chemical reactions initiated by light, is fundamentally shaping this landscape, particularly in solar energy conversion. This review provides a comprehensive and critical analysis of current trends in photochemistry that are directly enabling the development of next-generation renewable energy technologies. We delve into the operational principles, recent advances in materials, and persistent challenges across three pivotal photochemical systems: photoelectrochemical (PEC) devices, artificial photosynthetic systems for solar fuel production, and dye-sensitized solar cells (DSSCs). The discourse highlights the strategic shift from scarce, noble-metal-based components towards earth-abundant alternatives, the integration of molecular and solid-state systems in hybrid architectures, and the critical pursuit of long-term operational stability. While significant progress has been made in understanding charge transfer dynamics and tailoring material properties at the nanoscale, the path to widespread commercialization necessitates continued interdisciplinary innovation to overcome efficiency, durability, and scalability hurdles. This critical evaluation of the current state of the art aims to illuminate both the remarkable achievements and the fundamental scientific questions that remain at the forefront of photochemical energy research.

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compounds, BODIPY, BOPHY, Photocatalysis, developments of synthetic methodologies for the synthesis of novel organic compounds with unique theoretical and biological applications.

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1 Introduction

The Sun delivers a continuous and prodigious flux of energy to Earth, dwarfing humanity's total power consumption. Harnessing this resource through photochemical conversion, the transformation of light energy into storable chemical fuels or electricity, represents a paramount scientific challenge in the world. The process begins when a photon is absorbed by a material, promoting an electron to a higher-energy, excited state. This excited state is a crucial, energy-rich intermediate. The core objective of artificial energy conversion is to harness this transient energy to drive thermodynamically uphill chemical reactions, such as water splitting or carbon dioxide (CO₂)

reduction, before it is lost as heat or light.¹⁻⁴ Modern photochemical research is characterized by a powerful convergence of disciplines, including synthetic chemistry, materials science, nanoscience, and electrochemistry. These fields are directed at optimizing three sequential steps involving broad-spectrum light absorption, efficient charge separation, and rapid catalytic turnover.⁵⁻⁷ These steps manifest in several promising technological platforms, each with unique trade-offs between efficiency, stability, and cost. The overarching goal across all platforms is to develop technologies that are not only efficient but also economically viable and sustainable, requiring a holistic assessment from material sourcing to end-of-life recycling.^{8,9}

The fundamental photochemical process involves three sequential steps, *viz*, the absorption of a photon to create an excited state, the efficient separation of charge carriers (electrons and holes), and the directed use of these energetic charges to drive useful chemical reactions, such as water splitting or CO₂ reduction. Optimizing each step, while minimizing parasitic energy losses, requires a deep, synergistic understanding of molecular design, materials science, and interface engineering. A dominant and necessary trend is the strategic shift from scarce, noble-metal-based components (*e.g.*, Ru, Ir, Pt) toward catalysts and sensitizers made from earth-abundant elements (*e.g.*, Cu, Fe, Ni, Co).^{10,11} Also, the convergence of disciplines has given rise to several promising technological platforms. Photoelectrochemical (PEC) cells aim to directly produce hydrogen or hydrocarbons from sunlight and water.¹²⁻¹⁵ DSSCs offer a versatile, lower-cost photovoltaic alternative with unique aesthetic and diffuse-light capabilities.¹⁶⁻¹⁸ Concurrently, the field of artificial photosynthesis seeks to orchestrate molecular components into integrated systems that mimic nature's efficiency.¹⁹⁻²² While significant progress has been made, the



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research employs first-principles calculations and molecular modeling to guide the rational design of novel nanomaterials and molecular catalysts, with a focus on green organic transformations and sustainable oxidation processes. This synergistic approach provides deep mechanistic insights and accelerates the discovery of efficient catalytic systems.

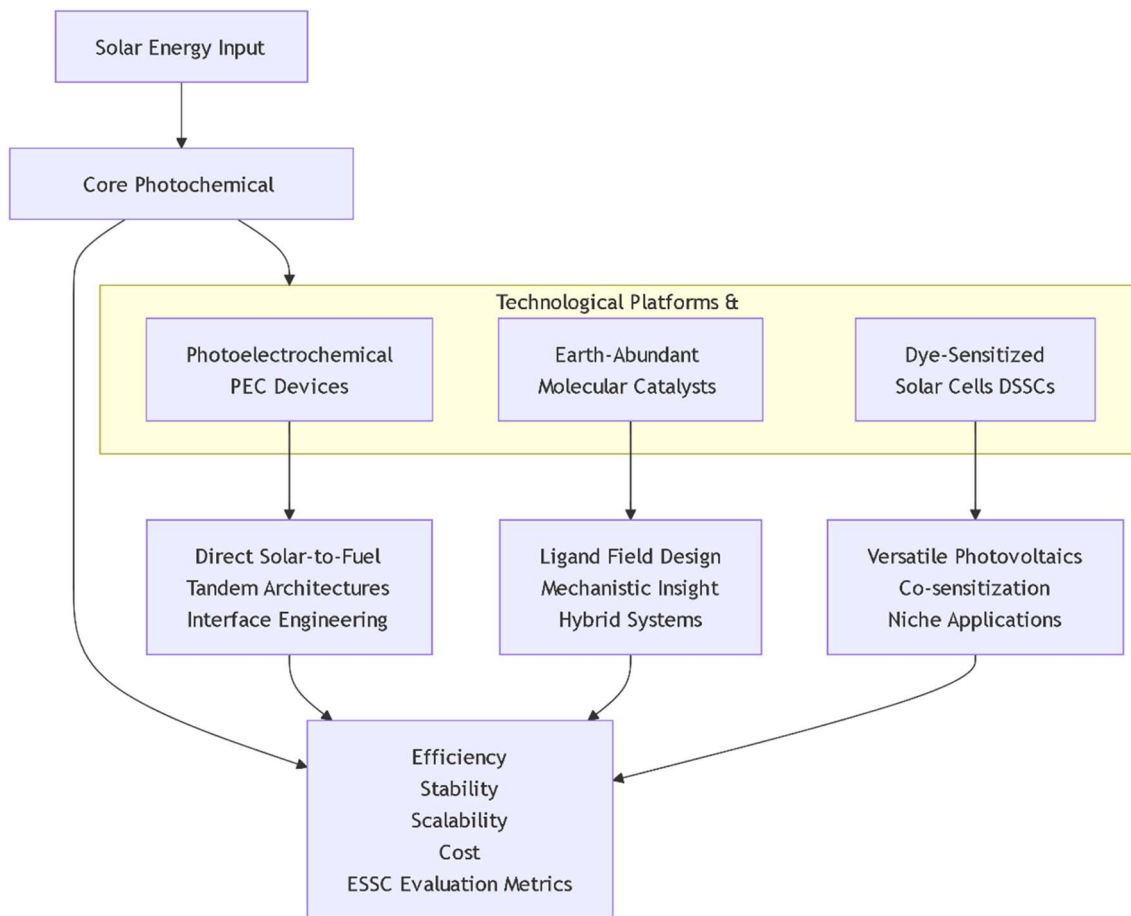


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Scheme 1 Conceptual map of photochemical energy conversion pathways.

path to commercialization hinges on simultaneously optimizing efficiency, stability, scalability, and cost, a complex, multi-parameter challenge.^{23–25}

While numerous reviews exist on individual technologies,^{26–29} such as PEC cells, artificial photosynthesis, or DSSCs, this review article provides a unified and critical perspective that bridges device-level engineering with molecular-level design (Scheme 1). The work is a critical evaluation of the progression from fundamental discovery to integrated system performance across these platforms, employing a consistent framework of efficiency, stability, scalability, and cost (ESSC) metrics to assess commercial viability. The article is structured to first examine advances at both the device architecture and molecular catalyst levels. It then explores applications in solar fuels and photovoltaics, before synthesizing the prevailing challenges and future research vectors. This holistic narrative, which moves from materials to devices to systems-level analysis, explicitly connects macroscopic engineering with molecular science under a common evaluative lens.

2 Advances in photochemical technologies: from materials to devices

The field of photochemical technology is undergoing a profound transformation, driven by a convergence of

innovative materials design and sophisticated device engineering. This evolution progresses from the molecular-scale synthesis of novel photoactive compounds to their integration into functional, scalable architectures for energy conversion and catalysis.^{30–34} Therefore, this section discusses advances at the device architecture level, focusing on integrated systems for direct solar-to-fuel conversion, followed by an examination of progress at the molecular and materials level, detailing the design of next-generation photocatalysts.^{35–38}

2.1 Device-level architectures for direct solar fuel production

2.1.1 PEC systems: principles and photoanode challenges. PEC cells represent an integrated device strategy for the direct conversion of sunlight into chemical fuels, most notably hydrogen *via* water splitting. A typical PEC cell consists of one or two semiconductor photoelectrodes (a photoanode and/or a photocathode) immersed in an aqueous electrolyte (Fig. 1). The fundamental processes are: (i) light absorption generating electron–hole pairs, (ii) charge separation driven by the built-in electric field at the semiconductor–liquid junction, (iii) surface catalysis for the oxygen evolution reaction (OER) at the photoanode and the hydrogen evolution reaction (HER) at the photocathode.^{39–43}

The photoanode, responsible for the OER, is often the performance-limiting component due to the reaction's kinetic



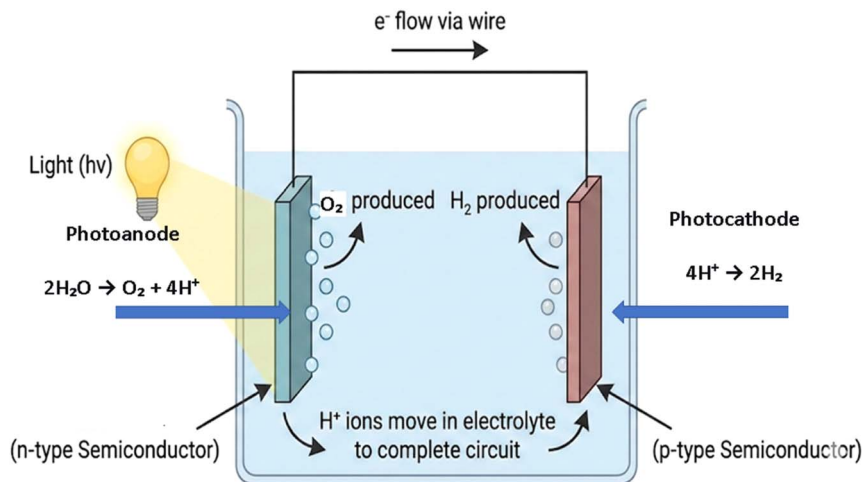


Fig. 1 PEC representation for water splitting.

sluggishness and thermodynamic demands.⁴⁴ Among visible-light-responsive metal oxides, Bismuth Vanadate (BiVO_4 , bandgap ~ 2.4 eV) has emerged as a benchmark photoanode material. However, its performance is hampered by poor charge carrier mobility and rapid surface recombination. Research strategies to overcome these limitations involve nanostructuring to shorten charge transport paths and the creation of heterojunctions (e.g., $\text{BiVO}_4/\text{WO}_3$) to enhance charge separation *via* built-in fields. Crucially, surface modification with OER co-catalysts like cobalt phosphate (Co-Pi) or nickel-iron oxyhydroxide (NiFeOOH) is essential to passivate surface traps and accelerate the reaction kinetics.^{45–48} Recent insights emphasize the need for kinetic synergy, where the hole transfer rate from the semiconductor bulk to the catalyst must outpace recombination (Fig. 2).

2.1.2 Photocathode development and tandem architectures. For the HER, efficient photocathodes are required. While

p-type silicon and indium phosphide (InP) show high performance, their cost and susceptibility to photocorrosion in electrolytes limit scalability. This has spurred research into alternative materials like copper-based chalcogenides (e.g., $\text{Cu}_2\text{ZnSnS}_4$, (CZTS)) and stable metal oxide heterostructures.^{49,50} A paradigm-shifting approach to overcoming the efficiency limits of single-absorber cells is the development of integrated tandem PEC cells (Fig. 3). These devices combine a high-bandgap photoanode (e.g., BiVO_4 , perovskite), and a low-bandgap photocathode (e.g., silicon (Si), Copper–Indium–Gallium–Selenide (CIGS)) in a monolithic stack. The top absorber captures high-energy photons for the OER, while transmitting lower-energy photons to the bottom absorber for the HER. This spectral splitting minimizes thermalization and transmission losses, enabling solar-to-hydrogen (STH) efficiencies exceeding 10%, a key benchmark for practicality.^{51,52} Realizing such devices demands exquisite interface engineering

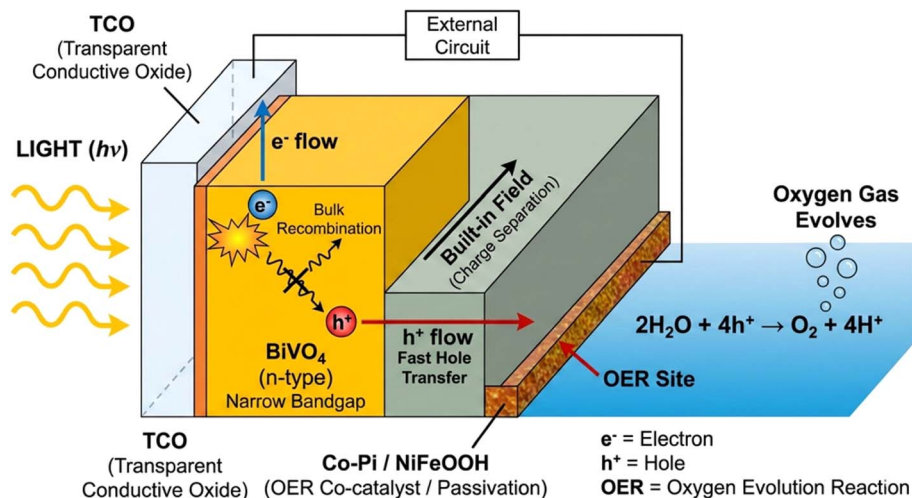


Fig. 2 Strategies for enhancing BiVO_4 photoanode performance, nanostructuring to reduce bulk recombination, and formation of a heterojunction (e.g., with WO_3) for improved charge separation, along with surface modification with an OER co-catalyst (e.g., Co-Pi, NiFeOOH) to accelerate kinetics and passivate surface states.



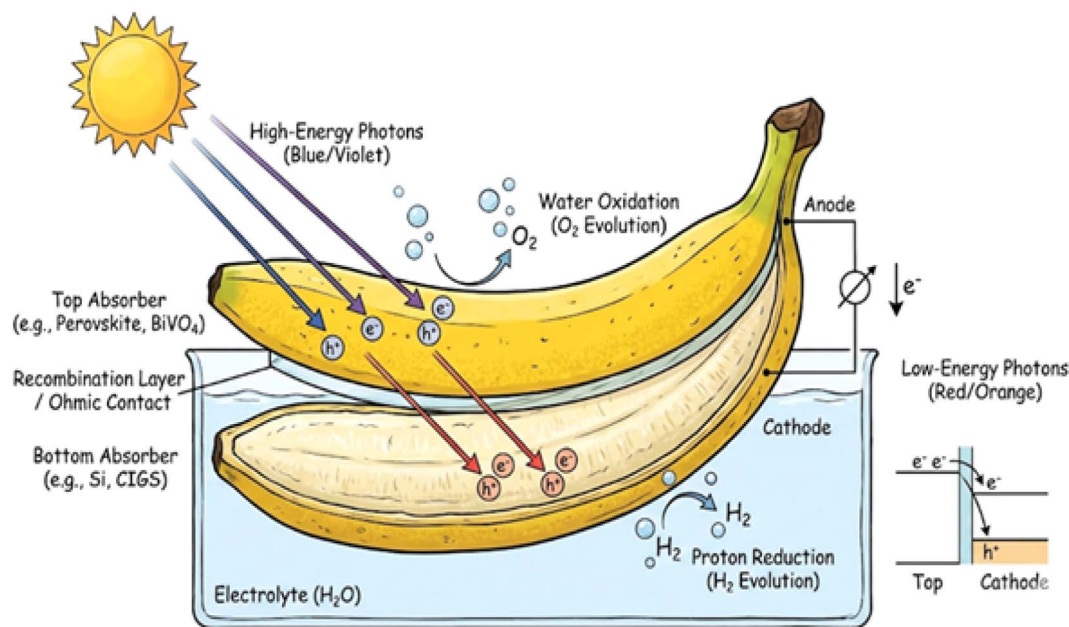


Fig. 3 Operating principle (banana illustration) of a tandem-PEC cell. A high-bandgap top absorber (e.g., perovskite, BiVO_4) harvests high-energy photons for water oxidation, while transmitting lower-energy photons to a low-bandgap bottom absorber (e.g., Si, CIGS) for proton reduction, enabling efficient use of the full solar spectrum.

between multiple functional layers (transport, protection, catalytic) to minimize parasitic recombination at every junction. Table 1 summarizes the performance metrics and key characteristics of representative state-of-the-art photoelectrodes.

2.2 Molecular and materials design for photocatalysis

2.2.1 Evolution from noble metals to earth-abundant complexes. Molecular photocatalysts are discrete compounds that absorb light and facilitate multi-electron redox reactions. Historically dominated by complexes of rare metals like ruthenium (Ru) and iridium (Ir), the field is undergoing a necessary paradigm shift towards earth-abundant first-row transition metals (e.g., Cu, Fe, Co, Ni) to ensure sustainability and scalability.^{53,54} Copper(i) complexes have emerged as successful replacements for Ru-based photosensitizers. They can form

metal-to-ligand charge-transfer (MLCT) excited states with competitive redox potentials and lifetimes, often enhanced by thermally activated delayed fluorescence (TADF).^{55,56} Meanwhile, Iron complexes are being re-evaluated through sophisticated ligand design that raises the energy of destructive metal-centered (MC) states, allowing access to luminescent and reactive charge-transfer states. For catalytic functions, nickel and cobalt complexes are displacing platinum and iridium/ruthenium oxides as cores for HER and OER catalysts, respectively (Fig. 4). Their activity is fine-tuned through precise ligand modifications.^{57–59}

2.2.2 Mechanistic insights and catalyst design principles. The transition to earth-abundant metals is driven by a deeper mechanistic understanding enabled by advanced spectroscopic tools like ultrafast transient absorption spectroscopy and time-

Table 1 State-of-the-art photoelectrodes for solar water splitting

Material/system	Type	Bandgap (eV)	Function	STH efficiency (%)	Key features/challenges	Ref.
$\text{BiVO}_4/\text{WO}_3$ heterojunction with Co-Pi	Photoanode	~2.4	OER	~6.2 (with bias)	Good visible light absorption; requires co-catalyst; modest stability	97 and 98
Ta_3N_5 with NiFeOOH	Photoanode	~2.1	OER	~3.5 (with bias)	Narrow bandgap; suffers from severe self-oxidation	99
p-Si with Pt/ TiO_2 protection	Photocathode	1.1	HER	~10 (in tandem)	High efficiency; requires complex protection layers	51
Sb_2Se_3 with Pt	Photocathode	~1.2	HER	~3.5	Earth-abundant; emerging material; stability under study	51
Perovskite/ BiVO_4 – Si tandem	Tandem cell	Varies	Full WS	>20 (PEC-PV)	Record efficiency; complex multi-layer fabrication; long-term stability is a major concern	100
CIGS-based tandem	Tandem cell	Varies	Full WS	~10–15	Good stability potential; scalable thin-film technology	101



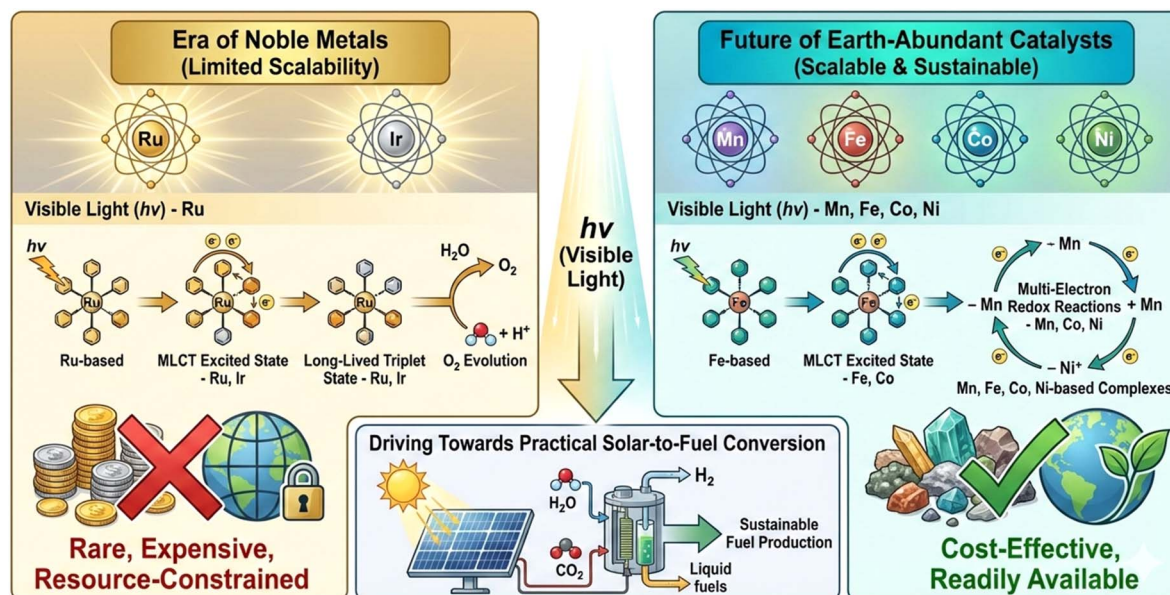


Fig. 4 Evolution of molecular photocatalysts from noble metals to earth-abundant alternatives (Cu, Fe).

resolved X-ray spectroscopy (Fig. 5). These techniques map excited-state dynamics on femtosecond timescales, revealing competing deactivation pathways.^{60–62} The key design principle is the rational manipulation of excited-state energetics through ligand architecture. The goal is to create a single, long-lived excited state with sufficient redox potential by controlling the ordering of ligand-field (LF), MLCT, and ligand-centered (LC) states. For iron complexes, this involves designing strong-field ligands to raise the energy of MC states above the desired CT state. This principles-based, predictive approach, supported by computational chemistry, is moving the field from serendipitous discovery to targeted engineering.^{63–66}

3 Applications in renewable energy: from laboratory concepts to integrated systems

3.1 Artificial photosynthesis: closing the carbon cycle

Artificial photosynthesis is a technological process designed to mimic the natural reactions by which plants convert sunlight, water, and carbon dioxide into energy-storing molecules. Its primary goal is to use solar energy to chemically reduce captured CO₂, combining it with protons from water to synthesize sustainable fuels and chemical feedstocks. By sourcing carbon from atmospheric or industrial CO₂ emissions, this process aims to create a circular economy, effectively closing the anthropogenic carbon cycle. A key objective is to achieve solar-to-chemical conversion efficiencies that significantly surpass the relatively low efficiency of natural photosynthesis in plants.⁶⁷ The technology fundamentally relies on advanced light-induced molecular transformations, typically driven by specialized photocatalysts or photoelectrochemical systems (Fig. 6).

These systems often employ semiconductor materials or molecular complexes to absorb light, generate charges, and catalyze the critical reactions of water oxidation and CO₂ reduction. Target outputs include energy-dense fuels such as hydrogen (from water splitting), methane, or methanol, which serve as renewable carriers for storing intermittent solar energy. As such, artificial photosynthesis represents a direct application of photochemical principles for sustainable energy storage and is a major focus of contemporary research in renewable energy technologies.^{68,69}

3.1.1 CO₂ reduction and solar fuels. The photochemical reduction of CO₂ seeks to convert this greenhouse gas into useful, energy-rich chemicals. Target products include

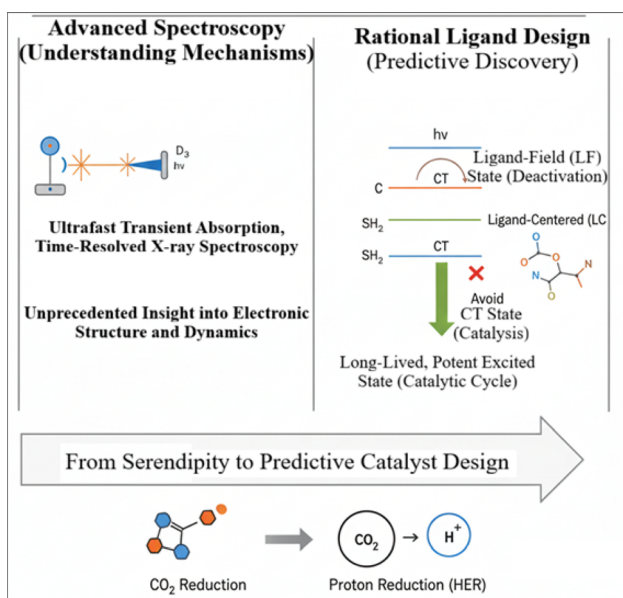


Fig. 5 Representation of catalyst design principles and mechanism.



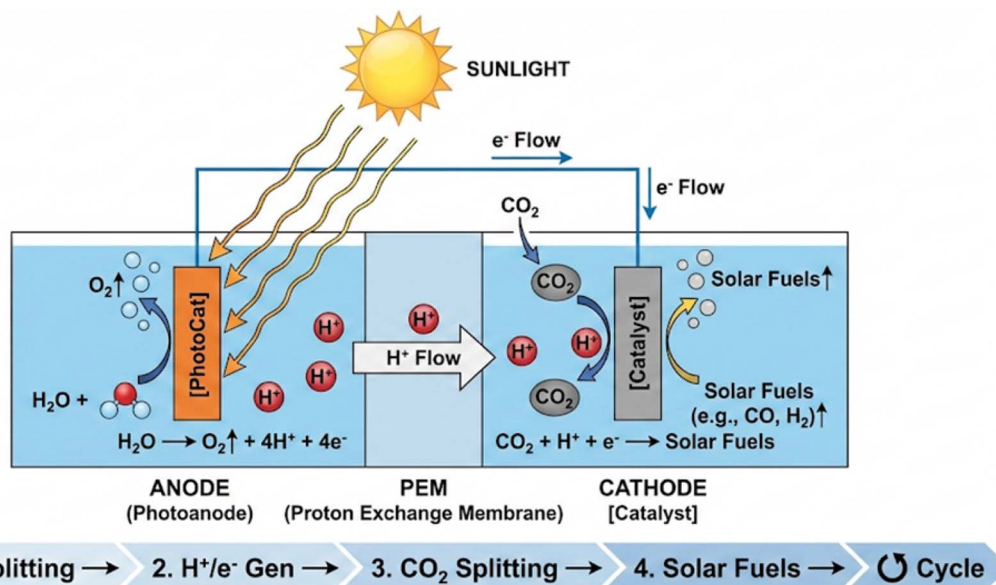


Fig. 6 The artificial photosynthesis cycle: solar energy drives the reduction of CO₂ to fuels (e.g., CO, CH₃OH) and the oxidation of water to O₂, mimicking natural photosynthesis but aiming for higher efficiency and different outputs.

fundamental feedstocks such as carbon monoxide, formic acid, and methanol. A central scientific challenge is the inherent thermodynamic stability and kinetic inertness of the CO₂ molecule.^{70–72} As illustrated in Fig. 7, overcoming this barrier demands the development of highly efficient and selective catalysts. These catalysts must manage complex multi-proton-coupled electron transfer processes to drive the reactions forward effectively. These catalysts are essential because reducing a single CO₂ molecule to a product like methanol requires multiple electrons and protons to be added in a specific sequence. The process involves unstable intermediate chemical species that must be carefully stabilized. Therefore, the catalyst's role is to lower the energy barriers for each step and orchestrate the precise coupling of protons and electrons at the right time. Effective management of this intricate sequence

is what determines the reaction's overall speed, energy efficiency, and selectivity for the desired fuel product. While early work used Re(I) and Ru(II) complexes, current research prioritizes earth-abundant molecular catalysts based on Mn(I), Co(II), and Ni(II). A key strategy for enhancing performance is second coordination sphere engineering, where pendant functional groups (e.g., phenolic protons) act as proton relays or stabilize key intermediates, thereby improving both activity and selectivity (Table 2).^{73,74}

3.1.2 Hybrid and heterogenized systems. To address challenges such as difficult catalyst recovery and limited stability in purely homogeneous systems, researchers are developing hybrid photochemical assemblies. These systems strategically integrate well-defined molecular catalysts, known for their precise tunability, with solid-state light absorbers, such as

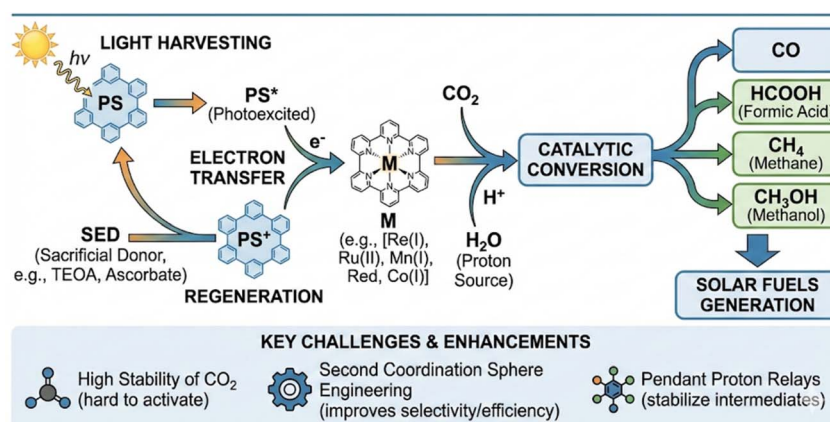


Fig. 7 Simplified mechanism of photocatalytic CO₂ reduction using a molecular catalyst (M), highlighting key steps: photoexcitation of a sensitizer (PS), electron transfer to the catalyst, CO₂ binding/activation, and proton-coupled electron transfers leading to product release.



Table 2 Representative molecular catalysts for photocatalytic CO₂ reduction

Catalyst (metal)	Major Product(s)	Selectivity (%)	Turnover number (TON)	Key design feature	Ref.
[Re(bpy)(CO) ₃ Cl]	CO	>90	~300	Seminal noble-metal catalyst; operates at low overpotential	71
[Mn(bpy)(CO) ₃ Br]	CO	>95	~1100	Earth-abundant alternative to Re; similar bipyridine ligand	82
Co-porphyrin with pendant phenol groups	CO/HCOOH	80 (CO)	~5000	Second-sphere proton relay enhances rate and selectivity	71 and 74
Ni(cyclam) ²⁺ derivatives	CO/H ₂	Varies	~10 ⁵	High durability; product selectivity sensitive to conditions	68
Fe-porphyrin/covalent organic framework (COF) hybrid	CO	>99	~1500	Heterogenized system; combines molecular specificity with solid-state stability	75 and 76

semiconductors or metal–organic frameworks (MOFs). This design merges the superior activity and selectivity of molecular species with the structural durability and efficient charge-separation properties of solid materials.^{75,76} For instance, a molecular catalyst based on ruthenium or manganese can be directly grafted onto the surface of a semiconductor like Cadmium Sulfide (CdS) or a carbon nitride sheet. This intimate contact drastically shortens the distance photogenerated charges must travel, minimizing wasteful recombination. Consequently, this architectural integration enhances the quantum efficiency of the overall process, directly boosting the yield of solar fuels. Thus, the hybrid approach represents a powerful strategy to harness the best features of both molecular and solid-state systems for practical artificial photosynthesis (Fig. 8).

3.2 DSSCs: versatility and aesthetic appeal

In 1991, Brian O'Regan and Michael Grätzel achieved a groundbreaking development by inventing the DSSC, a new type of photovoltaic device.⁷⁷ Their key innovation was the use of a nanostructured, wide-bandgap titanium dioxide semiconductor coated with light-absorbing dye molecules, which

effectively separated the processes of light absorption and charge transport.^{78,79} This biomimetic “artificial leaf” architecture offered a lower-cost alternative to conventional silicon solar cells and established foundational principles for modern photoelectrochemical and photocatalytic research. Such advancements have occupied a unique niche, offering advantages in manufacturing cost, performance under diffuse light, and design flexibility (color, transparency) compared to conventional silicon PV.⁸⁰

3.2.1 Operational principles and component optimization.

The core of a DSSC is a mesoporous film of a wide-bandgap semiconductor (typically Titanium dioxide, TiO₂) sensitized by a monolayer of a light-absorbing dye. Upon excitation, the dye injects an electron into the TiO₂ conduction band (Fig. 9). The oxidized dye is regenerated by a redox shuttle (e.g., I⁻/I₃⁻ or Co³⁺/Co²⁺ complexes) in the electrolyte, which is itself reduced at a platinum or carbon-based counter electrode.^{81,82}

The components of dye-sensitized solar cells have undergone significant and focused development. Early dye sensitizers were primarily ruthenium-based polypyridyl complexes, such as N3 and N719. Research later shifted toward metal-free organic dyes featuring a donor- π -acceptor, or D- π -A, molecular

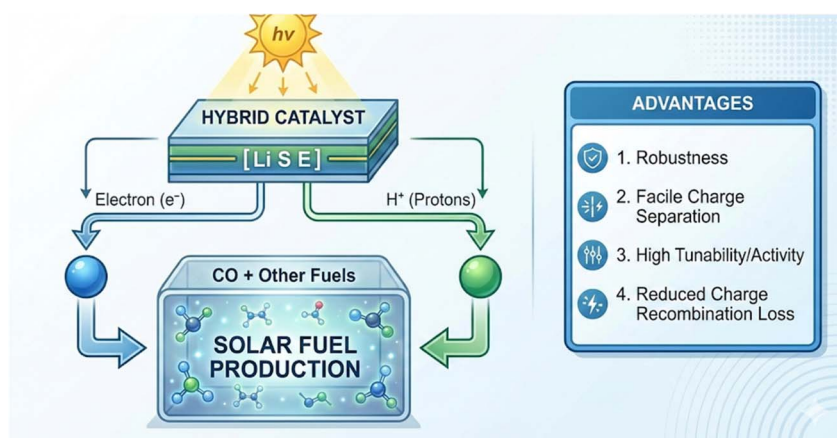


Fig. 8 Advanced features of hybrid-photocatalytic systems for CO₂ reduction.



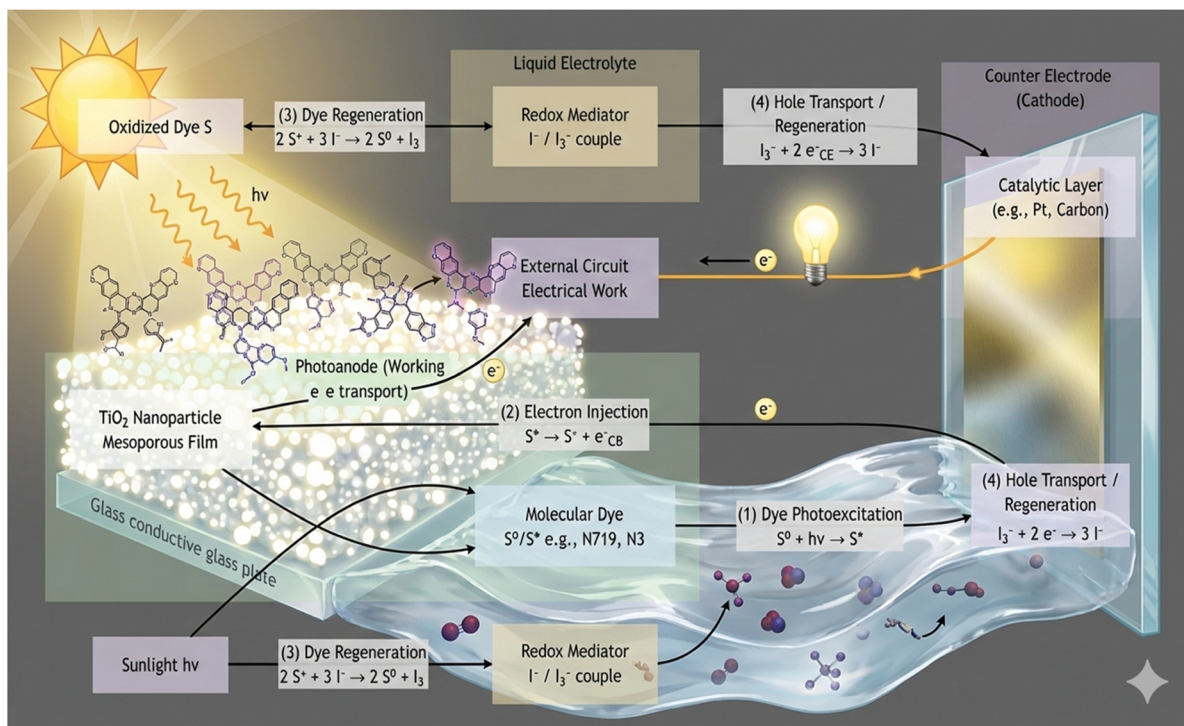


Fig. 9 Operational principle of a DSSC. Key steps: (1) dye photoexcitation, (2) electron injection into TiO_2 , (3) regeneration of the oxidized dye by the redox mediator (I^-/I_3^- shown), (4) hole transport to the counter electrode.

structure. Another important class of advanced sensitizers is porphyrin-based dyes, which have helped achieve record power conversion efficiencies exceeding 14%.^{81,83} Alongside dyes, the electrolyte system has also evolved substantially from its original form. The traditional liquid electrolyte relied on the iodide/triiodide (I^-/I_3^-) redox couple as a charge mediator. To address issues like corrosion and durability, alternative redox mediators such as cobalt ($\text{Co}^{3+/2+}$) complexes were introduced. Another major advancement has been the move toward solid-state hole-transport materials, like 2,2',7,7'-tetrakis(*N,N*-di-*p*-methoxyphenylamine)-9,9'-spirobifluorene (spiro-OMeTAD), to replace liquid electrolytes. These changes in electrolyte design improve

the long-term stability of the solar cell. They also simplify the sealing process of the device, which is crucial for practical manufacturing and deployment.^{84,85}

3.2.2 Emerging directions and critical perspective. Current research focuses on co-sensitization strategies using complementary dyes to achieve panchromatic absorption, and on developing DSSCs for niche applications where their properties are paramount: building-integrated photovoltaics (BIPV) due to color and transparency, and indoor light harvesting for powering low-energy Internet of Things (IoT) devices.^{84,86} While the emergence of perovskite solar cells (which originated from DSSC research) has overshadowed DSSCs in the pursuit of peak

Table 3 Evolution of key components in DSSCs

Component	Early generation (~1991–2005)	State-of-the-art/emerging	Key advantages/status	Ref.
Sensitizer	Ru-polypyridyl complexes (N3, N719)	Metal-free organic D- π -A dyes (e.g., Y123); porphyrins (e.g., SM315)	Lower cost, higher molar absorptivity; PCE >14% achieved	81 and 83
Redox mediator	Iodide/triiodide (I^-/I_3^-)	Cobalt complexes (e.g., $[\text{Co}(\text{bpy})_3]^{3+/2+}$); copper complexes; solid HTMs (spiro-OMeTAD)	Higher photovoltage; better stability; enables solid-state DSSCs	88 and 85
Counter electrode	Platinum (Pt) on FTO	Carbon materials (graphene, CNTs); conductive polymers (PEDOT)	Lower cost, comparable catalytic activity for I_3^- reduction	85
Primary application focus	General outdoor PV	BIPV; indoor light harvesting for IoT	Leverages aesthetic flexibility and superior diffuse-light performance	84 and 86



efficiency, DSSCs retain unique advantages in durability under low-light and high-temperature conditions, and in aesthetic integration. The evolutionary assessment has been organized in Table 3.

4 Challenges and future perspectives

Despite the compelling progress detailed herein, the path to the widespread deployment of photochemical energy technologies is fraught with scientific and engineering challenges that demand continued focused research. The paramount challenge across all systems is the simultaneous optimization of efficiency, stability, and cost, the pivot of energy technology. For PEC water splitting, corrosion of semiconductor materials in harsh aqueous electrolytes remains a fundamental issue, necessitating the development of more robust protection layers that are both conductive and optically transparent. In artificial photosynthesis, the selectivity of CO₂ reduction towards a single, high-value product remains elusive, and the scaling of these systems to industrially relevant levels is a monumental task that involves not only chemical engineering but also the development of efficient product separation and purification processes. For DSSCs and molecular systems, long-term photostability and thermal stability of the organic and molecular components under continuous operational stress are critical concerns.^{87–89}

Future research directions will likely involve several convergent strategies. The use of advanced computational modeling, including density functional theory (DFT) and machine learning, will accelerate the discovery and design of new materials with tailored optoelectronic properties. The exploration of novel nanoscale and heterostructured architectures, such as core-shell nanoparticles, nanowire arrays, and two-dimensional materials, will provide new avenues for controlling light-matter interactions and charge transport pathways.^{90–93} The integration of biological components, such as enzymes, with synthetic photochemical systems is an emerging frontier that could lead to highly selective and efficient hybrid biocatalysts for fuel production. Finally, a greater emphasis on life-cycle analysis (LCA) and techno-economic assessment (TEA) at the research stage will be crucial for guiding the development of technologies that are not only scientifically impressive but also economically viable and environmentally sustainable on a global scale.^{94–96}

5. Conclusions

In conclusion, the dynamic field of photochemistry is in the midst of a profoundly transformative era. This transformation is largely propelled by the world's urgent and escalating need for sustainable energy solutions. The collective research we have surveyed represents a strategic and coordinated front against energy challenges. One dominant trend is the meticulous refinement of photoelectrochemical (PEC) devices. These devices are engineered for the direct production of solar fuels, such as hydrogen. Through PEC systems, sunlight directly facilitates the splitting of water molecules. This process aims to store solar energy in a clean, chemical form. Concurrently, a significant

paradigm shift is moving research away from rare, expensive catalysts. The new focus is squarely on earth-abundant molecular photocatalysts. Catalysts based on iron, copper, or cobalt are now at the forefront of this investigation. This shift is crucial for ensuring the economic viability and widespread adoption of future technologies. Furthermore, scientists are engaging in sophisticated mimicry of natural photosynthesis. This bio-inspired approach seeks to replicate the elegance and efficiency of plant-based systems. Researchers are designing synthetic complexes that emulate natural light-harvesting antennae. They are also constructing molecular assemblies that mimic catalytic reaction centers found in nature. The goal is to achieve the high selectivity and low energy waste characteristic of biological systems. Alongside this, the persistent optimization of dye-sensitized architectures continues unabated. DSSCs are being steadily improved for better performance and stability. Novel organic and perovskite-sensitized materials are broadening the spectral absorption of these devices. Engineering of mesoporous semiconductor scaffolds enhances electron injection and transport. These four interconnected trends collectively represent a powerful, multifaceted assault on solar energy conversion. Each approach complements the others, creating a rich and diverse research landscape. Underpinning all these advancements is a deepening, atom-level understanding of fundamental mechanisms. Scientists are now unraveling complex photophysical pathways with unprecedented detail. The precise sequence of events following photon absorption—from excitation to charge separation is being mapped. Similarly, the intricate catalytic mechanisms that facilitate fuel-forming reactions are being decoded. This fundamental knowledge is critically enabled by a suite of cutting-edge characterization tools. Ultrafast laser spectroscopy captures events occurring on femtosecond time-scales. Advanced X-ray techniques provide atomic-resolution snapshots of catalysts in action. Sophisticated computational modeling predicts properties and guides the design of new materials. However, the path forward is not without its significant and persistent hurdles. Improving the overall efficiency of photon-to-fuel conversion remains a paramount challenge. The long-term durability of materials under constant photochemical stress is a major concern. Scaling laboratory breakthroughs to industrially relevant, manufacturable dimensions is a formidable task. The integration of components into robust, working systems adds another layer of complexity. Despite these challenges, the relentless pace of innovation in the field is undeniable. New discoveries and incremental improvements are reported in the literature virtually every day. This progress is fueled by a collaborative spirit that unites the global research community. Chemists, physicists, materials scientists, and engineers are working in concert across disciplines. This collaboration bridges the gap between molecular discovery and functional device engineering. Therefore, there is strong and justified cause for optimism about the future. The continued interplay between fundamental molecular science and applied research will be pivotal. Insights from quantum mechanics directly inform the synthesis of new light-absorbing molecules. Advanced materials engineering then translates these molecules into stable, functional films and devices. Finally, systems-level



integration assembles these components into practical, operational technology. This virtuous cycle of discovery and application will undoubtedly yield transformative results. It will lead to the next generation of efficient and affordable photochemical technologies. These future technologies will move beyond the laboratory to impact the global energy landscape. They are poised to solidify the role of sunlight as a cornerstone of our energy portfolio. Ultimately, the work in photochemistry today is lighting the path toward a sustainable, solar-powered future.

Author contributions

Abdulrahman A. Alsimaree: writing – original draft, visualization, data curation. Saeed S. Samman: writing – original draft, visualization, data curation. Jan Mohammad Mir: writing – review & editing, supervision, conceptualization. Hatem M. Altass: investigation, formal analysis, validation. Abdulaziz M. Almohyawi: investigation, conceptualization, writing – review & editing. Saleh A. Ahmed: supervision, project administration, funding acquisition, writing – review & editing.

Conflicts of interest

No potential conflict of interest was reported by the authors.

Data availability

No primary research results, software, or code have been included in this review article, and no new data were generated or analysed as part of this work.

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References

- 1 J. H. Montoya, L. C. Seitz, P. Chakthranont, A. Vojvodic, T. F. Jaramillo and J. K. Nørskov, *Nat. Mater.*, 2017, **16**, 70–81.
- 2 I. Rodriguez-Gutierrez, F. L. Souza and O. K. Varghese, in *Conversion of Water and CO₂ to Fuels Using Solar Energy: Science, Technology and Materials*, 2024, pp. 1–8.
- 3 M. Ashraf, M. Ayaz, M. Khan, S. F. Adil, W. Farooq, N. Ullah and M. Nawaz Tahir, *Energy Fuels*, 2023, **37**, 6283–6301.
- 4 C. Casadevall, A. Call, Z. Codolà, F. Acuña-Parés and J. L. Fillol, *An. Quim. RSEQ*, 2016, **112**, 133–140.
- 5 Y. Wang, H. Suzuki, J. Xie, O. Tomita, D. J. Martin, M. Higashi, D. Kong, R. Abe and J. Tang, *Chem. Rev.*, 2018, **118**, 5201–5241.
- 6 K. Fan, L. Wang and L. Tong, in *Conversion of Water and CO₂ to Fuels Using Solar Energy: Science, Technology and Materials*, 2024, pp. 19–45.
- 7 V. Balzani, A. Credi and M. Venturi, *ChemSusChem*, 2008, **1**, 26–58.
- 8 X. Xia, J. H. Pan, X. Pan, L. Hu, J. Yao, Y. Ding, D. Wang, J. Ye and S. Dai, *ACS Energy Lett.*, 2019, **4**, 405–410.
- 9 A. V. Emeline, A. V. Rudakova, V. K. Ryabchuk and N. Serpone, *Curr. Opin. Green Sustain. Chem.*, 2022, **34**, 100588.
- 10 G. Granqvist, *Adv. Mater.*, 2003, **15**, 1789–1803.
- 11 C. G. Granqvist, *Appl. Phys. A*, 1991, **52**, 83–93.
- 12 G. P. Smestad, F. C. Krebs, C. M. Lampert, C. G. Granqvist, K. L. Chopra, X. Mathew and H. Takakura, *Sol. Energy Mater. Sol. Cells*, 2008, **92**, 371–373.
- 13 J. Gong, C. Li and M. R. Wasielewski, *Chem. Soc. Rev.*, 2019, **48**, 1862–1864.
- 14 G. W. Crabtree and N. S. Lewis, *Phys. Today*, 2007, **60**, 37–42.
- 15 N. S. Lewis, *Chem. Rev.*, 2015, **115**, 12631–12632.
- 16 Y. W. Su, S. C. Lan and K. H. Wei, *Mater. Today*, 2012, **15**, 554–562.
- 17 G. Zhang, F. R. Lin, F. Qi, T. Heumüller, A. Distler, H. J. Egelhaaf, N. Li, P. C. Chow, C. J. Brabec, A. K. Jen and H. L. Yip, *Chem. Rev.*, 2022, **122**, 14180–14274.
- 18 K. A. Mazzio and C. K. Luscombe, *Chem. Soc. Rev.*, 2015, **44**, 78–90.
- 19 B. Ehrler, E. Alarcón-Lladó, S. W. Tabernig, T. Veeken, E. C. Garnett and A. Polman, *ACS Energy Lett.*, 2020, **5**, 3029–3033.
- 20 W. Shockley and H. J. Queisser, *J. Appl. Phys.*, 1961, **32**, 510–519.
- 21 D. Gust and T. A. Moore, *Science*, 1989, **244**, 35–41.
- 22 M. Freemantle, *Chem. Eng. News*, 1998, **76**, 37–46.
- 23 A. M. Al-Amri, *Polymers*, 2023, **15**, 3234.
- 24 Z. Peng, Y. Zhang, C. L. Choi, P. Zhang, T. Wu and Y. K. Chan, *Nanoscale*, 2023, **15**, 11403–11421.
- 25 N. Palavesam, S. Marin, D. Hemmetzberger, C. Landesberger, K. Bock and C. Kutter, *Flex. Print. Electron.*, 2018, **3**, 014002.
- 26 Y. Magazov, A. Aliyev, N. Zhumabay, Z. Taubaldiyeva, G. Zhigerbayeva and N. Nuraje, *RSC Adv.*, 2026, **16**, 1643–1661.
- 27 V. Dhiman, S. Singh, V. Srivastava, S. Garg and A. D. Saran, *Environ. Sci. Pollut. Res.*, 2025, **32**, 13299–13312.
- 28 B. D. Nguyen, I. H. Choi and J. Y. Kim, *Nanomaterials*, 2025, **15**, 1494.
- 29 T. Hisatomi, T. Yamada, H. Nishiyama, T. Takata and K. Domen, *Nat. Rev. Mater.*, 2025, **10**, 769–782.
- 30 P. Heinstejn, C. Ballif and L. E. Perret-Aebi, *Green*, 2013, **3**, 125–156.
- 31 E. Biyik, M. Araz, A. Hepbasli, M. Shahrestani, R. Yao, L. Shao, E. Essah, A. C. Oliveira, T. Del Cano, E. Rico and J. L. Lechón, *Eng. Sci. Technol., Int. J.*, 2017, **20**, 833–858.
- 32 R. J. Yang and P. X. W. Zou, *Int. J. Constr. Manage.*, 2016, **16**, 39–53.
- 33 A. V. Emeline, R. V. Mikhaylov, P. E. Lavrik, A. V. Kozhevina, K. M. Bulanin, P. D. Murzin, N. I. Glazkova, V. N. Kuznetsov, A. V. Rudakova, M. V. Mayevskaia and Y. M. Artemiev, *Rev. Adv. Chem.*, 2020, **10**, 73–111.
- 34 F. Schmidt, J. Wenzel, N. Halland, S. Güßregen, L. Delafoy and A. Czich, *Chem. Res. Toxicol.*, 2019, **32**, 2338–2352.



- 35 X. Li, P. M. Maffettone, Y. Che, T. Liu, L. Chen and A. I. Cooper, *Chem. Sci.*, 2021, **12**, 10742–10754.
- 36 C. Rodriguez-Seco, Y. S. Wang, K. Zaghbi and D. Ma, *Nanophotonics*, 2022, **11**, 1443–1484.
- 37 C. Y. Toe, J. Pan, J. Scott and R. Amal, *ACS ES&T Eng.*, 2022, **2**, 1130–1143.
- 38 X. Yzeiri, *J. Res. Appl. Chem.*, 2026, **8**, 45–67.
- 39 Q. Wang, J. Zhao and J. Luo, in *Water Photo- and Electro-Catalysis: Mechanisms, Materials, Devices, and Systems*, 2024, pp. 207–239.
- 40 K. H. Bevan, B. Miao and A. Iqbal, in *Conversion of Water and CO₂ to Fuels Using Solar Energy: Science, Technology and Materials*, 2024, pp. 183–202.
- 41 K. Fan, L. Wang and L. Tong, in *Conversion of Water and CO₂ to Fuels Using Solar Energy: Science, Technology and Materials*, 2024, pp. 19–45.
- 42 W. Yang, R. R. Prabhakar, J. Tan, S. D. Tilley and J. Moon, *Chem. Soc. Rev.*, 2019, **48**, 4979–5015.
- 43 W. H. Cheng, A. De La Calle, H. A. Atwater, E. B. Stechel and C. Xiang, *ACS Energy Lett.*, 2021, **6**, 3096–3113.
- 44 Q. Wang, J. Zhao and J. Luo, in *Water Photo- and Electro-Catalysis: Mechanisms, Materials, Devices, and Systems*, 2024, pp. 207–239.
- 45 G. McClea, J. Kennedy and A. T. Marshall, *J. Electrochem. Soc.*, 2025, **172**, 086501.
- 46 S. Corby, R. R. Rao, L. Steier and J. R. Durrant, *Nat. Rev. Mater.*, 2021, **6**, 1136–1155.
- 47 M. B. Vishlaghi, A. Kahraman, N. Österbacka, E. Usman, E. Erdem, A. Sennaroglu, J. Wiktor and S. Kaya, *J. Mater. Chem. A*, 2023, **11**, 16648–16658.
- 48 I. Grigioni, A. Polo, M. V. Dozzi, K. G. Stampelcoskie, D. H. Jara, P. V. Kamat and E. Selli, *ACS Appl. Energy Mater.*, 2022, **5**, 13142–13148.
- 49 Y. J. Jang and J. S. Lee, *ChemSusChem*, 2019, **12**, 1835–1845.
- 50 A. C. Salomao, M. dos Santos Araujo, H. L. Dos Santos, M. Medina, L. H. Mascaro and M. A. Andrade Junior, *ChemSusChem*, 2021, **14**, 4671–4679.
- 51 W. Yang, J. Park, H. C. Kwon, O. S. Hutter, L. J. Phillips, J. Tan, H. Lee, J. Lee, S. D. Tilley, J. D. Major and J. Moon, *Energy Environ. Sci.*, 2020, **13**, 4362–4370.
- 52 A. M. Fehr, A. Agrawal, F. Mandani, C. L. Conrad, Q. Jiang, S. Y. Park, O. Alley, B. Li, S. Sidhik, I. Metcalf and C. Botello, *Nat. Commun.*, 2023, **14**, 3797.
- 53 C. B. Larsen and O. S. Wenger, *Chem.–Eur. J.*, 2018, **24**, 2039–2058.
- 54 C. Förster and K. Heinze, *Chem. Soc. Rev.*, 2020, **49**, 1057–1070.
- 55 V. Ferraro, C. Bizzarri and S. Bräse, *Adv. Sci.*, 2024, **11**, 2404866.
- 56 P. Jin and C. Wang, *Phys. Chem. Chem. Phys.*, 2025, **27**, 14055–14072.
- 57 C. Bizzarri, in *Electrochemical Society Meeting Abstracts 247, the Electrochemical Society, Inc.*, 2025, p. 2730.
- 58 C. Li, X. Y. Kong, Z. H. Tan, C. T. Yang and H. S. Soo, *Chem. Phys. Rev.*, 2022, **3**, 021305.
- 59 K. Behm and R. D. McIntosh, *ChemPlusChem*, 2020, **85**, 2611–2618.
- 60 D. Li, F. Fan, C. Li and X. Wang, in *Water Photo- and Electro-Catalysis: Mechanisms, Materials, Devices, and Systems*, 2024, pp. 397–447.
- 61 K. T. Arul, T. T. Nga, C. L. Dong and W. C. Chou, in *Water Photo- and Electro-Catalysis: Mechanisms, Materials, Devices, and Systems*, 2024, pp. 363–395.
- 62 K. Fan, L. Wang and L. Tong, in *Conversion of Water and CO₂ to Fuels Using Solar Energy: Science, Technology and Materials*, 2024, pp. 19–45.
- 63 D. Arifin and A. W. Weimer, *Sol. Energy*, 2018, **160**, 178–185.
- 64 F. M. Hadi, R. C. Al-Zuhairy and H. S. Majidi, *Al-Rafidain J. Eng. Sci.*, 2025, **2**, 167–190.
- 65 Y. Zhao, W. Gao, S. Li, G. R. Williams, A. H. Mahadi and D. Ma, *Joule*, 2019, **3**, 920–937.
- 66 P. T. Cesana, B. X. Li, S. G. Shepard, S. I. Ting, S. M. Hart, C. M. Olson, J. I. Alvarado, M. Son, T. J. Steiman, F. N. Castellano and A. G. Doyle, *Chem*, 2022, **8**, 174–185.
- 67 B. Zhou, P. Zhou, W. Dong and Z. Mi, in *Conversion of Water and CO₂ to Fuels Using Solar Energy: Science, Technology and Materials*, 2024, pp. 309–339.
- 68 S. Fukuzumi, *Artif. Photosynth.*, Royal Society of Chemistry, 2025.
- 69 M. L. Lee, P. H. Liao, G. L. Li, H. W. Chang, C. W. Lee and J. K. Sheu, *Sol. Energy Mater. Sol. Cells*, 2019, **202**, 110153.
- 70 D. Arifin and A. W. Weimer, *Sol. Energy*, 2018, **160**, 178–185.
- 71 B. Krammer and T. Verwanger, in *Applied Photochemistry: when Light Meets Molecules*, ed. G. Bergamini and S. Silvi, Springer, Cham, 2016, pp. 978–3.
- 72 O. S. De La Pena, V. Antonio, L. Collado, P. Renones, E. Alfonso, F. Fresno, M. Liras and M. Barawi, *Acta Crystallogr., Sect. A: Found. Adv.*, 2014, **70**, C134.
- 73 R. Kathpalia and A. K. Verma, in *Plant Physiology Annual Volume 2023*, IntechOpen, 2023.
- 74 S. Zhao, Q. Liu, Y. Li, L. Feng, S. Fu, M. Mazarji and J. Pan, *Biofuel Res. J.*, 2024, **11**, 2082–2098.
- 75 J. Liu, Y. Y. Ren, W. J. Xia, B. Y. Deng and F. Wang, *J. Mater. Chem. A*, 2021, **9**, 19346–19368.
- 76 M. E. Louis, T. G. Fenton, J. Rondeau, T. Jin and G. Li, *Comments Inorg. Chem.*, 2016, **36**, 38–60.
- 77 B. O'Regan and M. Grätzel, *Nature*, 1991, **353**, 737–740.
- 78 S. K. Deb, S. Ferrere, A. J. Frank, B. A. Gregg, S. Y. Huang, A. J. Nozik, G. Schlichthörl and A. Zaban, in *Conference Record of the Twenty Sixth IEEE Photovoltaic Specialists Conference*, IEEE, 1997, pp. 507–510.
- 79 A. K. Pandey, V. V. Tyagi, A. Jeyraj, L. Selvaraj, N. A. Rahim and S. K. Tyagi, *Renewable Sustainable Energy Rev.*, 2016, **53**, 859–884.
- 80 J. Castillo-Seoane, L. Contreras-Bernal, A. J. Riquelme, S. Fauvel, Y. Kervella, J. Gil-Rostra, G. Lozano, A. Barranco, R. Demadrille, J. R. Sánchez-Valencia and A. Borrás, *Mater. Today Energy*, 2025, **49**, 101851.
- 81 P. G. S. C. Pradhan and S. Soman, in *Advances in Solar Energy Research*, Springer, Singapore, 2018, pp. 281–316.
- 82 F. Santos, D. Ivanou and A. Mendes, *Sol. RRL*, 2024, **8**, 2300574.
- 83 B. K. Korir, J. K. Kibet and S. M. Ngari, *Energy Sci. Eng.*, 2024, **12**, 3188–3226.



- 84 P. Mariani, L. Vesce and A. Di Carlo, in *2018 IEEE 4th International Forum on Research and Technology for Society and Industry (RTSI)*, IEEE, 2018, pp. 1–5.
- 85 M. Dhonde, K. Sahu, M. Das, A. Yadav, P. Ghosh and V. V. Murty, *J. Electrochem. Soc.*, 2022, **169**, 066507.
- 86 N. Pugazhenthiran, M. Kandasamy, P. Sathishkumar, S. Suresh, S. Karthick Kumar and S. Murugesan, *RSC Adv.*, 2021, **11**, 30566–30588.
- 87 J. Li and N. Wu, *Catal. Sci. Technol.*, 2015, **5**, 1360–1384.
- 88 T. Abbas, H. S. Yahya and N. A. Amin, *Energy Fuels*, 2023, **37**, 18330–18368.
- 89 A. V. Raghu and T. Tachikawa, in *Conversion of Water and CO₂ to Fuels Using Solar Energy: Science, Technology and Materials*, 2024, pp. 285–307.
- 90 G. Segev, J. Kibsgaard, C. Hahn, Z. J. Xu, T. G. Deutsch, C. Xiang, J. Z. Zhang, L. Hammarström, D. G. Nocera, A. Z. Weber and P. Agbo, *J. Phys. D: Appl. Phys.*, 2022, **55**, 323003.
- 91 S. A. Chowdhury, National Solar Energy Roadmap, 2021–2041, *Sustainable and Renewable Energy Development Authority (SREDA)*, 2020.
- 92 N. Taylor, O. G. Joanne, O. Eulaerts and M. Grabowska, *Clean Energy Technology Observatory: Direct Solar Fuels in the European Union – 2022 Status Report on Technology Development, Trends, Value Chains and Markets*, Publications Office of the European Union, 2022.
- 93 S. Zei, *Energy Convers.*, 2025, **1**, 100025.
- 94 A. Patra, R. Samal and C. S. Rout, *Catal. Today*, 2023, **424**, 113853.
- 95 S. Mohd, L. Balan, T. Gries, H. Alem, M. Lebrun, V. Falk and R. Schneider, *Catal. Sci. Technol.*, 2026, **16**, 123–135.
- 96 Y. Liu, X. Pan, Z. Qiu, L. Sun, P. Zhang, R. He, Z. Han, J. Ma, Z. Zhang and Y. Wang, *Fuel*, 2025, **393**, 135036.
- 97 J. Chi, Z. Wei, W. Fang, J. Yan, J. Wang, H. Zu, J. Cheng, H. Luo, Z. Ye, J. Liu and Z. Jiang, *Appl. Catal., B*, 2025, **365**, 124973.
- 98 I. Grigioni, A. Polo, M. V. Dozzi, K. G. Stampelcoskie, D. H. Jara, P. V. Kamat and E. Selli, *ACS Appl. Energy Mater.*, 2022, **5**, 13142–13148.
- 99 A. Kafizas, R. Godin and J. R. Durrant, in *Semiconductors and Semimetals*, ed. S. Hu and C. Xiang, Elsevier, 2017, vol. 97, pp. 3–46.
- 100 A. C. Salomao, M. dos Santos Araujo, H. L. Dos Santos, M. Medina, L. H. Mascaro and M. A. Andrade Junior, *ChemSusChem*, 2021, **14**, 4671–4679.
- 101 H. Kobayashi, N. Sato, M. Orita, Y. Kuang, H. Kaneko, T. Minegishi, T. Yamada and K. Domen, *Energy Environ. Sci.*, 2018, **11**, 3003–3009.

