

## Chemical Pathways in Solar Cells, Hydrogen Production, and Biofuels: A Comprehensive Review of Chemistry, Technology, and Sustainability

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### Abstract

Global reliance on fossil fuels, responsible for billions of tonnes of annual CO<sub>2</sub> emissions, continues to accelerate climate change. Renewable energy technologies are therefore essential to meet global decarbonization goals. Chemistry plays a central role in designing and advancing these technologies by dictating energy conversion pathways, materials stability, catalytic activity, and life cycle impacts. This review critically examines three renewable energy systems—solar cells, hydrogen production, and biofuels—by analyzing their chemical foundations, recent advances, and sustainability profiles. Advances in semiconductor chemistry have pushed solar cell efficiencies beyond 25%, while catalytic innovations are driving green hydrogen toward commercial feasibility. Similarly, lignocellulosic and algal biofuels demonstrate the promise of carbon-neutral fuels. However, challenges of material scarcity, instability, low energy return, and environmental trade-offs persist. Cross-cutting opportunities include green chemistry, hybridized systems, and machine learning–accelerated discovery. The review concludes with research gaps and future directions necessary to achieve a sustainable energy transition.

**Keywords:** Solar cells; Hydrogen production; Biofuels; Green chemistry; Renewable energy; Sustainability.

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### 1. Introduction

The 21st century energy landscape is undergoing an unprecedented transformation, yet global primary energy consumption remains dominated by fossil fuels, which account for nearly 80% of supply and generate over 33 gigatonnes of CO<sub>2</sub> annually (International Energy Agency [IEA], 2023). This dependency has driven rising greenhouse gas concentrations, biodiversity loss, and deterioration of air quality, thereby exacerbating the climate crisis. The Intergovernmental Panel on Climate Change (IPCC) has emphasized that limiting global warming to below 1.5 °C requires halving emissions by 2030 and achieving net zero by 2050. Meeting this goal demands not only the scaling up of existing technologies but also the discovery and optimization of new approaches that integrate chemistry, materials science, and process engineering. Against this backdrop, renewable and sustainable energy technologies have become indispensable pillars of decarbonization strategies worldwide.

Among the various pathways under exploration, solar photovoltaics, hydrogen production, and biofuels stand out for their chemical complexity, technological promise, and wide sustainability implications. Solar photovoltaics are critical for direct electricity generation, with crystalline silicon, thin films, and perovskite-based technologies demonstrating remarkable progress in

efficiency and cost reduction (Shockley & Queisser, 1961; Green et al., 2022; NREL, 2023). Hydrogen has emerged as a versatile energy carrier with potential to decarbonize hard-to-abate sectors such as steel, cement, and long-haul transport, though current production is still dominated by carbon-intensive steam methane reforming (Turner, 2004; IEA, 2022; Zhang et al., 2021). Biofuels, on the other hand, remain indispensable for transport and aviation, with pathways evolving from food-based feedstocks to lignocellulosic and algal biomass, which offer higher sustainability benefits if technological and cost barriers are overcome (Menon & Rao, 2012; Chisti, 2007; Demirbas, 2020).

The role of chemistry in advancing these technologies cannot be overstated. In photovoltaics, bandgap engineering, doping, defect passivation, and interface chemistry determine device efficiency and stability (Shockley & Queisser, 1961; Zhou et al., 2019). Hydrogen production pathways, from alkaline electrolysis to proton exchange membrane and solid oxide systems, are fundamentally dictated by catalytic surface reactions, electrolyte chemistry, and materials durability (Turner, 2004; Gao et al., 2023). Biofuel production is equally chemistry-intensive, involving biochemical and thermochemical transformations such as enzymatic hydrolysis of lignocellulose, catalytic upgrading of pyrolysis oils, and microbial fermentation engineered through synthetic biology (Menon & Rao, 2012; Hasunuma & Kondo, 2012). These examples underscore how chemistry serves as both an enabler and a bottleneck for sustainable energy transitions.

Existing reviews often emphasize engineering, economics, or policy perspectives, while fewer works explicitly address the unifying role of chemistry across these renewable energy systems (Lewis & Nocera, 2006). This gap is critical because the chemical mechanisms not only determine the feasibility and efficiency of each technology but also define their environmental footprints, resource demands, and scalability potential. A chemistry-centered synthesis therefore provides unique insights into cross-cutting challenges such as material scarcity, toxicity, lifecycle emissions, and recycling, while highlighting emerging opportunities in catalysis, nanomaterials, and machine learning-driven discovery (Seh et al., 2017; Kim et al., 2020).

The purpose of this review is to examine the chemical foundations, technological advances, and sustainability implications of solar cells, hydrogen production, and biofuels, while drawing attention to the interconnections that link these domains. By situating chemistry at the heart of the discussion, this article contributes to a holistic understanding of renewable energy pathways, clarifies research gaps that persist across the literature, and underscores opportunities for innovation. In doing so, it aligns with ongoing global efforts to achieve a carbon-neutral energy future and responds to the urgent call for interdisciplinary approaches to address the climate crisis. The following sections critically analyze the state of knowledge across these three domains, while emphasizing the central role of chemistry in enabling a sustainable and scalable energy transition.

## **2. Solar Cells: Chemistry at the Interface of Photons and Electrons**

## 2.1 Efficiency Evolution

The evolution of solar photovoltaic (PV) technology reflects a steady progression in semiconductor chemistry. First-generation crystalline silicon (c-Si) cells, developed in the mid-20th century, remain dominant due to their stability and maturity. Record laboratory efficiencies have reached 26.8%, while commercial modules typically operate at 20–22% (Green et al., 2022). However, silicon's energy-intensive purification and wafer processing pose sustainability challenges (Fthenakis & Kim, 2011).

Second-generation thin-film solar cells, including cadmium telluride (CdTe) and copper indium gallium selenide (CIGS), offered reductions in material use and greater flexibility (Kamat, 2013). Yet, their reliance on scarce or toxic elements (Cd, In, Te) has raised environmental and supply chain concerns.

The past decade has seen rapid progress in third-generation perovskite solar cells (PSCs). Since their introduction by Kojima et al. (2009), hybrid organic–inorganic lead halide perovskites have demonstrated remarkable optoelectronic properties, including high absorption coefficients, long carrier diffusion lengths, and tunable bandgaps. Laboratory efficiencies now exceed 26% (NREL, 2023). However, perovskites face critical barriers: chemical instability in moisture, heat, and UV light (Zhou et al., 2019), as well as toxicity associated with lead. Research efforts are focused on defect passivation, interface engineering, and the development of lead-free alternatives based on tin and germanium (Kim et al., 2020; Noel et al., 2014).

While PSCs have redefined the efficiency frontier, their chemical instability and toxicity remain unresolved, and the literature is still sparse on scalable recycling strategies.

## 2.2 Photochemical Mechanisms

The photovoltaic effect involves photon absorption, exciton generation, exciton dissociation, carrier transport, and collection (Shockley & Queisser, 1961). Key chemical challenges include:

- **Defect passivation:** Trap states at grain boundaries induce recombination; halide salts and fullerene derivatives are applied for surface chemistry control (Noel et al., 2014).
- **Interface chemistry:** Stability depends on transport layers (spiro-OMeTAD, CuSCN, NiOx), whose synthesis and doping chemistry directly impact cost and device durability (O'Regan & Grätzel, 1991).
- **Encapsulation:** Perovskite hydrolysis produces PbI<sub>2</sub>; fluoropolymers and cross-linking agents improve hydrophobicity (Zhou et al., 2019).

## 2.3 Sustainability Profile

Lifecycle emissions: 20–70 gCO<sub>2</sub>/kWh depending on technology and geography (Fthenakis & Kim, 2011). End-of-life recycling remains limited, especially for Cd- and Pb-based devices.

**Gap:** Stable, non-toxic absorbers; scalable tandem architectures; recyclable PV modules.

### 3. Hydrogen: From Water Splitting to Clean Fuel

#### 3.1 Chemical Routes

Hydrogen has re-emerged as a cornerstone of a decarbonized energy system, particularly for sectors where direct electrification is difficult (steel, cement, long-haul transport). However, the chemical pathways for hydrogen production vary significantly in terms of sustainability.

Currently, >95% of hydrogen is produced via steam methane reforming (SMR), a carbon-intensive process (IEA, 2022). Consequently, significant research has shifted toward water electrolysis, which—if powered by renewable electricity—produces near-zero emission “green hydrogen.”

Alkaline electrolysis, the most mature route, employs aqueous KOH or NaOH electrolytes with Ni- or steel-based electrodes. While relatively low-cost, it suffers from slower reaction kinetics (Gao et al., 2023). Proton exchange membrane (PEM) electrolysis utilizes a solid polymer membrane (e.g., Nafion) and platinum group metal catalysts, achieving higher efficiency (65–80%) and dynamic response, but at significantly higher cost due to catalyst scarcity (Zhang et al., 2021). Solid oxide electrolysis (SOE) operates at 700–900 °C, leveraging oxygen-ion conducting ceramics for up to 85% efficiency, though durability challenges limit commercialization (Turner, 2004).

Emerging approaches include photocatalytic water splitting, first demonstrated with TiO<sub>2</sub> by Fujishima and Honda (1972). Although current solar-to-hydrogen efficiencies remain <2% (Kudo & Miseki, 2009), nanostructured catalysts (Ni<sub>2</sub>P, MoS<sub>2</sub>) and heterojunction designs show promise (Seh et al., 2017). Another novel pathway is solar thermochemical hydrogen (STCH) production using metal oxide redox cycles (Abanades & Flamant, 2006).

While the literature highlights an urgent need for low-cost, earth-abundant catalysts, durable membranes, and scalable photocatalysts. Few studies comprehensively compare techno-economic feasibility across all routes.

#### 3.2 Catalytic Challenges

HER and OER suffer from sluggish kinetics, high overpotentials, and catalyst poisoning (CO, sulfur). Precious metals remain indispensable for high activity and durability (Zhang et al., 2021).

#### 3.3 Sustainability

- Gray H<sub>2</sub>: ~90–120 gCO<sub>2</sub>/MJ.
- Green H<sub>2</sub>: <5 gCO<sub>2</sub>/MJ when powered by renewables (IEA, 2022).
- Round-trip efficiency (electricity → H<sub>2</sub> → electricity): <40%.

**Gap:** Low-cost, durable, earth-abundant catalysts; scalable storage and transport infrastructure.

## 4. Biofuels: Chemical Conversion of Biomass

### 4.1 Generations of Biofuels

Biofuels have long been explored as renewable substitutes for fossil fuels, with development progressing through three generations.

First-generation biofuels, such as ethanol from corn/sugarcane and biodiesel from vegetable oils, are commercially established. However, they compete with food production and often have marginal greenhouse gas (GHG) benefits once land-use change is considered (Searchinger et al., 2008).

Second-generation biofuels, derived from lignocellulosic feedstocks (e.g., crop residues, forestry waste), avoid direct food competition and are more sustainable. Yet, their complex biomass chemistry requires harsh pretreatment to disrupt lignin and hemicellulose, followed by enzymatic hydrolysis and microbial fermentation (Menon & Rao, 2012). These processes remain costly and energy-intensive.

Third-generation biofuels focus on microalgae, which can yield lipids, carbohydrates, and proteins at high productivity. Algal cultivation in saline water or wastewater provides co-benefits such as nutrient recycling and CO<sub>2</sub> sequestration (Chisti, 2007). However, the literature repeatedly identifies harvesting, drying, and lipid extraction as major energetic and economic barriers (Lam et al., 2010). Advances in synthetic biology have enabled engineered *E. coli* and *S. cerevisiae* strains capable of consolidated bioprocessing (Hasunuma & Kondo, 2012). Thermochemical methods such as pyrolysis and gasification have also been enhanced with catalytic upgrading to produce drop-in fuels.

While the literature demonstrates feasibility, studies often neglect holistic life cycle analysis (LCA) and integration with carbon capture or co-product valorization, which are critical for true sustainability.

### 4.2 Thermochemical Routes

- **Pyrolysis:** 400–600 °C, anaerobic; yields bio-oil, syngas, char. Requires catalytic upgrading (zeolites, Ni-based catalysts).
- **Gasification:** >800 °C, limited O<sub>2</sub>/steam; yields syngas for Fischer–Tropsch synthesis.

### 4.3 Sustainability

- First-gen biofuels linked to deforestation and food price increases (Searchinger et al., 2008).
- Second-gen fuels achieve <20 gCO<sub>2</sub>/MJ if integrated with carbon capture (Hasunuma & Kondo, 2012).
- Algal biofuels could be carbon-negative when coupled with wastewater treatment (Chisti, 2007).

**Gap:** Energy-efficient pretreatment, lignin valorization, cost-effective algae harvesting.

## **5. Comparative Analysis and Sustainability Impact**

Renewable energy technologies are not equally mature, efficient, or sustainable. Their impact must be assessed using multiple dimensions: energy efficiency, lifecycle greenhouse gas (GHG) emissions, resource intensity, energy return on investment (EROI), and economic feasibility. Table 1 summarizes key comparative metrics.

### ***5.1 Efficiency and Energy Return***

Solar photovoltaics (PV) exhibit the highest energy conversion efficiencies among the three pathways, with crystalline silicon (c-Si) modules operating at 20–22% and laboratory perovskite–silicon tandem cells surpassing 30% (Green et al., 2022; NREL, 2023). Hydrogen electrolysis achieves 60–80% efficiency depending on the technology, with solid oxide electrolysis cells (SOECs) offering the highest theoretical potential (>85%) but limited by durability. Biofuels, in contrast, have lower EROI values: 30–35% for first-generation biofuels, 20–30% for lignocellulosic ethanol, and <10% for algal biodiesel (Chisti, 2007; Lam et al., 2010). This makes them less favorable purely in energetic terms but valuable for transport and aviation sectors where liquid fuels remain indispensable.

### ***5.2 Lifecycle Greenhouse Gas Emission***

Lifecycle assessments (LCA) reveal substantial variation. Solar PV systems emit 20–70 gCO<sub>2</sub>-eq/kWh over their lifecycle, dominated by energy-intensive silicon purification (Fthenakis & Kim, 2011). With renewable-powered manufacturing and recycling, this figure could fall below 15 gCO<sub>2</sub>-eq/kWh. Hydrogen’s footprint depends almost entirely on its production pathway: “grey hydrogen” from SMR emits 90–120 gCO<sub>2</sub>-eq/MJ, while “green hydrogen” from renewable-powered electrolysis can achieve <5 gCO<sub>2</sub>-eq/MJ (IEA, 2022). Biofuels range widely: corn ethanol yields ~70 gCO<sub>2</sub>-eq/MJ, often comparable to gasoline, while lignocellulosic and algal fuels can achieve <20 gCO<sub>2</sub>-eq/MJ if coupled with carbon capture and utilization (CCU) or co-product valorization (Menon & Rao, 2012; Demirbas, 2020).

### ***5.3 Resource and Environmental Trade-offs***

Resource intensity presents a major bottleneck. PV technologies require critical raw materials: silicon, indium, gallium, tellurium, and lead. Perovskites, while promising, pose toxicity risks that complicate end-of-life disposal (Kim et al., 2020). Hydrogen faces infrastructure challenges: compression, liquefaction, and pipeline transport all demand substantial energy inputs. Biofuels are constrained by land, water, and nutrient use. First-generation biofuels directly compete with food systems, while algal biofuels, though decoupled from agriculture, face water-intensive harvesting and dewatering steps (Chisti, 2007; Lam et al., 2010).

### ***5.4 Economic Competitiveness***

Solar PV is currently the most competitive, with levelized cost of electricity (LCOE) falling to ~\$0.02–0.04/kWh in favorable regions, often below fossil fuels (IEA, 2023). Hydrogen costs vary: grey hydrogen is ~\$1.5–2/kg, while green hydrogen remains ~\$4–6/kg but is projected to fall below \$2/kg by 2030 with scale and catalyst innovation (Gao et al., 2023). Biofuels remain costly: corn ethanol is competitive at \$0.6–0.8/L, but lignocellulosic ethanol and algal biodiesel remain >\$1.5–2/L without subsidies (Demirbas, 2020).

### 5.5 Comparative Sustainability Outlook

From a sustainability perspective, solar PV currently offers the highest impact per unit cost and lowest lifecycle footprint when deployed at scale. Green hydrogen is indispensable for decarbonizing hard-to-electrify sectors but requires breakthroughs in catalysts, membranes, and infrastructure to scale economically. Biofuels occupy a niche role in aviation, shipping, and rural energy systems, where liquid fuels are irreplaceable, but require integration with waste streams, CCU, and biorefineries to become sustainable.

**Table 1. Comparative Summary of Solar Cells, Hydrogen Production, and Biofuels**

Technology	Efficiency Range	Lifecycle Emissions	Key Chemical Challenges	Emerging Solutions
<b>Solar Cells</b>	15–26% (Si); >25% (Perovskite)	20–70gCO <sub>2</sub> -eq/kWh	Lead toxicity in PSCs  ; Scarcity of In, Te in thin films	Lead-free perovskites (Sn, Ge halides)  ; Circular economy PV modules
<b>Hydrogen</b>	60–80% (Electrolysis); <2% (Photocatalysis)	<5 gCO <sub>2</sub> -eq/MJ (green H <sub>2</sub> )	Membrane degradation under high current  ; Low quantum efficiency in photocatalysis	Earth-abundant electrocatalysts; Photoelectrochemical cells; Integration with renewable-powered grids
<b>Biofuels</b>	20–40% energy yield (varies by type)	Variable: Negative for 1 <sup>st</sup> gen; lower for 2 <sup>nd</sup> / 3 <sup>rd</sup> gen	Food vs fuel, pretreatment energy demand, high cost of algae fuels	Synthetic biology, consolidated bioprocessing, catalytic upgrading

### 6. Conclusion and Future Directions

This review has critically examined three major renewable energy pathways—solar photovoltaics, hydrogen production, and biofuels—through the lens of chemistry. While all three technologies are essential for global decarbonization, their sustainability profiles, readiness levels, and challenges differ significantly.

Solar PV is already the most competitive renewable electricity source, with crystalline silicon firmly established and perovskites pushing efficiency boundaries. Yet, long-term sustainability requires addressing material toxicity, supply chain bottlenecks, and circular recycling. Hydrogen is indispensable for decarbonizing heavy industry, transport, and seasonal storage, but catalyst scarcity, electrolyzer durability, and infrastructure gaps hinder rapid deployment. Biofuels provide renewable liquid fuels for aviation, shipping, and rural contexts, but food–fuel conflicts, low EROI, and processing costs limit their contribution unless coupled with waste feedstocks, synthetic biology, and biorefinery integration.

Across all pathways, several cross-cutting challenges emerge:

1. Material scarcity and toxicity (In, Te, Pb in PV; Pt/Ir in PEM electrolyzers).

2. Stability and durability limits, from perovskite degradation to membrane breakdown in electrolysis.
3. Economic and infrastructural barriers, particularly for hydrogen distribution and biofuel scaling.
4. Lifecycle sustainability gaps, as few studies holistically integrate emissions, water use, land use, and circularity.

To overcome these barriers, future research directions should prioritize:

1. Green chemistry and materials innovation: lead-free perovskites, earth-abundant catalysts (Ni, Fe, Co), recyclable polymers, and lignin valorization.
2. Hybridized and integrated systems: PV–electrolysis coupling for direct solar hydrogen, biorefineries co-producing fuels and chemicals, and PV–perovskite tandems for >30% efficiency.
3. Advanced computational tools: machine learning and AI-driven screening of catalysts, semiconductors, and enzymes to accelerate discovery.
4. Circular economy and policy frameworks: scalable recycling for PV and batteries, carbon pricing to incentivize green hydrogen, and sustainability certification for biofuels.
5. Interdisciplinary collaboration: bridging chemistry with microbiology, materials science, and process engineering to tackle challenges holistically.

In conclusion, while solar cells currently provide the greatest near-term impact, hydrogen and biofuels remain indispensable for a comprehensive energy transition. Chemistry sits at the core of all three technologies, determining efficiency, durability, and environmental footprint. By aligning chemical innovation with systems integration and sustainability principles, the next decade can unlock transformative advances, accelerating the global shift toward a carbon-neutral energy future.

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