



Review article

SiC-based heterostructures and tandem PEC cells for efficient hydrogen production

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ARTICLE INFO

Keywords:

Silicon carbide
Heterostructures
Van der Waals heterostructures
DFT modeling
Tandem PEC cells
Hydrogen production

ABSTRACT

Achieving solar-to-hydrogen (STH) conversion efficiencies above 10 % is within reach with silicon carbide (SiC), a wide-bandgap semiconductor offering unique properties for photoelectrochemical (PEC) water splitting. This review integrates recent advances in novel van der Waals heterostructure designs, Janus-based SiC composites, and eco-friendly synthesis routes to improve efficiency and scalability. In addition, it provides a systematic correlation of density functional theory (DFT) predictions with experimental performance metrics, highlighting critical gaps and optimization pathways. Additionally, comprehensive modeling of electronic structures, band alignments, and surface reactions to optimize SiC-based configurations, including type-II heterojunctions with materials such as MoS₂ and TiO₂. Key performance metrics, such as photocurrent density and STH efficiencies, are evaluated alongside experimental advancements. Despite significant progress, challenges such as long-term photoelectrode stability, scalable fabrication, and cost reduction persist. We discuss strategies to address these issues, including eco-friendly etching techniques and novel material combinations, and propose future research directions. This review highlights that SiC-based tandem systems achieve STH efficiencies up to 6.3 % and stability exceeding 100 days, with DFT modeling suggesting potential beyond 10 %

1. Introduction

Photoelectrochemical (PEC) water splitting offers a sustainable pathway for hydrogen production, addressing global energy demands and climate change. Hydrogen, a clean and versatile energy carrier, powers fuel cells, stores solar energy, and decarbonizes sectors such as transportation and industry [1–4]. However, PEC systems struggle with photoelectrode limitations, achieving solar-to-hydrogen (STH) efficiencies – typically below 10 % – far from the >20 % target for commercial viability [5,6].

Recent advances have also highlighted the potential of PEC systems to drive nitrogen reduction reactions, expanding the scope of sustainable energy conversion beyond water splitting. These studies demonstrate that integrating SiC-based heterostructures and related semiconductor materials can enable efficient ammonia production under mild conditions, underscoring the versatility and importance of these approaches [7–10].

In PEC processes, sunlight irradiates electrodes in an aqueous

electrolyte, converting the energy of photons into electrochemical energy. To split molecules of water, the bandgap of photoelectrode material must be equal to or greater than the energy of the incident photons. A theoretical minimum of 1.23 eV per electron is needed to produce hydrogen and oxygen from water, aligning with the energy of visible light photons. In practice, however, the efficiency of semiconductor-based photocatalysis is often reduced by energy losses and other challenges.

Challenges include poor light absorption, inefficient charge separation, and instability in aqueous electrolytes. Stable wide-bandgap materials such as TiO₂ are limited to UV absorption, while narrower bandgap semiconductors such as Si or GaAs corrode despite capturing visible light [11,12]. Silicon carbide (SiC) with various crystal structures (polytypes), is promising for PEC due to its tunable bandgap (2.36–3.2 eV), enabling tailored UV and visible light absorption [13–16]. This tunability optimizes SiC for different solar spectrum regions, a key advantage for PEC applications. Its chemical inertness, mechanical strength, and thermal stability make it good for harsh PEC environments

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Received 15 May 2025; Received in revised form 4 August 2025; Accepted 19 August 2025

Available online 21 August 2025

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[17,18]. High carrier mobility and heterostructure compatibility enhance charge separation, as demonstrated by nanoporous 3C-SiC achieving photocurrents of 2.30 mA/cm^2 [19].

Heterostructures integrating SiC with 2D materials such as MoS₂, phosphorene, or TiO₂ improve PEC efficiency through type-II band alignments, which spatially separate charge carriers [20–24]. SiC based vdW heterostructures, which stack 2D materials via weak van der Waals (vdW) forces, enhance charge transfer, reduce recombination, and broaden spectral utilization [21,25–28]. Such heterostructures exhibit enhanced photocurrent densities, underscoring SiC's potential in PEC systems [29–32].

Density functional theory (DFT) modeling is pivotal for optimizing SiC-based PEC systems, elucidating electronic structures, band alignments, and surface reactions [33–35]. DFT reveals how doping or strain tunes SiC bandgap and designs vdW heterostructures for improved charge separation [36–38]. Advanced techniques, such as the Bethe-Salpeter equation, clarify excitonic effects, critical for optimizing light absorption and charge separation in PEC devices, bridging experimental and predictive design efforts.

Despite advancements, scaling SiC-based PEC systems for industrial applications remains challenging. Key obstacles include photoelectrode stability under illumination, scalable fabrication, and cost reduction of SiC and associated materials. Addressing these demands a multidisciplinary approach, integrating materials science, electrochemistry, and computational modeling to enhance system design and performance.

This review explores SiC-based tandem PEC systems, heterostructures, and vdW heterostructures, which enhance charge separation and spectral utilization. Tandem PEC systems pair wide-bandgap SiC photoanodes with narrow-bandgap photocathodes to maximize light absorption and generate sufficient photovoltage for unassisted water splitting, often achieving higher STH efficiencies than single photoelectrode STH efficiencies. Challenges include band misalignment, interfacial recombination, and integration complexity.

Although several reviews have discussed general semiconductor photoelectrodes such as TiO₂, Si, and III–V compounds for photocatalytic applications and PEC water splitting [39–44], a focused and systematic analysis dedicated specifically to SiC-based systems have been lacking. SiC exhibits unique properties—including a tunable wide bandgap, exceptional chemical and thermal stability, high carrier mobility, and compatibility with advanced heterostructures—that differentiate it from conventional semiconductors. Moreover, challenges such as scalable synthesis of nanostructured SiC, interface engineering in heterojunctions, and efficient utilization of visible light require targeted discussion. Therefore, this review aims to fill the gap by providing a comprehensive summary of SiC-specific strategies, performance metrics, and future directions in SiC-based heterostructures and tandem PEC cells for efficient H₂ production.

To ensure comprehensive coverage of relevant advances in SiC based heterostructures for PEC water splitting, we performed a structured literature search across Web of Science. Studies were included if they (i) reported experimental or computational investigations of SiC-based heterostructures, (ii) evaluated PEC performance metrics such as solar-to-hydrogen (STH) efficiency, photocurrent density, or stability under illumination, and (iii) focused on semiconductor band structure engineering. Review articles, purely theoretical works lacking PEC performance data, or reports not related to SiC were excluded.

Data was extracted manually by the authors and tabulated for key PEC indicators, including band alignment, photovoltage, charge carrier mobility, and theoretical versus experimental STH efficiency. Special attention was given to recent studies involving novel heterojunction configurations, 2D Janus materials, and AI-assisted screening workflows. This strategy ensures a reproducible foundation for the synthesis and evaluation of current trends and emerging opportunities in the field.

2. Properties of silicon carbide

SiC is promising for PEC applications due to its tailorable physical, chemical, and electronic properties. This section examines SiC electronic characteristics, chemical stability, and advantages over other materials, supported by evidence.

Electronic properties of SiC vary by polytype, with 3C-SiC (cubic, 2.36 eV), 4H-SiC (hexagonal, 3.2 eV), and 6H-SiC (hexagonal, 3.0 eV) most relevant for PEC [45–47]. 3C-SiC absorbs visible light up to 525 nm, ideal for solar PEC, while 4H-SiC and 6H-SiC target UV. High carrier mobility, especially in 4H-SiC, facilitates efficient charge transport, reducing recombination losses. SiC thermal stability, mechanical strength, and radiation resistance enhance durability in harsh PEC conditions, including extreme environments [17,48–52].

SiC is inert to acids, alkalis, and temperatures up to 1600°C, SiC forms a protective SiO₂ layer via strong Si-C bonds, ensuring longevity electrochemistry [53,54]. SiC surpasses common PEC materials such as Si, TiO₂, ZnO, and GaN due to:

- Light absorption and stability, unlike Si with bandgap 1.1 eV, which corrodes despite broad absorption, 3C-SiC balances visible light capture with stability [55]. In contrast to III–V semiconductors, SiC offers superior stability and lower toxicity.
- In terms of environmental compatibility, SiC is non-toxic and resistant to photocorrosion.
- SiC yields higher hydrogen outputs due to enhanced charge separation [56].
- Thermal advantage, SiC 3.7 W/cm-K conductivity exceeds GaN's 1.3 W/cm-K [17].

Nanostructured SiC is promising in optics and photonics to its large surface area and adjustable light emission. These features make it appropriate for efficient and durable photoelectrodes. To meet the demands of such applications, various synthesis methods have been developed to produce SiC nanostructures with controlled morphologies, optimized for photocatalytic and PEC reactions.

The methods differ significantly in complexity, cost, and their ability to deliver nanostructures tailored for specific applications. Producing SiC coatings for photoelectrodes demands careful oversight of quality, uniformity, and substrate adhesion. In contrast to nanopowders, which can be created through diverse methods, thin film coatings necessitate precise management of thickness and structure, restricting the range of suitable techniques. Methods such as chemical vapor deposition (CVD), molecular beam epitaxy (MBE), ion beam synthesis of SiC on Si, and the coordinated atomic substitution approach are the primary techniques for creating thin SiC films. These processes ensure high purity and crystallinity of the material but involve intricate technological setups and rigorous control of parameters such as temperature, pressure, and the composition of the reaction environment [57–65]. One effective synthesis method is single-step thermal plasma pyrolysis, which transforms rice husk into SiC-SiO₂ core-shell nanostructures without requiring catalysts. By leveraging agricultural waste, thermal plasma pyrolysis ensures environmental sustainability and significantly reduces raw material costs [66]. There could also be a significant reduction in raw material costs, as rice husk is widely available and often classified as agricultural waste. Due to the intimate contact between silica and carbon in its structure, rice husk possesses a high surface area that facilitates SiC formation at lower temperatures. Furthermore, life cycle assessment studies have shown that using rice husk as a feedstock significantly reduces the environmental footprint of SiC production, owing to both the renewable origin of the precursor and the low energy input required [67]. This supports the ecological and economic feasibility of rice husk derived SiC for scalable PEC applications. In contrast, microwave heating of a porous precursor at 1300°C for 20 minutes facilitates rapid and uniform growth of SiC whiskers, driven by microwave plasma activation. An energy-efficient method yields high-purity

nanostructures, but careful temperature control is critical to prevent oxidation and the formation of amorphous SiO_2 [68].

For applications requiring enhanced catalytic performance, embedding SiC nanoparticles into ferrierite zeolites during synthesis boosts catalytic activity by 2.2 times, owing to intimate contact between SiC and the catalytic phase. This approach excels in energy-efficient catalysis by maximizing surface interactions [69]. Similarly, carbothermal reduction combined with a template method produces submicron ZrC-SiC-C microspheres with interlocked structures. Yet, the high temperatures required increase energy consumption, reducing its cost-effectiveness for large-scale production [70]. To be suitable for PEC tandem cells, SiC nanostructures with high surface area and tailored photoluminescent properties are essential to maximize light absorption and charge carrier generation. Porous SiC nanosheets, synthesized in situ using graphite flakes, achieve a surface area of up to $149 \text{ m}^2/\text{g}$ and demonstrate a hydrogen production rate of $51.0 \text{ } \mu\text{mol}/\text{g}\cdot\text{h}$, driven by efficient gas-solid reactions. Such high activity makes them a top candidate for photocatalysis [71].

Polycrystalline SiC nanostructures, with bandgaps of 2.57–2.74 eV and photoluminescence at 330 nm, are well-suited for ultraviolet photocatalysis, though their lower surface area slightly reduces efficiency compared to nanosheets [72]. But despite the high cost, the use of some techniques for producing SiC is justified by the creation of highly efficient structures. Such techniques may include laser writing of N-doped 3C-SiC [73], photo-assisted etching [74], photonic cavities formation for light trapping [75], etc. The environmental impact of synthesis methods for nanoporous SiC is critical and warrants attention. Anodization in HF produces nanoporous 3C-SiC with a photocurrent of $2.30 \text{ mA}/\text{cm}^2$ and 93 % light absorption [19], but HF toxicity and handling challenges hinder scalability and eco-friendliness. In contrast, plasma-assisted KOH etching provides a rapid, sustainable alternative, achieving an etching rate of $540 \text{ nm}/\text{min}$ for 4H-SiC [76]. Additionally, nanoporous 4H-SiC enhances photocurrent via high carrier mobility and efficient charge transport [17].

Figure 1 illustrates schematic diagram comparing charge separation and diffusion in (a) planar 3C-SiC and (b) nanoporous 3C-SiC photoanodes. In planar SiC, photons with energy $h\nu$ are absorbed by the material and penetrate to a depth known as the penetration depth $D\lambda$. Upon absorption, the energy of the photons is transferred to electrons, leading to the formation of electron-hole pairs: electrons (e^-) move in one direction, while holes (h^+) move in the opposite direction. The separation of these charge carriers occurs under the influence of an electric field in the region known as the depletion layer width W_{dep} . Additionally, the diffusion length L_D is important, as it indicates the average distance that carriers can travel before recombining, that is, before they combine and lose their energy. In contrast, porous SiC has a complex internal structure due to the presence of pores, which increase the surface area of the material.

Photons entering the porous material are repeatedly reflected and scattered within the pores, significantly increasing the effective path length [19]. This enhances the probability of light absorption, and as a result, the generation and separation of electron-hole pairs become more intense.

To identify the most suitable synthesis methods for photocatalytic tandem cells and PEC applications, a comparison of their optimality and cost is essential. Optimality is evaluated based on the ability to produce nanostructures or heterostructures with high surface area, purity, photoluminescent properties, and efficient charge separation, while cost considers raw materials, energy consumption, and equipment complexity. Table 1 provides a detailed comparison of the most recent experimental methods of nanostructured SiC production.

The unique properties of SiC make it a promising material for PEC applications. However, to realize its full potential, it requires combination with other semiconductors in heterostructures, which will be discussed further below.

Table 1
Comparison of SiC production methods.

Synthesis Method	Optimality	Comment	Reference
Thermal Plasma Pyrolysis	SiC-SiO ₂ nanostructures with decent surface area, suitable for heterojunctions	Utilizes agricultural waste (rice husk) and requires no catalysts.	[66]
Microwave Heating	Uniform SiC whiskers with high purity and surface area	Energy-efficient.	[68]
Embedding in Zeolites	Limited photoluminescence restricts direct photocatalytic use.	Complex synthesis and equipment costs.	[69]
Carbothermal Reduction	Thermally stable SiC for heterostructures such as ZrC-SiC-C.	High-temperature requirements increase energy costs.	[70]
Molten Salt Shielded Method	Produces diverse, photoluminescent nanostructures (e.g., 2H/3C-SiC heterojunctions)	Complex salt composition control and scaling challenges	[72]
Hot-Wire CVD	High-quality fibers with minimal defects	Sophisticated equipment and gas control systems	[77]
Pulsed Electrical Discharges	Small nanoparticle size is promising for heterostructures; variable performance and optimization need reduce current suitability.	Moderate equipment costs	[78]

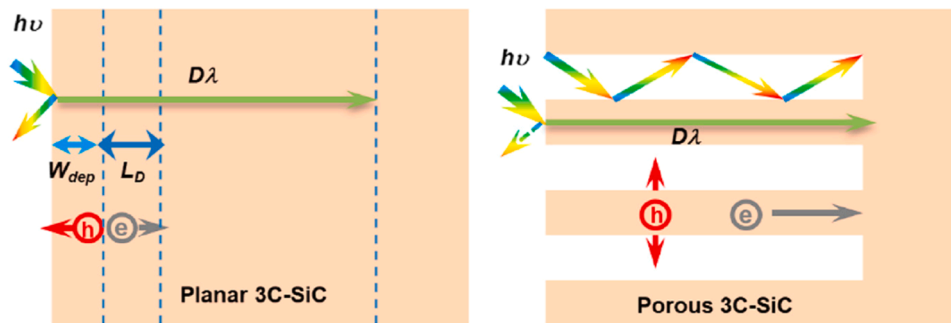


Fig. 1. Schematic illustration comparing charge separation and diffusion processes in planar 3C-SiC (left) and nanoporous 3C-SiC (right) photoanodes. Photo-generated electron-hole pairs are separated in the depletion region (W_{dep}). In planar SiC, carriers recombine over the diffusion length (L_D), while in porous SiC, enhanced light scattering within pores increases the absorption path length and promotes charge collection. Blue arrows indicate electron transport to the back contact; red arrows show hole transfer to the electrolyte (ACS, 2021 [19]).

3. SiC-Based Heterojunctions

Heterojunctions, interfaces between dissimilar semiconductors, enhance charge carrier separation and transport in PEC systems, particularly via type-II alignments that spatially separate electrons and holes [20–24]. In a typical Type-II heterojunction, the conduction band minimum (CBM) and valence band maximum (VBM) of the two semiconductors are staggered. Upon illumination, photogenerated electrons transfer from the higher-energy CBM of one semiconductor to the lower-energy CBM of the other, while holes migrate in the opposite direction. This spatial separation reduces recombination and enables efficient redox reactions on different surfaces. For SiC, heterostructures such as SiC-PAMAM-ZnO achieve ~87 % OER efficiency over 24 hours without photocorrosion [79]. Similarly, n-3C-SiC/p-Si heterostructures protect Si from corrosion, ensuring stable HER for 9 hours at 38 mA/cm² [80]. However, interface defects arising from lattice mismatch or incompatible surface chemistries can act as recombination centers, reducing overall efficiency. For instance, the lattice mismatch between SiC and MoS₂ is approximately 4 %, which may introduce strain and defects at the interface. Recent studies indicate that lattice mismatch exceeding 15–20 % in metal-semiconductor heterostructures results in high-density interface defects, significantly accelerating charge carrier recombination and degrading optoelectronic performance [81]. Even in cases of moderate mismatch, maintaining defect-free epitaxial growth remains challenging. To mitigate these issues, strategies such as the use of buffer layers, non-epitaxial growth induced by cation exchange reactions, and vdW heterointerfaces have been proposed. VdW interfaces, characterized by gaps of ~0.3–0.5 nm, can accommodate lattice misfit and suppress dislocation formation [81–83]. For example, 2D-material-assisted epitaxy has demonstrated that freestanding membranes with minimal lattice mismatch constraints can be fabricated via vdW and remote epitaxy methods [84]. However, maintaining atomically clean interfaces remains challenging, as residual contamination, thickness variations in 2D layers, and poor wettability can induce morphological defects that increase recombination rates and limit practical efficiency. While wafer reuse and scalable lift-off techniques offer potential cost reductions, the complexity of layer transfer, defect monitoring, and thermal management still pose critical barriers for large-scale integration. The stability of 2D materials in aqueous environments remains a concern, necessitating protective coatings or alternative material choices. Zhu et al. investigated the use of a-SiC:H heterostructures as photocathode protective layers and demonstrated operational stability of >100 hours and photocurrent of ~8 mA/cm² with predicted STH >10 % (measured under AM1.5 light source) [85].

Advanced fabrication strategies further improve SiC-based heterojunctions by addressing interface challenges and expanding functionality. A low-temperature (200°C) bonding method using vacuum ultraviolet/ozone activation integrates single-crystalline SiC with Si, SiO₂, and glass substrates, forming ultra-thin, high-quality interfaces that reduce defects and enhance PEC performance [86]. Similarly, a novel approach fabricates WZ-GaN/3C-SiC heterostructure nanowires by leveraging stacking faults in 3C-SiC as nucleation sites for controlled WZ-GaN growth, enabling tailored morphologies and epitaxial alignment for applications in optics, electronics, and photocatalysis [87].

To address SiC wide bandgap limitation, which restricts its use with Vis and NIR light, a SiC/Ge/graphene heterostructure incorporates Ge as a VIS-NIR-absorbing layer and graphene to form a Schottky junction, achieving high light absorption in the 500–1200 nm range for optoelectronic applications [30]. Additionally, high-quality (111)-oriented 3C-SiC films grown on 2H-AlN/Si templates via chemical vapor deposition exhibit improved structural quality for films thinner than 300 nm, owing to the suitable lattice match between 3C-SiC and AlN, despite some twinned domains and 6H-SiC inclusions. This growth process also enhances AlN structural quality by reducing dislocations, though it reduces AlN insulating properties due to cross-doping with SiC [88]. These methods highlight the potential of fabrication techniques to overcome

limitations and broaden the utility of SiC-based heterojunctions.

Multilayered heterostructures with varying bandgaps enhance charge separation and PEC efficiency. BP-SiC, with a 1.23 eV direct bandgap and type-II alignment, excels in exciton dissociation and visible-light absorption (10⁵ cm⁻¹), suitable for water splitting at pH 0–3 [89]. These properties – efficient light absorption due to the direct bandgap, effective charge separation from type-II alignment, and stability in acidic conditions – make BP-SiC suitable candidate for PEC water splitting reactions. Design requires initial layers to transmit longer wavelengths deeper into the layered structure.

In addition to conventional type-II and multilayer heterostructures, recent studies have demonstrated various experimental SiC-based Z-scheme photocatalysts with enhanced charge separation and redox activity. In Z-scheme configurations, photogenerated electrons from the conduction band of one semiconductor recombine with holes from the valence band of the other, enabling the remaining electrons and holes to maintain strong reducing and oxidizing capabilities, respectively. For example, AgCl/SiC heterostructures synthesized via mechanochemical ball milling exhibited outstanding photocatalytic performance, pH stability, and reusability [90]. Similarly, WO₃/SiC direct Z-scheme systems showed significantly improved photodegradation rates of organic pollutants due to the preserved strong oxidation and reduction capabilities of photogenerated carriers [91]. Moreover, dual Z-scheme InVO₄/SiC composites have been reported to effectively reduce CO₂ into CO under visible-light irradiation, achieving CO yields up to 142.6 μmol·g⁻¹ [92]. In another approach, Ag₃PO₄/Ag/SiC Z-scheme photocatalysts were developed with silver nanoparticles acting as electron mediators, further expanding the versatility of SiC-based Z-scheme architectures. These findings underline the broad potential of SiC as a component in both simple and multi-component Z-scheme photocatalytic systems [93].

Computational modeling and simulations play a key role in guiding the design and optimization of such advanced heterostructures, as detailed in the following section.

4. Simulation of SiC-based composition

While DFT modeling provides valuable insights into the electronic structure and interfacial mechanisms of SiC-based systems, it is important to recognize inherent limitations. Standard DFT calculations typically assume defect-free, perfectly ordered structures under vacuum conditions, neglecting solvent interactions, temperature effects, and dynamic processes occurring in real devices. Moreover, commonly used functionals such as PBE tend to underestimate bandgap energies, while hybrid functionals like HSE06 increase computational cost and remain sensitive to parameter selection. These factors can lead to discrepancies between theoretical predictions and experimental observations, underscoring the necessity of experimental validation and the integration of complementary simulation techniques, such as ab initio molecular dynamics or explicit solvation models.

The interface between the semiconductor and the electrolyte is pivotal for charge transport, recombination, and the kinetics of surface reactions. Modeling of the semiconductor-water interface reveals that the adsorption of water molecules strongly depends on the surface structure and the composition of the photocatalyst. Some semiconductive materials show notable differences in hydrogen bond dynamics due to variations in interfacial interactions and surface chemistry, which directly influence the efficiency of charge separation and the overall stability of the system, with the rate of redox reactions being a key determinant [94,95].

Calculations performed using the Perdew-Burke-Ernzerhof (PBE) functional with a plane-wave basis set are widely used due to computational efficiency. However, PBE typically underestimates bandgap values compared to experimental results. To improve accuracy, hybrid functionals such as HSE06 are often applied for band structure and optical property predictions. Furthermore, recent machine learning (ML) methods have been developed to predict corrected bandgaps and

electronic structures based on PBE outputs, offering reliable estimations with reduced computational cost. DFT modeling optimizes SiC-based PEC systems by analyzing electronic structures, bandgaps, and surface properties, guiding material design and performance enhancement. One important application of DFT is to study the kinetics of reactions on the SiC surface. Bhati et al. performed DFT and the VASPsol packages and investigated the kinetic barrier of the Hare step in the HER on 3C-SiC (110) depending on the surface charge (0 to $-10 \mu\text{C}/\text{cm}^2$). Under photoexcitation ($\lambda = 515 \text{ nm}$), the barrier decreases, improving the catalytic activity of the photocathode [96,97]. It highlights the importance of modeling surface effects, as noted by Zhang et al., correlating the surface morphology and defects of SiC with its photocatalytic performance [96,97].

In addition to surface modeling, modifications such as doping and mechanical strain are employed to enhance the properties of SiC. Incorporating transition metals like Mo and W reduces the bandgap, thereby improving visible light absorption and addressing the challenge of SiC bandgap. Similarly, mechanical compression or tensile strain alters the energy levels, as observed in the ZnO/SiC heterostructure, where the bandgap is reduced to 2.52 eV, enhancing carrier mobility and optical absorption [97,98].

A recent DFT study further explored strain engineering effects in a type-II SiC/WS₂ van der Waals heterojunction. Two stable configurations (Systems A and B) were identified, both exhibiting direct bandgaps of 1.778 eV and 1.820 eV, respectively, and favorable optical absorption in the visible region. Biaxial strain ranging from -6% to $+10\%$ revealed a non-linear impact on bandgap and carrier effective mass. Notably, compressive strain (-2%) reduced the hole-to-electron effective mass ratios to as low as 0.901 and 0.910, enhancing charge separation. The system also showed promising photocatalytic performance under compressive strain, meeting the criteria for spontaneous water splitting at strain levels of -4% , -2% , and 0% . The most efficient configuration (System B at -4%) achieved a theoretical STH of 16.91 %, highlighting the strong tunability of SiC/WS₂ heterostructures via mechanical modulation. These findings emphasize the critical role of strain in optimizing PEC properties of SiC-based heterojunctions and provide foundational

guidance for future material design [99].

Alongside doping and strain, vdW heterostructures – combining SiC with two-dimensional materials such as graphene, MoS₂, hBN, and GaN through weak vdW interactions – show significant promise for PEC applications. The vdW heterostructures, typically exhibiting type-II band alignment, promote efficient charge separation and reduce recombination. However, computations reveal that, despite the expected properties of vdW heterostructures, external factors can significantly influence and optimize their characteristics. For example, mechanical strain not only alters the energy levels but also leads to notable transitions, such as a shift from a direct to an indirect bandgap in SiC-CrSe₂, as well as a switch from type-II to type-I band alignment in strained SiC-CrS₂ and SiC-CrSe₂ vdW heterostructures [100]. This tunability underscores the importance of external factors for practical applications of low dimension structures in thermoelectric devices and optoelectronics.

Table 2 summarizes the simulated properties of 15 heterostructures. Such, Al₂CO/SiC exhibits a direct bandgap of 2.27 eV and high absorption in the visible and UV ranges [101].

Recent first-principles calculations have demonstrated that SiC-based heterostructures can achieve significant STH efficiencies. For example, Li et al. investigated the SiC/PtSe₂ vdW heterostructure using the HSE06 hybrid functional and reported a theoretical STH efficiency of 34.7 %. The model considered an indirect bandgap of 1.52 eV, enhanced optical absorption surpassing the monolayer components, and favorable Gibbs free energy changes for both HER and OER ($\Delta G_{\text{PDS}} = 2.03 \text{ eV}$). These results underline the potential of SiC-based systems to exceed the conventional STH thresholds and support the feasibility of achieving efficiencies above 10 % [102]. BlueP/SiC displays a bandgap of 1.409 eV and an absorption coefficient of $2.082 \times 10^5 \text{ cm}^{-1}$ at 404 nm [103]. All structures demonstrate thermal and dynamic stability, with absorption coefficients up to $1 \times 10^6 \text{ cm}^{-1}$, outperforming standalone materials [104,105].

Hou and Wang [106] simulated hexagonal lattices of SiC and MoS₂ monolayers, suggesting a high potential for creating stable SiC/MoS₂ heterostructures with controlled interlayer exciton lifetimes of $\sim 10^{-6}$ to $\sim 10^{-9}$ seconds through manipulating the stacking sequence. Hou and

Table 2
Modeling results of semiconductor SiC and various vdW heterostructures.

	Electrode Material	Shape and Size of Nanostructures	Bandgap	Absorption Coefficient/ ABPE	Source
1	Al ₂ CO/SiC	2D multilayer heterostructure, lattice mismatch of 4 %	2.27 eV	Ultraviolet and visible regions	[101]
2	XSe/SiC (X = Mo, W)	3.404 Å and 3.612 Å interface distance for MoSe/SiC and WSe/SiC heterostructures, respectively	1.117 eV and 1.426 eV for MoSe/SiC and WSe/SiC, respectively	569.1 nm and 393.2 nm for MoSe/SiC and WSe/SiC, respectively	[120]
3	2D ZnO/SiC	ZnO and SiC layers with lattice constants of 3.262 Å, 3.138 Å for ZnO and SiC, respectively	2.86 eV and 2.74 eV for patterns I -II, respectively	Under strain absorption peak reaches $4 \times 10^5 \text{ cm}^{-1}$	[121]
4	SiC/GaN	Monolayers stacked in different configurations, with G2 being the most stable	3.331 eV	Under strain absorption peak $3.4 \times 10^5 \text{ cm}^{-1}$	[122]
5	SiC/PtS ₂	Lattice mismatch of 4.45 %	1.52 eV	Absorption peak $5.19 \times 10^5 \text{ cm}^{-1}$. STH = 34.7 %	[102]
6	2D SiC containing graphene and silicene nanodomains	Substituting Si atoms with C atoms and C atoms with Si atoms for graphene and silicene, respectively	2 eV	Visible range	[123]
7	2D GeC-SiC	1.875 Å and 1.847 Å bond lengths for GeC and SiC, respectively	1.978 eV, 2.278 eV, and 2.686 eV, depending	Absorption coefficient $1 \times 10^6 \text{ cm}^{-1}$ in the UV range	[124]
8	BlueP and XC (X = Ge, Si)	Lattice constants of 3.096 Å and 3.275 Å for SiC and BlueP, respectively	1.409 eV	Absorption peak is $2.082 \times 10^5 \text{ cm}^{-1}$ at 404 nm	[103]
9	SiC and Janus MS ₂ (M = Mo, W)	Lattice constants around 3.17-3.18 Å for both SiC-MoS ₂ and SiC-WSe ₂	1.74-2.34 eV for different models	Strong visible light absorption, with peaks in the ultraviolet region	[125]
10	SiC and VXY (X = Cl, Br and Y = Se, Te)	Lattice constants of 3.25 Å, 3.255 Å, 3.353 Å, 3.397 Å, and 3.485 Å for SiC, and VClSe, VBrSe, VClTe, and VBrTe, respectively	2.05 eV, 2.35 eV, 1.96 eV, 1.52 eV	Visible region	[126]
11	SiC, SiS, and P monolayers	Lattice constants of 3.19 Å for SiS-SiC	2.22 eV and 2.21 eV for SiS-SiC and SiS-P respectively	Exciton peaks at 1.63 eV and 1.45 eV for SiS-P and SiS-SiC, respectively	[127]
12	GaN/SiC	Layered structures of GaN and SiC, with atom-alignment configurations	2.05 eV,	Visible-light absorption	[128]
13	β-AsP/SiC	Stacking of 14 atoms in a supercell structure with 3 As atoms, 3 P atoms, 4 Si atoms, and 4 C atoms	1.65 eV	10^5 cm^{-1} in the visible and ultraviolet light range. STH energy conversion efficiency calculated to be 5.9 %	[129]

Wang optimized 12 stacking modes as illustrated in Figure 2 (six symmetric structures were formed: 1-AA, 1-AA', 1-AB, 1-AB', 1-A'B', and 1-A'B upper panel, and six additional structures -AA, 2-AA', 2-AB, 2-AB', 2-A'B', and 2-A'B in the lower panel). Calculations for four stacking configurations (1-AA, 1-A'B, 2-AA, 2-A'B) revealed that 2-AA and 2-A'B exhibit the most intense peaks, driven by interlayer excitons with binding energies of 0.46–0.54 eV. In 2-A'B, electric field accelerates recombination, reducing the exciton lifetime to 1.02×10^{-7} s. Configurations 1-A'B and 2-A'B produce bright excitons with high absorption intensity due to spin-conserved transitions, while 1-AA and 2-AA yield dark excitons with low intensity due to spin-flip transitions, as confirmed by including spin-orbit coupling [106].

In addition to evaluating electronic structures and bandgaps, first-principles calculations can be extended to estimate the theoretical STH conversion efficiency of photocatalysts. Recent studies have demonstrated that combining density functional theory with kinetic and thermodynamic modeling enables estimation of STH efficiency limits for various heterostructures. For example, Fu et al. [107] showed that intrinsic vertical electric fields in two-dimensional materials can enhance carrier separation and extend absorption into the infrared, with predicted STH efficiencies reaching up to 32 %. Fan et al. [108] proposed a Z-scheme PEC mechanism in $\text{MoSe}_2/\text{SnSe}_2$ and $\text{WSe}_2/\text{SnSe}_2$ van der Waals heterostructures, where spatial separation of the hydrogen and oxygen evolution reactions on distinct layers enables spontaneous full water splitting. Their simulations reported STH efficiencies of up to 10.5 %, without the need for external bias or sacrificial agents, offering a viable route toward scalable PEC devices.

Furthermore, Li et al. [109] established that Z-scheme heterostructures have a theoretical STH efficiency limit of ~ 37.8 %, higher than that of type-I and type-II configurations (~ 17.1 %). Building on this, Zhang et al. [110] systematically screened 46 Janus group-III

chalcogenide monolayers and identified multiple vdW heterostructures with type-II band alignment, lattice mismatch < 5 %, and photovoltaic power conversion efficiencies exceeding 20 %, notably $\text{Ga}_2\text{Te}-\text{GaInS}_2$ at 23.69 %. Although these values are specific to PV applications, the underlying band engineering principles are transferable to PEC systems. Finally, the integration of SiC with Janus two-dimensional materials, such as MoSse monolayers, has been proposed as an effective strategy to introduce intrinsic electric fields that promote efficient charge separation and improve redox kinetics. Theoretical studies suggest that such Janus-based SiC heterostructures could potentially achieve STH efficiencies exceeding 20 %, offering a promising direction for the rational design of advanced photocatalysts [111]. Furthermore, recent first-principles calculations on Janus SiC/ SnSse vdWHs underscore their potential for high-efficiency PEC applications. These vdWHs exhibit a type-II band alignment and benefit from both an intrinsic dipole in the Janus SnSse layer and an interfacial electric field arising from charge redistribution between SiC and SnSse . This dual-field structure strongly promotes spatial separation of photo-generated electron-hole pairs, thus enhancing redox kinetics. The reduced bandgap in the heterostructure improves optical absorption across the visible and infrared regions, resulting in a predicted STH of 41.5 %. Additionally, biaxial tensile strain further increases photocurrent density by 31 %, highlighting the tunability of optoelectronic properties via external mechanical modulation. These findings provide a robust design pathway for high-performance Z-scheme PEC systems based on low-dimensional SiC heterostructures [112]. In addition to SiC/ SnSse , Janus-type heterojunctions based on g-SiC and SMoSiN_2 have also shown promise as direct Z-scheme photocatalysts. Recent DFT calculations revealed that g-SiC/ SMoSiN_2 heterojunctions with opposite polarization directions (denoted Pup and Pdown) possess direct bandgaps of 1.72 eV and 1.61 eV, respectively, along with excellent thermodynamic and dynamical stability. These heterostructures exhibit a built-in electric field directed from g-SiC toward SMoSiN_2 , which acts as an internal driving force for efficient charge separation. Importantly, this configuration enables a direct Z-scheme mechanism that preserves strong redox potential for both HER and OER. The system demonstrates exceptionally high carrier mobility – up to $7867.56 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$ – and strong visible-light absorption on the order of 10^5 cm^{-1} . Under neutral pH conditions, the photogenerated carriers drive spontaneous hydrogen and oxygen evolution reactions without the need for external bias or sacrificial agents. The calculated STH reaches 27.53 %, surpassing the conventional theoretical limit for PEC water splitting. These findings highlight g-SiC/ SMoSiN_2 vdW heterojunctions as highly promising candidates for next-generation Z-scheme PEC architectures [113].

Challenges inherent to traditional first-principles simulations include limited accuracy in modeling complex solid-liquid interfaces, slow computational workflows, and often limited correlation with experimental PEC performance. These limitations have motivated the increasing integration of artificial intelligence (AI) and ML into computational materials discovery pipelines [114,115]. By augmenting DFT with surrogate models, ML can accelerate the screening of candidate materials, predict key performance metrics, and facilitate the design of high efficiency heterostructures. This integration has further enabled the development of digital twins – computational frameworks that couple experimental feedback with predictive simulations to optimize PEC device design and operation.

A notable demonstration of this approach was presented by Biswas et al. [116], who implemented a hierarchical ML-DFT workflow using multi-fidelity surrogate models trained on ~ 1000 halide perovskite compositions computed with both PBE and HSE06 functionals. Their model enabled high-throughput screening of over 150,000 ABX_3 perovskites, identifying over 3000 thermodynamically stable candidates with suitable bandgaps and STH efficiencies exceeding 20 %, with some approaching 24 %. This work underscores the value of surrogate models for navigating vast chemical spaces with high accuracy.

In the context of SiC-based PEC systems, Ma et al. investigated three

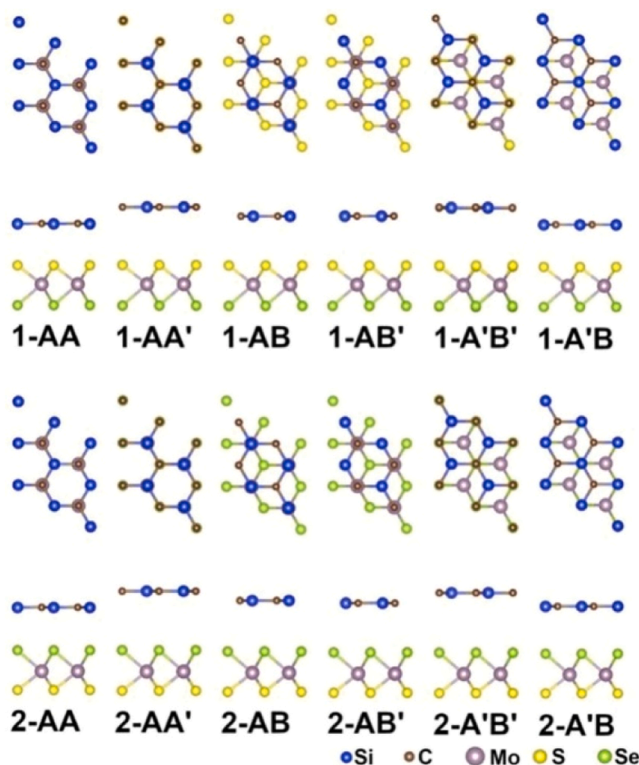


Fig. 2. The top and side views of SiC/ MoSse . Upper panel: six different stacking modes by rotating the top SiC monolayer at different special angles compared with MoSse monolayer; lower panel: the obtained other six structures through changing the relative positions of S and Se atoms (Elsevier 2021 [106]).

potential photocatalytic materials – $\text{Si}_4\text{C}_4\text{HF}_3\text{Br}_2\text{I}_2$, $\text{Si}_4\text{C}_4\text{F}_3\text{ClBr}_3\text{I}$, and $\text{Si}_4\text{C}_4\text{F}_3\text{ClBr}_2\text{I}_2$ (with 1.96 eV, 2.16 eV, and 1.71 eV, respectively), which are suitable for photocatalytic water splitting compared to monolayer SiC, by combination ML and DFT (Figure 3a). The band edge positions of listed materials align with the redox potentials for H^+/H_2 and $\text{O}_2/\text{H}_2\text{O}$ at pH 0 and 7 and exhibit low effective mass (m^*) and high electron mobility ($10^3 \text{ cm}^2 \text{ V}^{-1} \cdot \text{s}^{-1}$), confirming their ability to drive water splitting (Figure 3b). Partial charge density reveals that the CBM is localized on the upper surface (Si, C, and halogens like H, F, Cl), while the VBM is concentrated around Br and I on the lower surface, enhancing charge separation for hydrogen and oxygen evolution reactions (Figure 3c).

Optical absorption (Figure 3d) shows the materials absorb three times more visible and infrared light than monolayer SiC, with a redshift due to smaller bandgaps. For the HER (Figure 3e), the ΔGH is around -0.28 eV to -0.31 eV without light, requiring a small energy barrier to form H_2 . Under light, photogenerated electrons drive HER spontaneously. For the OER (Figure 3f), the maximum ΔGO_2 is 1.53 eV for $\text{Si}_4\text{C}_4\text{F}_3\text{ClBr}_3\text{I}$ without light, but illumination provides enough $U_{\text{h}} = 1.62 \text{ V}$ for a spontaneous reaction. Finally, AI MD simulations confirm the dynamic and thermodynamic stability of these materials, supporting their potential for photocatalytic applications [117].

Despite such theoretical promise, real-world PEC systems often suffer

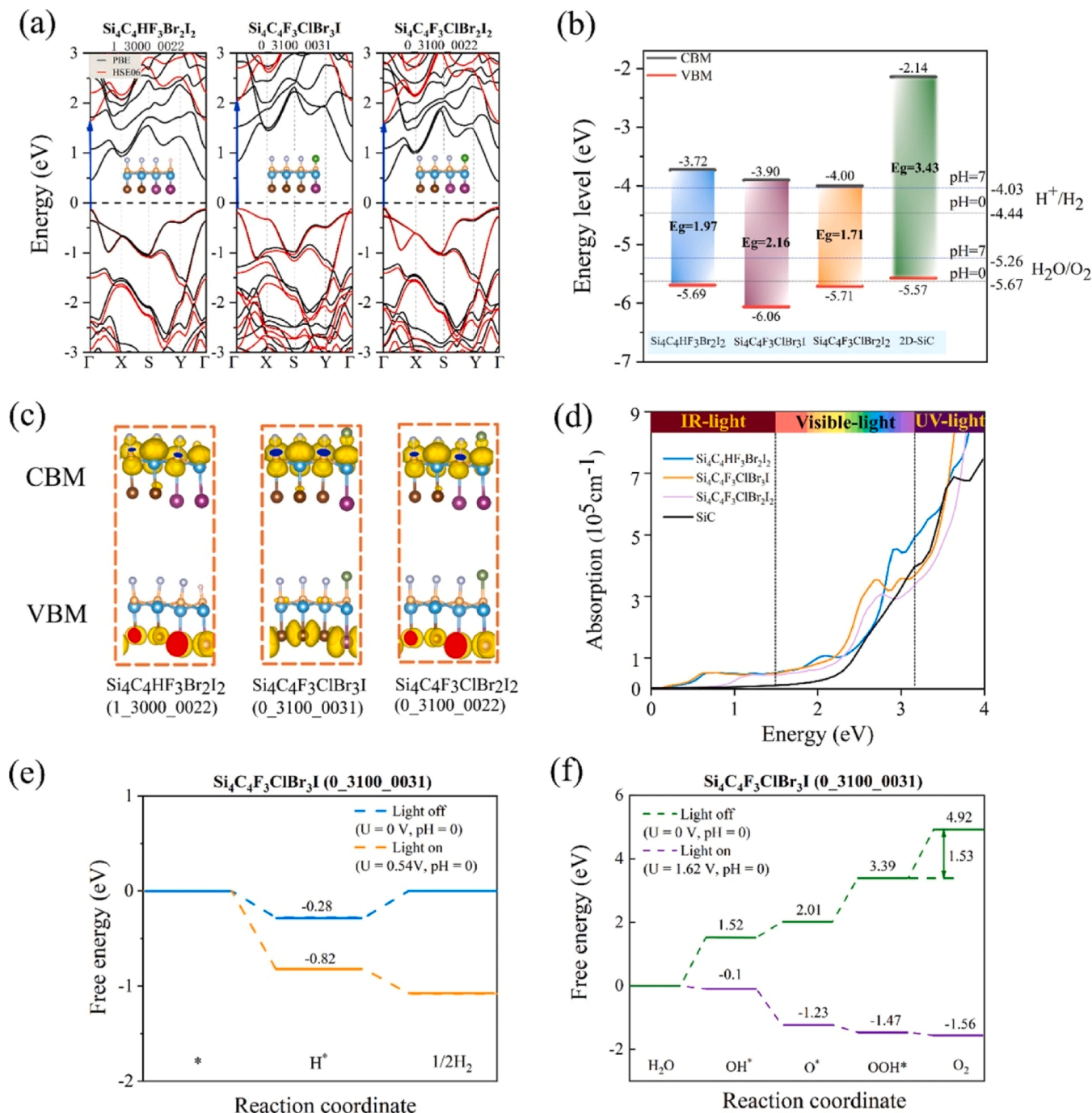


Fig. 3. Structural, electronic, optical property and catalytic activity diagrams of potential photocatalytic materials. (a) Band structures and the side views after relaxation. The blue arrow points from VBM to CBM. The blue, orange, light pink, silver, green, brown, and purple balls represent Si, C, H, F, Cl, Br, and I atoms, respectively. (b) Band alignment. (c) Partial charge density of CBM and VBM. (d) Optical absorption coefficient. These results are obtained by the calculations based on the HSE06 functional. Free energy diagrams of (e) HER and (f) OER for $\text{Si}_4\text{C}_4\text{F}_3\text{ClBr}_3\text{I}$ (0_3100_0031) under different conditions (Elsevier, 2024 [117]).

from a persistent performance gap: while simulations may predict STH efficiencies above 30 %, experimental values for SiC based photoelectrodes typically remain below 8 %. This discrepancy arises from idealized modeling assumptions—such as defect-free, perfectly crystalline interfaces – and the neglect of practical factors like lattice mismatch (>4 %), charge recombination at grain boundaries, catalyst degradation, and optical losses in multilayer electrodes. Bridging this gap requires a more holistic integration of ML-enhanced simulations with experimental characterization to guide iterative design and fabrication processes.

Beyond computational screening, ML is also increasingly being applied to experimental PEC datasets, despite the challenges posed by sparse and noisy data. For example, a recent study developed clustering-augmented ML models combined with SHAP (Shapley Additive Explanations) to predict photocurrent density in hematite and BiVO₄ photoanodes [118]. This approach identified key descriptors (e.g., dopant radius, donor density, interface roughness) even with limited datasets, achieving R² values exceeding 0.85. In a related review, Liang et al. [119] highlighted the utility of interpretable ML methods – such as random forests and Bayesian optimization—in optimizing co-catalyst loading, interfacial morphology, and band alignment in heterostructured systems which collectively emphasize that surface and interface engineering, informed by data-driven approaches, is increasingly critical in achieving high-efficiency PEC devices.

Based on charge transfer mechanisms and band alignment, we systematically categorize SiC-based heterostructures into three main types as (i) type-II heterojunctions, (ii) Z-scheme systems, and (iii) Janus configurations, each offering distinct advantages for PEC applications

The demonstrated advantages of SiC based heterostructures provide the basis for their use in more complex systems. Tandem PEC cells, which combine multiple photoactive layers to maximize the solar spectrum, are a natural extension of these advances. In the next section, we discuss how SiC heterostructures can be integrated into tandem systems to improve solar-to-hydrogen conversion efficiency. These stable structures outperform single materials.

SiC can be integrated into tandem photoelectrochemical systems in combination with several metal oxides such as TiO₂, WO₃, and BiVO₄, which are listed in Tables 3–6. These combinations leverage the wide bandgap and chemical stability of SiC as the bottom photoelectrode and the visible-light absorption of the oxide as the top photoanode. For example, tandem architectures combining TiO₂ photoanodes and 3C-SiC photocathodes have been reported to improve durability, although their STH efficiencies remain lower (<1 %) compared to Si/metal oxide tandems. In contrast, BiVO₄/Si tandem cells have achieved efficiencies exceeding 5 %, albeit with challenges related to photocorrosion. Therefore, while SiC-based tandem systems offer superior stability and tunability, their overall performance still requires optimization relative

Table 3
Performance of BiVO₄ based Tandem PEC Cells for Water Splitting.

Cell Configuration	STH Efficiency (%)	Stability	Source
NiOOH/FeOOH/BiVO ₄ /SnO ₂ /TTO/ TOPCon Si	1.72	24 h	[155]
n+p-Si/Nb ₂ O ₅ /NiPt W:BiVO ₄ /NiCo (O-OH) ₂	3.9	50 h	[156]
CoBi/BiVO ₄ /TiO ₂ a-Si	3.0		[157]
BiVO ₄ TOPCon Si	0.24		[158]
W:BiVO ₄ a-Si:H/nc-Si:H	5.2		[151]
BiVO ₄ /Cu ₂ O/NiFe-LDH BiVO ₄ / Cu ₂ O-C/TiO ₂	1.18		[159]
Co(OH) ₂ /BiVO ₄ Carbon-based PSC	4.6		[160]
Cu ₂ ZnSnS ₄ BiVO ₄	8.0	168 h	[161]
Nanocone/Mo:BiVO ₄ /Fe(Ni)OOH Perovskite	3.2		[162]
Perovskite/BiVO ₄	1.3	96 h	[163]
CoPi/W:BiVO ₄ SHJ (dual photoanode)	2.1		[164]

Table 4
Performance of Hematite-Based Tandem PEC Cells for Water Splitting.

Cell Configuration	STH Efficiency (%)	Source
p-Si/TiO ₂ /Fe ₂ O ₃ TiO ₂ /TiO ₂	0.18	[173]
α-Fe ₂ O ₃ LFO:Cr	0.0026	[174]
Fe ₂ O ₃ /NTO/Co-Pi Perovskite PSC	3.25	[175]
Ti-Fe ₂ O ₃ /FeS/FeOOH Si	4.7	[176]
Fe ₂ O ₃ (ALD-modified) CH ₃ NH ₃ PbI ₃	3.4	[177]

Table 5
Performance of WO₃-Based Tandem PEC Cells for Water Splitting.

Cell Configuration	STH Efficiency (%)	Source
BiVO ₄ /WO ₃ Porphyrin-Dye	5.7	[182]
WO ₃ /BiVO ₄ c-Si PV	2.3 (front), 3.2 (back)	[183]
SS/a-Si WO ₃	>3.0	[184]

Table 6
Performance of TiO₂-Based Tandem PEC Cells for Water Splitting.

Cell Configuration	STH Efficiency (%)	Stability	Source
CdS/CdSe/TiO ₂ CdS/CdSe/TiO ₂	2.78		[188]
BiFeO ₃ /TiO ₂ NT/N719 DSSC	0.0033	6 h	[189]
TiO ₂ /FeS/FeOOH	1.353	200 h	[190]
BiOI/TiO ₂ DSSC	1.34		[191]
GaInP ₂ /GaAs/TiO ₂ /TiN/Ni ₅ P ₄	11.4–13.2	>200 h	[192]
GaAs/TiO ₂ /Ni-Pi	9.5	110 h	[193]

to state-of-the-art configurations involving silicon or perovskites.

4.1. SiC in tandem PEC cells

Tandem PEC systems connect photoanode and photocathode in series to optimize light absorption and charge separation. The essence of a tandem-scheme PEC system is that the top photoelectrode must be transparent to longer wavelengths, allowing sufficient photon transmission to the bottom photoelectrode, with both needing to be current-matched to balance photon absorption [130,131]. The photoanode generates holes for oxygen evolution, while the photocathode produces electrons for hydrogen evolution. Different bandgaps broaden spectral coverage, reducing losses. Z-scheme designs enhance photocurrent via efficient charge transfer [132].

Traditionally, PEC systems are classified into three configurations: photocathode-based, photoanode-based, and hybrid tandem cells, where both the photoanode and photocathode are active. Figure 4 illustrates schematic diagram of a tandem photoelectrochemical cell consisting of a TiO₂ photoanode and a 3C-SiC photocathode. The tandem configuration is designed to optimize light absorption and charge separation for efficient water splitting. In hybrid tandem cells, light is absorbed by both the photoanode and the photocathode materials, increasing the overall conversion of photons into chemical energy [133].

In PEC/PV systems, PV cells boost voltage for charge separation, with electrons recombining in the PV and hydrogen evolving at the cathode. Figure 5 represents simplified schematic of a photoelectrochemical/photovoltaic (PEC/PV) tandem cell configuration, using a photoanode/PV setup as an example. This Fig. demonstrates how the PEC and PV components are integrated to enhance overall solar-to-hydrogen efficiency [134]. Another promising approach involves the separation of hydrogen and oxygen evolution into distinct cells. The authors of [135] demonstrated a method for producing hydrogen and oxygen in separate compartments connected solely by metallic wires. This strategy eliminates the need for membranes, which can introduce energy losses and complicate the system’s design [135].

The scientific community is also increasingly interested in various types of solar concentrators, such as Fresnel lenses, parabolic mirrors,

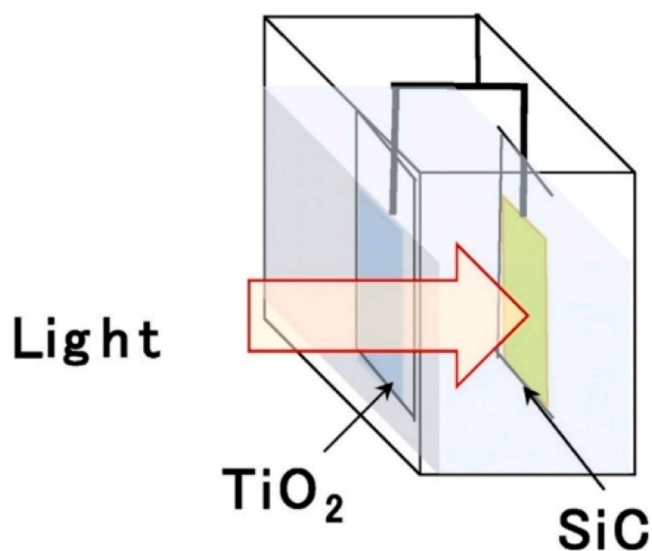


Fig. 4. Schematic diagram of a tandem PEC cell composed of a TiO_2 photoanode and a SiC photocathode. The illustration shows visible light transmission through the TiO_2 layer to the underlying SiC, enabling sequential photon absorption [133].

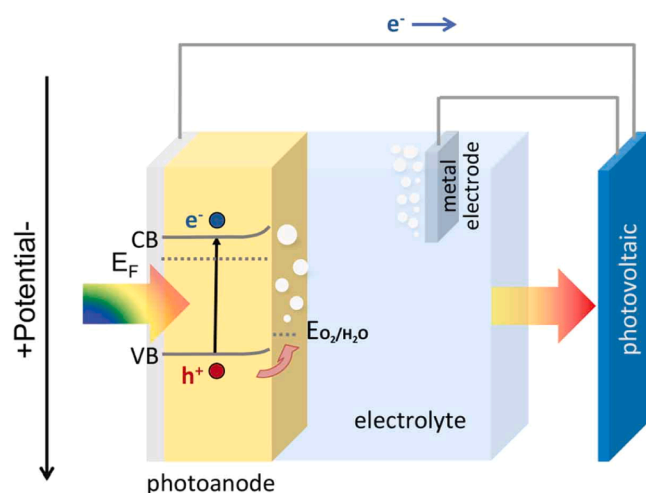


Fig. 5. Simplified illustration of the PEC/PV tandem cell configuration (taking the photoanode/PV as an example) (with permission of Creative Commons CC BY license Taylor & Francis 2018).

and tracking systems, which maximize solar energy capture and focus it on photoelectrodes. However, while these technologies enhance light utilization, they also introduce additional costs [136].

Incorporating cocatalysts into the photoelectrode modifies the energy levels, facilitating charge transfer and accelerating surface reactions. This enhances the efficiency of PEC water splitting by reducing the energy barriers for hydrogen and oxygen evolution (Figure 6a).

By introducing mid-gap states through doping or defects, the semiconductor bandgap is altered to enhance light absorption. These states allow the material to capture lower-energy photons, improving its ability to utilize the visible spectrum for PEC applications (Figure 6b). A Z-scheme system, using two narrow-bandgap semiconductors, optimizes charge separation and enables efficient, unassisted water splitting. The configuration shows the electron and hole transfer pathways, mimicking natural photosynthesis to drive the complete water splitting reaction without external bias (Figure 6c) [137]. However, Z-scheme systems use two photocatalysts for efficient water splitting, though modeling defects remains complex [138], and often demand the sacrificial reagents to prevent back-reactions, while heterostructures such as CdS/SnS_x enhance efficiency without them [139,140].

Along with catalyst materials and electrolyte composition, system temperature boosts PEC efficiency but can degrade stability, as seen in $\text{CaBi}_6\text{O}_{10}$ electrodes [141–143]. Thus, it is crucial to consider thermal effects during the operation of photocatalytic systems to prevent structural deterioration and long-term efficiency losses.

The US Department of Energy targets $\geq 20\%$ STH efficiency for commercial water splitting. On the way to the required 20 %, researchers are trying out different variations and combinations of photoactive materials. Many combinations do not find practical application not only because of their low efficiency, but also because of their complex designs or rapid degradation reactions of the photoelectrodes. The perovskite/Si combination exceeds the efficiency threshold at lower costs, with scalable devices up to 342 cm^2 [144]. Overall, perovskites and their derivatives exhibit high catalytic activity, tunable band gaps, and adjustable energy levels due to their structural flexibility and diverse chemical compositions [145]. However, despite these advantages, the instability of surface states and material degradation limit their widespread application [146]. Systems based on integrations PEC with solar cells operates with reduced external power needs [147], but requires additional technological solutions for the production of photovoltaic devices.

Tandem systems, combining different bandgap semiconductors, enhance STH efficiency without external energy, gaining significant attention [148,149]. However, many of these systems rely on metal oxide photoelectrodes, which, despite their potential, face significant challenges that impact overall performance. Metal oxide photoelectrodes in tandem PEC cells face limitations [150]. BiVO_4 (2.4 eV) absorbs up to 520 nm, and BiVO_4/Si tandem configurations have been reported to achieve STH efficiencies exceeding 5 % under simulated AM

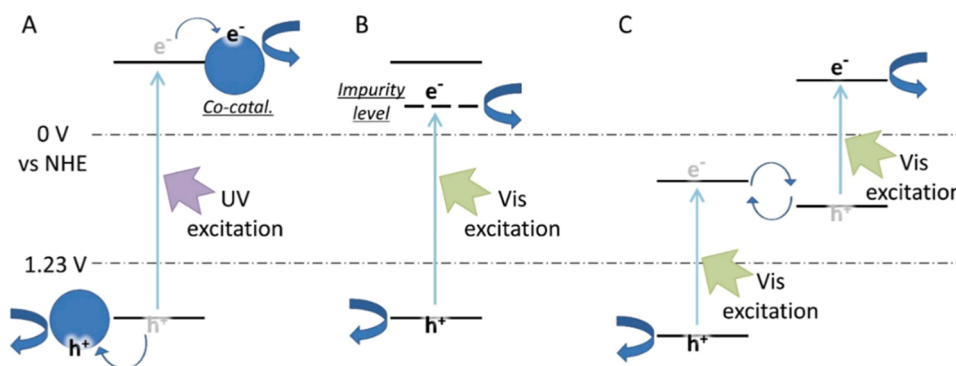


Fig. 6. Schematic of energy diagrams of wide-bandgap semiconductors with (A) cocatalysts and (B) impurity energy level. (C) is a typical Z-scheme using two narrow bandgap semiconductors (with permission by MDPI 2024 [137]).

1.5G illumination without external bias [151]. However, they require protective layers due to photocorrosion [151–154]. To provide a comprehensive view of current tandem PEC cell performance, Table 3 summarizes the STH efficiencies and stability of various configurations, particularly those involving BiVO₄.

Table 3 shows that BiVO₄ and Si dominate tandem PEC systems, achieving STH efficiencies up to 8 % (Cu₂ZnSnS₄||BiVO₄, AM 1.5G, 100 mW/cm², unassisted two-electrode configuration) and photocurrents up to 5.82 mA/cm² (Nanocone/Mo:BiVO₄/Fe(Ni)OOH||Perovskite). However, BiVO₄ short carrier diffusion length and Si susceptibility to photocorrosion limit long-term stability and scalability.

Fe₂O₃ (2.0–2.2 eV) is stable, absorbs up to 600 nm, but low conductivity limits STH to ~5 % despite doping improvements [165–172].

Table 4 summarizes the performance of various Fe₂O₃ based tandem PEC cells for water splitting.

α -Fe₂O₃ based tandem cells achieve modest STH efficiencies (up to 4.7 %) and photocurrents (up to 4.24 mA/cm²), but performance is limited by short carrier lifetimes and poor conductivity.

Tungsten trioxide (2.5–2.7 eV) is stable in acidic pH, absorbs up to 460 nm, yet low mobility hinders efficiency [178–180]. Table 5 summarizes the performance of tandem PEC cells utilizing WO₃ as a photoanode for water splitting [181].

Titanium dioxide (3.0–3.2 eV) is UV-limited (<400 nm), stable, but requires doping for visible light use [134,185–187]. Table 6 summarizes the performance of tandem PEC cells utilizing TiO₂ as a photoanode or photocathode for water splitting. Table 6 includes configurations with

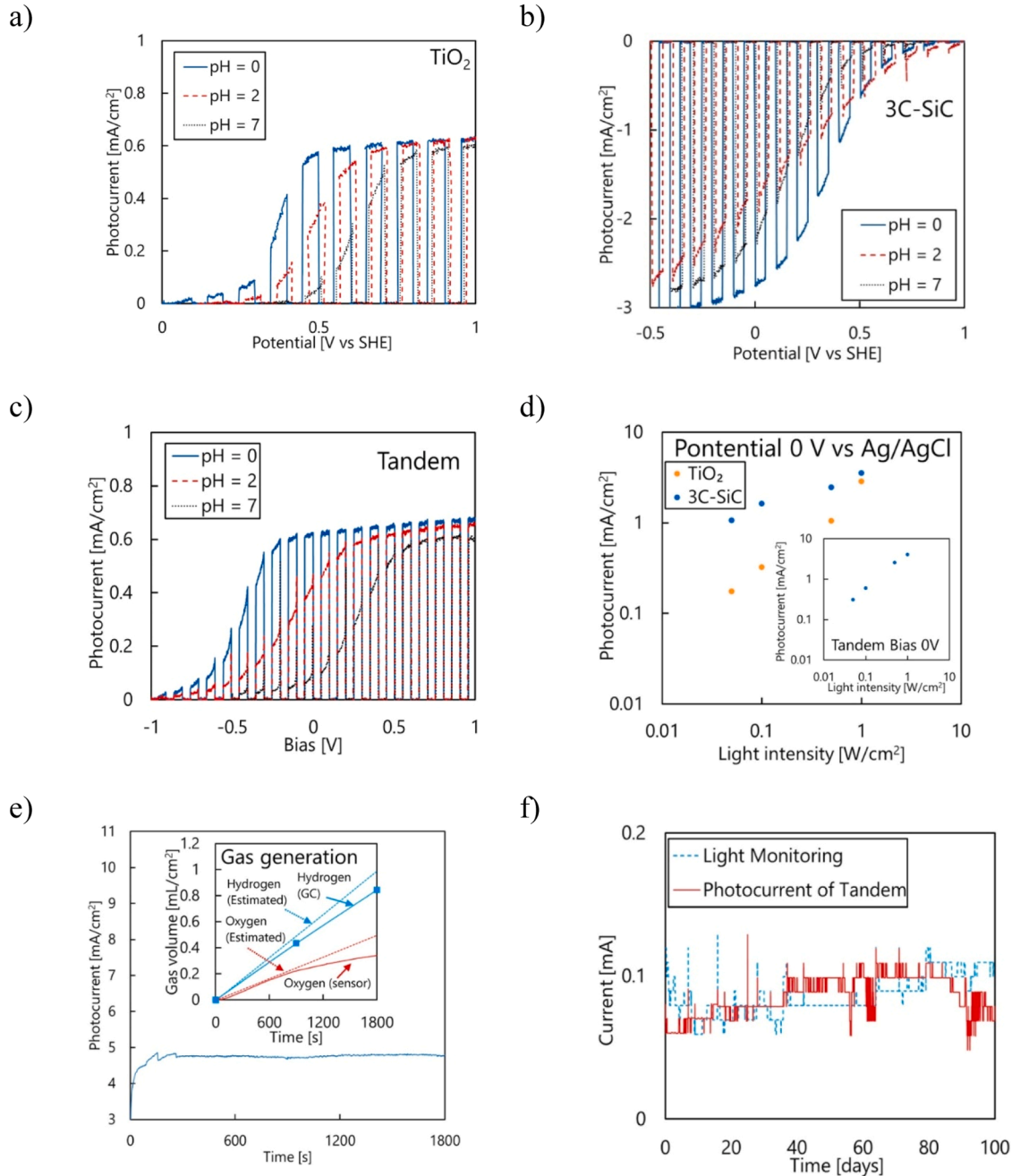


Fig. 7. Performance characteristics of TiO₂/3C-SiC tandem PEC cells. (a–c) pH dependence of photocurrent densities under broadband illumination at 0.1 W/cm²; (d) light intensity dependence of photocurrents for individual and tandem electrodes (inset: photocurrent vs. intensity); (e) long-term stability test under white light illumination at 1 W/cm² and 0.4 V bias over 1800 s, with evolved gas volumes (H₂, O₂) measured via gas chromatography and oxygen detector; (f) photocurrent response under 405 nm LED illumination (0.5 W/cm²) without external bias [133].

CdS/CdSe, BiFeO₃, GaAs, and III-V photocathodes, reporting STH efficiency, and stability under 1 sun illumination (AM 1.5G).

TiO₂-based tandem PEC systems suffer from several critical limitations that hinder their commercial viability for water splitting. The wide bandgap of TiO₂ restricts absorption to the UV region, resulting in low STH efficiencies in simpler configurations (e.g., 0.0033 % for BiFeO₃/TiO₂||TNT/N719 DSSC [189], 1.34 % for BiOI/TiO₂||DSSC [191]), necessitating complex sensitization (e.g., CdS/CdSe [188]) or integration with high-cost III-V semiconductors (11.4–13.2 % STH for GaInP₂/GaAs/TiO₂/TiN/Ni₅P₄ [192]) to achieve competitive performance. Photocurrents are modest (e.g., 2.08 mA/cm² for TiO₂/FeS/FeOOH [190]), and stability is often short, even though systems demonstrate seawater splitting with 200 h stability [190]. The reliance on toxic (e.g., CdS/CdSe) or expensive materials (e.g., GaAs) and complex fabrication hampers scalability and environmental sustainability. Incomplete performance metrics for several configurations indicate inconsistency, underscoring the need for materials which offer a tunable bandgap, high carrier mobility, and superior stability for more efficient and durable PEC systems, including potential seawater applications. As shown in Zhang et al. investigation [133], coupling physicochemical properties of TiO₂ and 3C-SiC in tandem system offers competitive conditions for hydrogen generation. Briefly, [133] demonstrates that the photocurrent of a TiO₂ photoanode increases under low pH, confirming its high efficiency in acidic environments (Figure 7a).

In contrast, the photocurrent of a 3C-SiC photocathode exhibits minimal dependence on pH and reaches its maximum at pH = 0 due to suppressed charge recombination (Figure 7b). Consequently, the TiO₂/3C-SiC tandem system exhibits enhanced photocurrent at low pH, benefiting from the surface properties of both materials (Figure 7c). Under illumination with an intensity of 1 W/cm², this structure delivers a stable photocurrent of 4.75 mA/cm² and maintains long-term stability over 100 days (Figure 7d-f).

A major challenge in SiC-based PEC systems is ensuring long-term stability under illumination. Photoelectrodes often suffer from photocorrosion in aqueous electrolytes, where photogenerated holes oxidize the semiconductor surface. Photocorrosion persists in tandem systems. Polymer electrolytes reduce it but may lower photoactivity [150,194]. For SiC, this can lead to the formation of SiO₂, which passivates the surface but may also block charge transfer. To address this, conformal coatings such as TiO₂ or Al₂O₃ have been employed, extending stability from hours to over 100 days in systems like TiO₂/3C-SiC [195].

Strategies to reduce anodic corrosion in SiC include:

- Photonic crystals: 3C-SiC with protective coatings (e.g., g-CN, NiO) enhances absorption and stability.
- Redox molecules: Oxidize photoholes to protect SiC surfaces.
- Catalysts: Co-Pi redirects photoholes to OER [196–198].

Another challenge is the scalable fabrication of nanostructured SiC. While anodization in HF produces high-performance nanoporous SiC, the use of toxic HF limits scalability. Alternative methods, such as plasma-assisted KOH etching, offer an eco-friendly solution with high etching rates (540 nm/min for 4H-SiC) [76], but further optimization is needed for industrial adoption.

Analyzing discussed above, a key challenge in tandem PEC cells is the scarcity of stable, efficient p-type photocathodes for water reduction. While n-type photoanodes such as WO₃ and Fe₂O₃ have advanced, p-type options such as TiO₂/GaP show low photocurrents and stability [199]. Summarizing metal oxide material limitations, SiC-based heterojunctions and tandem systems offer a promising solution. SiC excels as a photoanode or photocathode, particularly with TiO₂, BiVO₄, or perovskites, to boost STH efficiency.

Oxynitride perovskites, such as SrTaO₂N on GaN/SiC substrates, demonstrate significant potential for enhancing the efficiency of PEC water splitting. These materials absorb light up to 550 nm, exhibit a high transmittance coefficient (>60 %), and begin generating photocurrent at

a low onset potential of approximately -0.4 V relative to the reversible hydrogen electrode (RHE), reaching a photocurrent density of 6 μA/cm² at 1.23 V relative to RHE – surpassing similar photoanodes like LaTiO₂N and CaNbO₂N [200]. Figure 8, depicts PEC reaction using a GaN/SiC semiconductor structure coated with SrTaO₂N layers of 60 nm and 30 nm thickness.

Under light illumination, electron-hole pairs are generated after which electrons move to the electrode, reducing water to H₂ (2H⁺ + 2e⁻ → H₂), while holes oxidize water at the surface, producing O₂ (2H₂O + 4h⁺ → O₂ + 4H⁺) (Figure 8a). Voltammetric characteristics show that adding SrTaO₂N increases the photocurrent, with the 30 nm layer outperforming the 60 nm layer and bare GaN/SiC due to lower charge transfer resistance (Figure 8b). Photocurrent versus time plots reveal stability, as SrTaO₂N-coated structures maintain a current of 6 μA/cm² over 180 seconds (Figure 8c). The energy diagram illustrates that SrTaO₂N creates a hole-blocking barrier, enhancing charge separation, with the valence and conduction band levels of SrTaO₂N and GaN aligning with the H⁺/H₂ and O₂/H₂O reaction potentials, enabling efficient water splitting (Figure 8d) [200].

Since transparency is critical for enabling the necessary light spectrum to penetrate the lower layers, as depicted in Figure 9 (a schematic diagram of a wireless, stand-alone PEC tandem cell, showcasing a self-contained system for solar-driven water splitting without external wiring or bias), the thickness of the active layers plays a pivotal role. This thickness not only affects light transmission but also impacts charge transport, as discussed earlier. A comparative analysis of photoanodes featuring 30-nm and 60-nm GaN layers revealed that a 30-nm layer is sufficient to ensure effective charge transport while maintaining adequate transparency [200]. This balance between optical and electrical properties is essential for optimizing the performance of such advanced PEC systems.

While metal oxide tandem cells such as BiVO₄/Si achieve STH efficiencies up to 10 % [151–154], SiC-based systems as TiO₂/3C-SiC currently demonstrate lower efficiencies (0.74 %) [195]. However, SiC offers superior stability, with systems maintaining performance over 100 days compared to 168 hours for Cu₂ZnSnS₄||BiVO₄ [161]. This trade-off between efficiency and durability underscores the need for further optimization of SiC-based systems to enhance their efficiency while leveraging their inherent stability. Table 7 shows the summary of recent progress in SiC based tandem photoelectrochemical water splitting reactions.

The data in the Table 7 indicate that SiC-based photoelectrodes hold significant potential for solar water splitting but require further development. The TiO₂/3C-SiC configuration stands out due to its durability, though it needs enhancement in efficiency.

Amorphous SiC (a-SiC:H) serves as a promising photoelectrode material for PEC water splitting, offering a clean pathway to hydrogen production using sunlight due to its wide bandgap exceeding 2.0 eV, which ensures proper band-edge alignment with the electrolyte for efficient water splitting. This wide bandgap, achieved through carbon incorporation during RF-PECVD fabrication with SiH₄, H₂, and CH₄ gas mixtures, enhances corrosion resistance in harsh electrolytic environments, making a-SiC:H durable for up to 150 hours in pH 2 buffered electrolytes [85]. In contrast, increasing the electrolyte pH from 0 to 2 significantly reduces corrosion without affecting the photocurrent output, which remains robust at around 6 mA/cm² at -1.4 V versus Ag/AgCl after a hydrofluoric acid dip to remove detrimental SiO_x layers formed upon air exposure [85]. Additionally, a-SiC:H integration with a-Si:H tandem photovoltaic devices shifts the flat band potential favorably below the H₂O/O₂ half-reaction potential, facilitating water splitting with photocurrents ranging from 3 to 5 mA/cm² under AM1.5 light intensity in hybrid PEC configurations [201]. Furthermore, the use of gradient boron doping and high-quality nano-crystalline silicon (nc-Si:H) junctions, combined with micro-textured photonic structures, enables a-SiC:H-based photocathodes to achieve current densities of -5.1 mA/cm² at 0 V versus the reversible hydrogen electrode, demonstrating

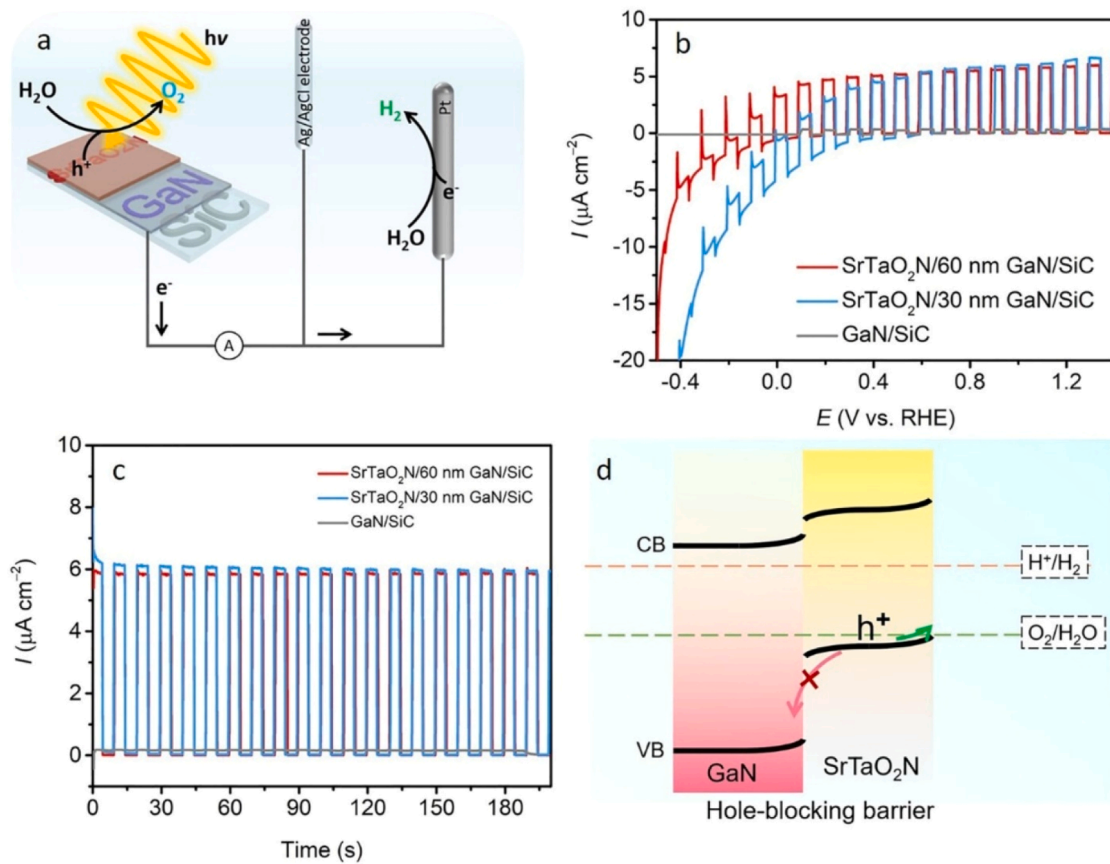


Fig. 8. (a) Scheme of the PEC water splitting cell. (b) LSV and (c) CA curves at 1.23 VRHE of SrTaO₂N/GaN/SiC photoanodes and bare substrate recorded under interrupted AM 1.5G illumination in 0.1 M NaOH electrolyte. (d) Schematic illustration of the hole transfer path in the laminated structure for water oxidation. (with permission Taylor & Francis copyright 2022 [200]).

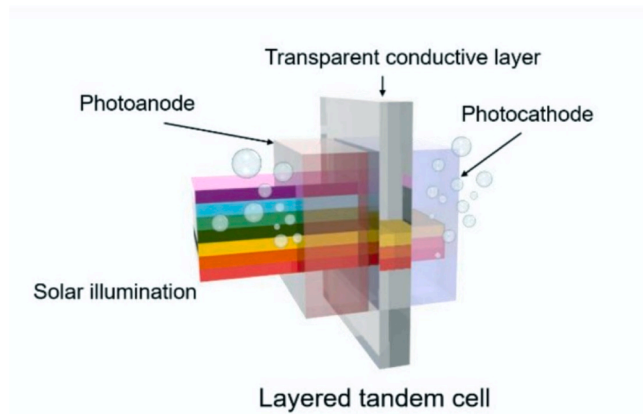


Fig. 9. Scheme of a wireless stand-alone PEC tandem cell. (with permission Taylor & Francis copyright 2022 [200]).

cost-effective and earth-abundant material advantages [181].

However, the formation of SiO_x layers on a-SiC:H surfaces when exposed to air reduces photocurrent and shifts the onset potential cathodically, posing a challenge for consistent performance unless mitigated by chemical treatments [85]. Chemically, hydrogen production reactions may etch the electrode, particularly when physical defects are present, accelerating corrosion [202].

Physical defects such as pinholes or spikes in textured TCO substrates can initiate delamination, compromising the structural integrity of the a-

Table 7

SiC-based PEC cells.

Cell Configuration	STH Efficiency (%)	Stability	Source
a-SiC:H photoelectrode with a-Si:H tandem PV	1.0	≥150 hours	[201]
TiO ₂ /3C-SiC tandem structure	0.74	≥100 days	[195]
Monolithic a-SiC:H PEC cathode with a-SiC:H/nc-Si:H PV	6.3		[181]
a-SiC:H photoelectrode with a-Si:H tandem PV	1.6	≥100 hours	[202]
a-SiC:H(p)/a-SiC:H(i) with a-Si:H tandem PV	1.6		[203]
a-SiC:H(p)/a-SiC:H(i) with a-Si:H tandem/micromorph PV	>10 (theoretical)	≥100 hours	[85]

SiC:H layer, as confirmed by SEM and EDS studies. Furthermore, the absence of hydrogen-evolution catalysts in these systems may limit efficiency compared to catalyst-enhanced configurations, and simulations suggest that while a STH efficiency exceeding 10 % is feasible, achieving this in practice requires overcoming physical and chemical degradation mechanisms [85]. In contrast, the hybrid PEC/PV systems show promise in real-world setups, producing 0.83 mA/cm² at zero bias in a two-electrode configuration with a ruthenium oxide counter electrode, indicating practical viability for hydrogen production [201]. Summarizing above, systems based on a-SiC:H show high potential efficiency; however, their stability is a weak point. To achieve an optimal balance of high efficiency and durability, future research should focus on optimizing materials, developing protective strategies, and conducting

comprehensive testing.

Advances in the development of SiC-based tandem PEC cells highlight their potential for sustainable hydrogen production, but scalability and durability issues remain. We conclude by summarizing the progress and outlining future research directions.

5. Conclusions and outlook

SiC has emerged as a highly promising material for PEC water splitting, offering a unique combination of properties that address the limitations of traditional semiconductors. Its tunable bandgap (2.36–3.2 eV) allows for optimized light absorption across the solar spectrum, while its exceptional chemical stability and high carrier mobility make it ideal for the harsh conditions of PEC environments. The integration of SiC into heterostructures and tandem PEC cells has demonstrated significant enhancements in charge separation and spectral utilization, leading to improved STH efficiencies. Notable examples include SiC-based vdW heterostructures and tandem systems such as $\text{TiO}_2/\text{3C-SiC}$, which have achieved impressive photocurrents and long-term stability. DFT modeling has been instrumental in optimizing these systems, providing critical insights into electronic structures, band alignments, and surface reactions.

Despite the promising advancements in SiC-based tandem PEC cells, achieving STH efficiencies exceeding 10 % remains a significant challenge. Key limitations include interface defects in heterostructures, stemming from lattice mismatches, which act as recombination centers and reduce charge separation efficiency. Additionally, while SiC exhibits exceptional chemical stability, the overall system durability is often compromised by photocorrosion of other tandem components, such as narrow-bandgap photocathodes, in aqueous environments. Furthermore, the scalability of high-performance SiC nanostructures is hindered by the cost and complexity of fabrication methods like CVD and MBE, which require precise control and high energy inputs. Addressing these challenges demands targeted strategies, such as interface engineering with buffer layers to minimize defects, the development of protective coatings to enhance stability, and the exploration of cost-effective, scalable synthesis techniques leveraging sustainable precursors.

Moreover, future studies could investigate the use of SiC with emerging 2D materials, such as transition metal dichalcogenides or MXenes, to create heterostructures with enhanced properties. Advanced DFT techniques, including the incorporation of excitonic effects through methods such as the Bethe–Salpeter equation, could provide deeper insights into charge transfer dynamics and light absorption. Investigating the role of defects and doping in SiC nanostructures may also lead to improved catalytic activity and stability. Experimental validation of DFT predictions will be essential to ensure the accuracy of computational models and to refine theoretical approaches. Collaborative efforts between theorists and experimentalists will accelerate the development of optimized SiC-based PEC systems. The utilization of rice husk-derived SiC is estimated to reduce raw material costs, primarily due to the low price and wide availability of agricultural waste feedstock [66]. According to life cycle assessments, the energy invested in SiC production can be recovered within two years of operation in PEC systems, making it a sustainable option. Additionally, the environmental impacts of SiC-based PEC systems should be evaluated comprehensively, including energy consumption during production and end-of-life disposal. Such analyses are currently lacking but are essential to ensure alignment with green energy principles.

By addressing these challenges, SiC-based PEC systems could play a pivotal role in achieving the >20 % STH efficiency target set by the US Department of Energy, paving the way for scalable and sustainable hydrogen production. Continued multidisciplinary efforts, combining materials science, electrochemistry, and computational modeling, will be essential to unlock the full potential of SiC in sustainable energy systems.

To advance the development of SiC-based PEC systems toward

practical implementation, several technical milestones should be prioritized. These include achieving interface defect densities below 10^{10} cm^{-2} to reduce recombination losses, fabricating large-area electrodes exceeding 100 cm^2 with uniform thickness and crystallinity, and developing scalable methods for integrating protective coatings to ensure operational stability beyond 1000 hours. Additionally, improving light absorption through optimized texturing and tandem configurations is essential for surpassing the 10 % STH efficiency threshold. Collaborative research efforts focusing on these objectives will be critical to bridging the current performance gap between laboratory-scale demonstrations and commercially relevant devices. AI and ML algorithms are expected to play an increasingly important role in the design of SiC-based PEC systems. For example, AI models can be trained on large DFT databases to predict optimal combinations of semiconductors with tailored band alignments and defect tolerances. ML techniques can also accelerate the identification of synthesis parameters that maximize stability and efficiency, while generative models may be applied to design novel heterostructure configurations. The integration of these tools into experimental workflows will be essential to expedite the development of scalable, high-performance PEC devices.

Funding information

The author(s) declare that financial support was received for the research, authorship, and/or publication of this article. This research has been funded by the Science Committee of the Ministry of High Education and Science of the Republic of Kazakhstan (Grant No. AP23490626 “Research and development of ZnO/BiVO_4 and $\text{Cu}_2\text{O}/\text{ZnO}$ photoelectrodes to create highly efficient tandem light-driven hydrogen production systems”).

CRediT authorship contribution statement

N.B. Bakranov: Writing – review & editing, Supervision, Project administration, Methodology, Investigation, Funding acquisition. **Zh. Kuli:** Writing – review & editing, Resources, Methodology, Formal analysis. **Zh.O. Mukash:** Writing – review & editing, Methodology, Investigation, Funding acquisition, Conceptualization. **D.I. Bakranova:** Writing – review & editing, Validation, Investigation, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

During the preparation of this work the authors used ChatGPT (Version 4.0) to improve the English language of this manuscript. All content was subsequently reviewed and edited by the authors, who take full responsibility for the final version of the publication.

Data availability

Data will be made available on request.

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