Energy LAB

HIGHLIGHT

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Energy and mass transfer at interfaces in solar-driven photocatalytic CO_2 reduction reactions

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Solar-driven photocatalytic CO_2 reduction represents a transformative approach to renewable energy storage and carbon neutrality. By converting low-density, intermittent solar energy into stable, energy-dense green chemicals, this technology addresses critical limitations in renewable energy utilization and promotes a circular carbon economy. However, its industrial-scale application is hindered by inefficiencies in energy and mass transfer across key interfaces. This highlight introduces the fundamental challenges and recent advancements in optimizing three critical interfaces: the light harvesting interface, charge transfer interface, and catalytic reaction interface. We discuss strategies to enhance light absorption, charge carrier dynamics, and reactant adsorption/desorption, providing insights into the design of efficient photocatalytic systems for CO_2 reduction.

Global energy transition demands innovative solutions to harness renewable energy and mitigate carbon emissions.[1] Solar-driven photocatalytic CO_2 reduction, which converts CO_2 and water into hydrocarbons using sunlight, tackles two major challenges: stabilizing intermittent solar energy into storable chemical bonds and closing the anthropogenic carbon cycle. Despite decades of research, practical applications remain hindered by low solar-to-fuel conversion efficiencies (<5%), primarily due to inefficiencies in energy and mass transfer at functional interfaces.[2] This process is governed by three critical interfaces (Figure 1): (i) light harvesting interface,[3] (ii) charge transfer interface,[4] and (iii) catalytic reaction interface.[5]

Light harvesting interface governs the absorption and conversion of solar energy into photogenerated charge carriers. However, suboptimal spectral utilization and inefficient exciton transport to catalytic centers remain significant barriers. Recent advances prioritize broadening the absorption spectrum of photocatalysts to harness visible and near-infrared (NIR) light, beyond the ultraviolet (UV) range traditionally utilized. Synthesis of multi-gap semiconductor composites combining materials with complementary absorption profiles — for example, TiO_2 (UV-active) coupled with perovskites or chalcogenides (visible to NIR-active) — has demonstrated synergistic spectral extension and improved solar-to-fuel efficiency.[6] Photon upconversion converts low-energy photons (e.g., NIR) into higher-energy photons (e.g., visible/UV), enabling the use of otherwise wasted solar energy. Incorporation of plasmonic nanoparticles (e.g., Au, Ag) exploits localized surface plasmon resonances to amplify the local electromagnetic field and enable photon upconversion, converting low-energy photons into higher-energy carriers usable in photocatalysis.[7] Typically, lanthanide-doped upconversion materials have been successfully employed to convert NIR photons into visible or UV light, effectively recycling otherwise wasted energy. Moreover, engineering heterojunctions with well-aligned, layered or gradient energy levels — through multilayer or gradient assemblies — facilitates directional photon-to-charge conversion pathways, suppressing electron-hole recombination and maximizing full-spectrum solar utilization.[8] Additionally, optimizing the energy level alignment and minimizing lattice mismatch between components can significantly facilitate exciton transfer and charge separation. Incorporating surface modifications can improve interface stability and reactivity, thereby maximizing overall photocatalytic efficiency and promoting effective solar energy utilization.

Charge transfer interface controls the separation, transfer, and utilization of photogenerated charge carriers, which are essential for photocatalytic CO_2 reduction. Built-in electric fields (BIEFs) at heterojunctions generate steep energy gradients that spatially separate charge carriers, minimizing recombination. Prompt migration of carriers to active sites is essential; however, defect states and trap centers within photocatalysts frequently capture carriers, leading to recombination and efficiency loss. Innovative interface engineering focus on mitigating these recombination pathways by optimizing structural order, tailor energy band alignment, and improving carrier mobility. Heterojunction architectures, particularly Z-scheme systems, markedly enhance charge separation by combining semiconductors with complementary band structures and matching energy potentials. For instance, the In_2O_3/Nb_2O_5 S-scheme heterojunction enables ultrafast electron transfer ($1.5\times10^{12}\ s^{-1}$) for CO_2 photoreduction, achieving 48.7 $\mu mol\cdot g^{-1}\cdot h^{-1}$ CO yield with 92.3% selectivity.[9]

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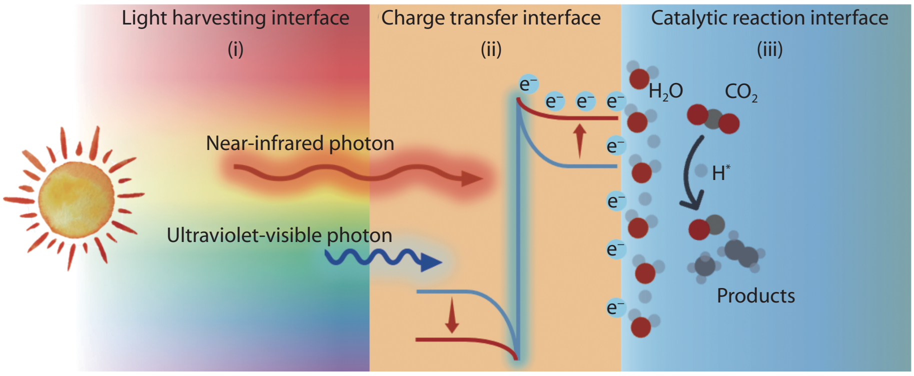

Fig. 1 The three primary interfaces governing photocatalytic performance: (i) light harvesting, (ii) charge transfer, and (iii) catalytic reaction surface

Atomic intercalation modifications, such as Co/Cu_3-TPA-COF incorporation, further adjust electronic structures to promote efficient charge migration while suppressing recombination. Cutting-edge spatiotemporal imaging techniques offer critical mechanistic insights by tracking hot-electron dynamics and anisotropic trapping phenomena, guiding rational interface design.[10] Collectively, these strategies address intrinsic defects and recombination issues, thereby advancing the charge carrier utilization in solar-driven photocatalytic CO_2 reduction systems.

Catalytic reaction interface plays a critical role in reactant adsorption/desorption, activation energy barriers, and reaction kinetics — all determinants of product's yield and selectivity. Optimizing this interface is essential for improving the efficiency and selectivity of photocatalytic CO_2 reduction.[11] Inefficient transfer of photogenerated carriers to surface active sites frequently leads to suboptimal CO_2 reduction performance. Modifying the surface electronic structure and active sites enhances charge transfer efficiency and minimizes interfacial energy losses. Development of hybrid catalysts combining multiple catalytic sites enables optimized CO_2 adsorption as well as selectivity in product desorption. Furthermore, tuning surface morphology to increase active site accessibility and modifying electronic properties accelerates reaction kinetics. Targeted surface engineering can also direct reaction pathways towards desired products, improving both selectivity and overall conversion efficiency. Recent advancements in operando spectroscopy, particularly time-resolved X-ray absorption spectroscopy (XAS), have provided unprecedented insights into the dynamic processes occurring at the catalytic reaction interface of photocatalytic systems. These techniques allow for real-time monitoring of electronic and structural changes during photocatalytic CO_2 reduction, offering a deeper understanding of the mechanisms governing charge transfer and catalytic reactions. For instance, time-resolved XAS has elucidated the strong interfacial bonding results in stable Cu–O–Si sites that maintain their structure during the CO_2 reduction reaction, without significant reconstruction.[12] Additionally, complementing experimental advances, machine learning (ML) has emerged as a transformative tool for accelerating interface optimization. Neural network models trained on high-throughput datasets of photocatalyst performance can predict optimal bandgap alignments, defect configurations, and surface adsorption energies with atomic-scale precision.[13] By integrating active learning frameworks with robotic synthesis platforms, ML bridges the gap between mechanistic understanding and scalable photocatalyst design, addressing the combinatorial complexity inherent in multi-interface systems.[14]

Optimizing energy and mass transfer at the light harvesting, charge transfer, and catalytic reaction surface interfaces is critical for advancing solar-driven photocatalytic CO_2 reduction. Although recent advances demonstrate significant performance improvements, challenges persist in finely tuning interfacial properties to achieve robust operation under real-world conditions. Future efforts should emphasize integrated interface engineering strategies that simultaneously address multiple interfacial processes, supported by the development of novel materials, advanced characterization techniques, and innovative system designs. By addressing these critical barriers, solar-driven photocatalytic CO_2 reduction can emerge as a practical and sustainable technology for renewable energy conversion and carbon management, contributing meaningfully to global decarbonization efforts.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

AUTHOR CONTRIBUTIONS

S. Bai, W. Zheng, and Q. Huang contributed equally. S. Bai and W. Zheng wrote the original draft of this paper; all authors were involved in discussing and reviewing the draft and approved the final version.

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