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Article

Solar Photothermal CO_2 Conversion: Harnessing Light and Heat for Carbon Neutrality: A Mini Review

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Abstract: Photothermal CO_2 conversion is a promising strategy for sustainable solar fuel production, which integrates photocatalytic and thermocatalytic processes to enhance solar energy utilization, reaction kinetics, and product selectivity. By coupling photon-induced charge excitation with localized thermal effects, photothermal systems enable the efficient activation of thermodynamically stable CO_2 molecules under relatively mild conditions. This review provides a comprehensive overview of the fundamental principles underlying photocatalysis and thermocatalysis, and their synergistic effects in photothermal catalysis. It discusses photonic–thermal coupling, plasmonic and non-plasmonic pathways, and major CO_2 conversion routes such as hydrogenation and artificial photosynthesis. Advances in the design of efficient nanostructured catalysts, focusing on light absorption, heat management, charge dynamics, and optofluidic reactors, are also highlighted. Despite significant progress, challenges remain, such as the unclear thermal and nonthermal contributions, which limit mechanistic understanding and catalyst design. Insufficient insight into energy transfer, deactivation, and local reaction environments also hinders the efficiency. Practical issues, such as stability, light penetration, heat control, and scalability, limit industrial use. Future research should integrate operando characterization, modeling, and machine learning to understand the structure–performance relationships and develop efficient catalysts. Photothermal CO_2 conversion is advancing rapidly, with the potential for carbon-neutral energy production through efficient solar-driven catalytic processes.

Keywords: Photothermal catalysis; CO_2 conversion; Solar fuels; Machine learning

1. Introduction

The swift progress of global industry has resulted in humanity's excessive dependence on fossil fuels, leading to rising CO_2 emissions and environmental concerns. The global energy sector is experiencing a profound shift aimed at lowering carbon emissions and combating the escalating damage caused by climate change (Riffat and Samaei, 2025). Current trends indicate that the world will likely exceed the 1.5°C global warming cap set by the Paris Agreement (World Meteorological Organization, United Nations Climate Change, 2015), as many areas are already experiencing notable temperature increases (Al-Assad, 2025). Moreover, reports from international organizations such as the IEA, IRENA, and Ember underscore a clear link between higher renewable energy adoption and lower carbon intensity (Uyar and Hayber, 2025). In this scenario, solar energy has emerged as a highly promising renewable alternative due to its abundance, sustainability, and minimal environmental impact. Solar energy, available in the form of light and heat, can be harnessed through photovoltaic and photothermal technologies to produce electricity and chemical fuels (Gao et al., 2022, Liang et al., 2026).

Solar-driven catalysis, utilizing sunlight as photonic and thermal energy, offers a sustainable path for energy conversion and storage. Among these methods, photothermal catalysis, facilitated by carefully

designed nanostructured catalysts, has garnered significant attention as an effective strategy for solar fuel production. This approach combines the benefits of photocatalysis and thermocatalysis, enhancing the utilization of the solar spectrum. Notably, solar-driven fuel generation through photothermal catalysis includes hydrogen production from water splitting and carbon-based fuel synthesis via CO_2 reduction (Liang et al., 2026, Rehan et al., 2025a). Solar photothermal CO_2 conversion presents a promising route for achieving carbon neutrality by effectively combining light and heat to drive efficient chemical transformations. This process enables the sustainable reduction of CO_2 into value-added fuels and chemicals, paving the way for a greener energy future (Ramos‐Fernandez et al., 2025).

Despite its potential, the mechanisms governing photothermal processes, particularly photon, hot carrier, and thermal effect interactions under multi-field coupling, remain inadequately understood. This gap limits system efficiency and highlights the need for strategies to enhance light absorption, charge separation, heat management, and multi-electron transfer, while suppressing electron–hole recombination (Guene Lougou et al., 2024). Catalysis serves a dual function in shifting toward renewable energy systems. It aids in converting biomass into fuels and allows renewable energy to drive catalytic reactions. Photocatalysis is a prime example, while thermocatalytic processes can be powered by solar energy when combined with solar concentration technologies. Crucially, sustainable development demands substantial reductions in CO_2 emissions and the stabilization of atmospheric concentrations, as highlighted in projections by the International Energy Agency (Fresno et al., 2023). The increasing interest of researchers in solar photothermal CO_2 conversion is well explained by the number of publications from 2016 to 2026 (Figure 1).

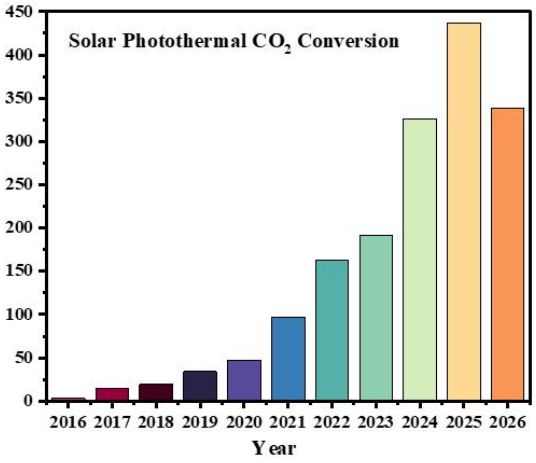

Figure 1. Solar photothermal CO_2 conversion publication from Scopus database (2016-2026).

Photothermal catalysis functions at the intersection of photocatalysis and thermocatalysis, merging photon-induced charge excitation with thermally activated reaction pathways. This dual capability enables the simultaneous reduction of activation energy and the enhancement of reaction kinetics through localized heating effects. Consequently, photothermal catalysis is particularly effective in activating thermodynamically stable molecules like CO_2 under moderate conditions, offering higher reaction rates than conventional photocatalysis and requiring less energy than thermocatalysis. As a result, it has garnered significant attention in recent years. Among its various applications, CO_2 conversion is the most extensively studied, with major products including CO and CH_4, while the formation of higher-value products, such as methanol, ethanol, and C^{2+} hydrocarbons, remains comparatively less explored (Fresno et al., 2023). As a result, the conversion and utilization of CO_2 have become pivotal research areas. Transforming CO_2 into value-added products like CO through catalytic processes offers both environmental and economic advantages, highlighting significant potential for future advancements. Particularly, photothermal catalysis has demonstrated the ability to efficiently convert CO_2 under relatively mild conditions (Guo et al., 2025).

Carbon dioxide (CO_2) is not only a significant greenhouse gas but also a plentiful and cost-effective carbon feedstock. Converting it into high-energy fuels offers a promising approach to simultaneously combat climate change and tackle energy shortages. Notably, the solar-driven production of syngas from CO_2 and H_2O presents an appealing method for storing solar energy in the form of chemical bonds (Wang et al., 2019). Carbon monoxide (CO) is a crucial intermediate that acts as a fundamental building block in the synthesis of methanol and long-chain hydrocarbons. However, efficiently converting CO_2 into fuels while maintaining net-zero emissions presents a significant challenge. This endeavor necessitates the development of advanced catalytic systems that can effectively utilize the entire solar

spectrum and facilitate efficient energy conversion and storage. Various catalytic approaches, including thermal, photocatalytic, and photothermal processes, have been explored, each offering distinct advantages in terms of reactivity, selectivity, and stability (Guene Lougou et al., 2024).

This review delves into photothermal catalysis as a burgeoning and promising approach for the solar-driven conversion of CO_2 into synthetic fuels. It systematically explores the fundamental principles, including thermodynamics, reaction mechanisms, and kinetics, alongside key methodologies for catalyst design and performance evaluation. Additionally, it examines recent advancements in photothermal materials and highlights strategies to enhance optical absorption, heat management, and catalytic efficiency. It highlights the crucial need to integrate operando characterization, modeling, and machine learning to understand structure–performance relationships and develop efficient catalysts. The challenges and future opportunities in this field are also critically analyzed, aiming to provide insights into the development of efficient and sustainable solar-driven CO_2 conversion systems. The literature for this mini review was systematically searched across Scopus, Web of Science, and Google Scholar for the period 2016–2026 using keywords including 'photothermal CO_2 conversion', 'photothermal catalysis'. Only peer-reviewed articles, reviews, and book chapters focused on photothermal CO_2 conversion to fuels with clear performance metrics and last 10 years literature were included, while non-English publications, conference abstracts without full data, and studies lacking quantitative activity reporting were excluded.

2. Fundamental Insights into Photocatalysis, Thermocatalysis, and Photothermal Catalysis

The fundamental principles of photocatalysis, thermocatalysis, and photothermal catalysis have been comprehensively examined in recent scholarly reviews and book chapters (Guene Lougou et al., 2024, Wang et al., 2024). This text provides a succinct overview to elucidate their primary mechanisms and distinctions.

2.1. Photocatalysis

Photocatalysis predominantly occurs in semiconductor materials. When photons possessing energy equal to or exceeding the bandgap energy (E_{BG}) are absorbed, electrons (e^-) are excited from the valence band (VB) to the conduction band (CB), resulting in the formation of corresponding holes (h^+) in the VB. These electron–hole pairs, referred to as photoinduced charge carriers, can migrate to the catalyst surface and engage in reduction and oxidation reactions. Nonetheless, the recombination of charge carriers remains a significant limitation, markedly diminishing photocatalytic efficiency. Consequently, enhancing charge separation and mobility is essential for improving performance. In certain instances, thermal energy, provided either by light-induced heating or external sources, can augment photocatalytic activity by facilitating charge carrier excitation, separation, and migration. However, this thermal contribution alone is generally inadequate to independently drive the reaction, and thermocatalysis plays a negligible role under such conditions (Hong et al., 2022).

2.2. Thermocatalysis

Thermocatalysis encompasses a series of interconnected physical and chemical processes. In a typical gas-phase reaction occurring over a porous catalyst, seven sequential steps can be delineated: (1) film diffusion of reactants, (2) pore diffusion of reactants, (3) adsorption of reactants, (4) surface reaction, (5) desorption of products, (6) pore diffusion of products, and (7) film diffusion of products. Among these, steps (4)–(6) are predominantly chemical in nature, whereas the remaining steps are governed by physical transport processes. The overall reaction rate is dictated by the rate-limiting step, which is the slowest among these processes. Optimal adsorption strength and appropriate binding of intermediates are essential for effective catalysis. Furthermore, active sites are frequently associated with surface defects, unsaturated valences, or electronic irregularities. In thermocatalytic systems, light can function as an alternative heating source through photothermal conversion. The heat generated by light absorption can either substitute conventional heating or lower the required reaction temperature. Under such conditions, photocatalytic contributions are minimal. Instead, the role of light is primarily linked to thermal effects, although it may also influence catalyst microstructure or elementary reaction steps (Wang et al., 2024).

2.3. Photothermal Catalysis

Photothermal catalysis encompasses catalytic processes wherein both light and heat concurrently facilitate the reaction. The predominant mechanism within a given system may involve photocatalysis,

thermocatalysis, or a synergistic integration of both, resulting in distinct photothermal effects across various reactions, as illustrated in Figure 2. Generally, any catalytic process characterized by light absorption, heat generation, and chemical transformation can be classified under photothermal catalysis. Thermal energy may be derived from intrinsic photothermal materials (self-heating) or from external heating sources (assisted heating) (Song et al., 2022). For clarity, these different contributions are often categorized to elucidate their roles in specific reaction systems (Gao et al., 2022). A significant advantage of photothermal catalysis is its synergistic effect, wherein the combined influence of light and heat yields catalytic performance that exceeds the sum of individual photocatalytic and thermocatalytic contributions. A comparative summary of these processes is presented in Table 1. This synergy facilitates reduced reaction severity, enhanced reaction rates, and the emergence of novel catalytic pathways. These aspects will be examined in detail in the subsequent sections.

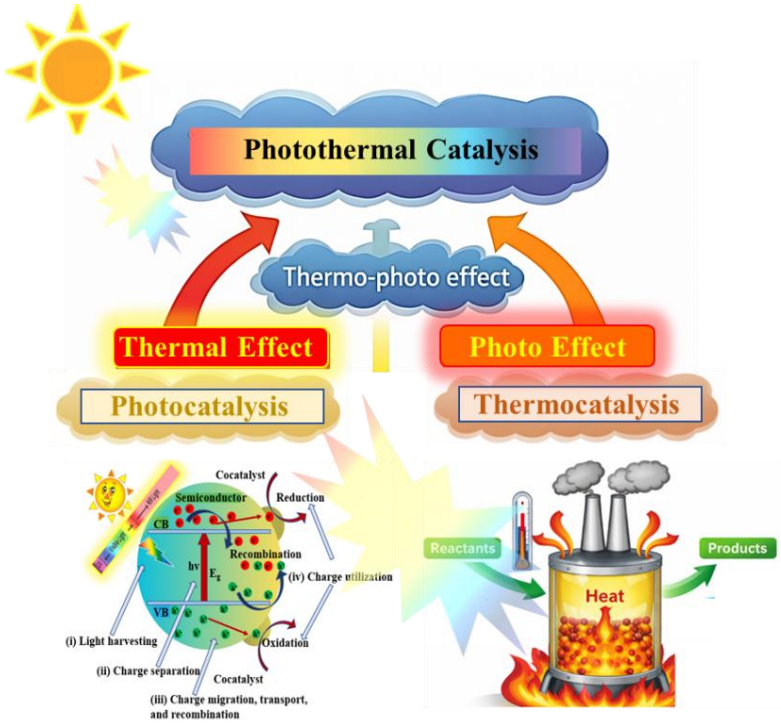

Figure 2. Conceptual illustration of the synergistic interaction between photonic and thermal energy in photothermal catalysis.

Table 1. Overview of photothermal catalysis types for fuel generation (Gao et al., 2022, Fresno et al., 2023).

Aspect/ Description	Photocatalysis	Thermocatalysis	Photothermal Catalysis
Driving force	Photochemistry	Thermochemistry	Photochemistry & thermochemistry
Phenomena	Introducing heat into photocatalysis	Introducing light into thermocatalysis	Coupling photocatalysis and thermocatalysis
Excitation Type	Photon excitation	Heat excitation	Photon & heat excitation
Gibbs free Energy ΔG	ΔG > 0 (with catalyst, lower)	ΔG < 0 (with catalyst, higher)	Can occur for ΔG > 0 and ΔG < 0 processes
Processes involved/ Mechanism	Photo-reduction, photo-excitation, formation, absorption, generation, conversion	Thermo-reduction	Photocatalysis and thermocatalysis (occur concurrently or sequentially)
Catalyst requirement	Semiconductor (bandgap dependent)	Metals/oxides (thermally stable)	Hybrid systems (plasmonic metals + semiconductors)
Limitations	Fast e^-–h^+ recombination, low efficiency	High energy consumption, carbon	Mechanism complexity, still early-stage

		footprint	development
Industrial feasibility	Limited	Mature technology	Emerging for solar fuels

To rigorously substantiate claims of nonthermal or synergistic contributions in photothermal CO_2 conversion, authors must report seven critical data points: (1) catalyst surface temperature under illumination ($T_{surface}$), measured via IR camera, Raman thermometry, or EXAFS calorimetry; (2) dark catalytic rate (R_{dark}) at the same $T_{surface}$ using external heating; (3) action spectrum or wavelength-dependent rates across UV, vis, and NIR bands; (4) intensity dependence over ≥ 3 irradiance levels with corresponding $T_{surface}$; (5) apparent activation energies (E_a) for both light-driven and dark conditions; (6) complete carbon balance and product selectivity; and (7) a control experiment using an inert photothermal absorber (e.g., carbon black/SiO_2) to establish the maximum thermal-only contribution. If any of these are missing, claims of nonthermal or synergistic effects must be explicitly qualified as preliminary. This framework ensures reproducibility and enables meaningful cross-study comparison.

3. Fundamentals of Photothermal CO_2 Conversion

3.1. Photonic and Thermal Synergies

Heterogeneous photocatalysis is fundamentally driven by the generation of electron–hole pairs when a semiconductor is exposed to photons with energy equal to or greater than its bandgap. These photogenerated charge carriers can migrate to the catalyst surface and participate in redox reactions with adsorbed species. However, their efficiency is often limited by rapid recombination, necessitating strategies to enhance charge separation and utilization. In contrast, thermal heterogeneous catalysis primarily relies on the intrinsic reactivity of surface active sites, particularly low-coordination atoms or defect sites, which provide energetically favorable pathways for bond cleavage and formation. Although catalysis reduces the activation energy barrier, reaction rates remain strongly temperature-dependent, influenced by thermodynamics, adsorption–desorption equilibria, and surface reaction kinetics. Consequently, many industrial catalytic processes operate at elevated temperatures (typically several hundred degrees Celsius), which increases energy consumption and may lead to catalyst deactivation through sintering or coking.

From a thermodynamic standpoint, thermal catalysis is constrained to facilitating spontaneous (Gibbs free energy downhill) reactions, often necessitating elevated temperatures and pressures to achieve favorable conditions. In contrast, photocatalysis permits thermodynamically uphill reactions, such as water splitting and CO_2 reduction, by transforming photon energy into chemical energy. These processes are, in essence, photosynthetic in nature, although they are commonly classified as photocatalysis (Fresno et al., 2023). The photothermal effect, characterized by the conversion of absorbed radiant energy into heat, adds an additional dimension to catalytic processes by enabling localized temperature increases at active sites. In the context of CO_2 conversion, thermal activation typically results in higher reaction rates (often reaching $mmol.g^{-1}.h^{-1}$), whereas photochemical activation allows for operation at lower bulk temperatures and may introduce alternative reaction pathways with distinct selectivity. Notably, reduced operating temperatures can suppress undesired side reactions such as coke formation, thereby enhancing catalyst stability.

The synergistic integration of photonic and thermal effects can be applied to critical CO_2 conversion reactions, including the dry reforming of methane, the reverse water–gas shift, the Sabatier reaction, and methanol synthesis (Fresno et al., 2018):

$$CO_2 + CH_4 \rightarrow 2CO + 2H_2 \quad (1)$$

$$CO_2 + H_2 \rightarrow CO + H_2O \quad (2)$$

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O \quad (3)$$

$$CO_2 + 3H_2 \rightarrow 2CH_3OH + H_2O \quad (4)$$

3.2. Decoupling Thermal and Nonthermal Effects in Photothermal Catalysis

Thermal effects that occur during catalytic reactions can significantly influence the temperature at active sites, thereby impacting catalytic activity, selectivity, and stability. In the field of photothermal

catalysis, a primary challenge is to ascertain whether thermal and photochemical contributions operate independently as additive energy sources or synergistically to create new reaction pathways through interfacial coupling. Clarifying this distinction is essential for both comprehending the underlying mechanisms and designing advanced catalysts in a rational manner. When catalytic performance is predominantly driven by localized heating from photothermal conversion, the primary mechanism is thermal. In such instances, catalyst design should focus on maximizing solar absorption, enhancing photothermal conversion efficiency, and optimizing heat transfer and confinement to achieve elevated local temperatures at active sites. Conversely, when nonthermal effects are significant, catalytic enhancement arises from photoexcited charge carriers (such as hot electrons and holes) that directly participate in surface reactions. In these cases, it is crucial to enhance charge carrier generation, separation, lifetime, and interfacial transfer (Yang et al., 2026).

It is essential to quantitatively distinguish between these two contributions to the total energy. By separating thermal from nonthermal effects, one can accurately determine the true source of catalytic activity and refine reaction pathways with enhanced precision. Recent progress has introduced valuable methods in this area. For example, a systematic assessment of the relative roles of localized heating and hot carriers in photothermal ammonia synthesis was achieved using a temperature determination method based on the Le Châtelier principle. Moreover, operando techniques like EXAFS-based calorimetry have facilitated real-time observation of temperature changes in catalytic nanoparticles (such as Ni) during CO_2 conversion, providing deeper insights into reaction kinetics and energy transfer processes. These methods are significant steps toward a thorough understanding of photothermal catalytic mechanisms (Bian et al., 2023).

3.3. Routes for Photothermal Catalysis

Photothermal catalysis can be broadly classified into plasmonic and non-plasmonic pathways, based on the underlying mechanisms and types of catalysts involved (Wang et al., 2020).

3.2.1. Plasmonic Photothermal Catalysis

In plasmonic systems, the photothermal effect is predominantly induced by localized surface plasmon resonance (LSPR), which results from the collective oscillation of conduction electrons in metallic nanoparticles when exposed to light irradiation. This phenomenon facilitates strong light absorption and the production of energetic charge carriers, commonly known as hot electrons and hot holes.

These hot carriers can participate in catalytic processes via two main pathways:

- **In the indirect transfer pathway**, where hot carriers are generated within the plasmonic metal and subsequently transferred to adjacent adsorbates or semiconductor supports.
- **The direct transfer pathway**, involving immediate injection of hot carriers into adsorbates or neighboring materials via chemical interface damping (CID) (Fresno et al., 2023).

The direct route is typically more effective as it minimizes energy losses linked to carrier relaxation. Additionally, the non-radiative decay of plasmons leads to localized heating, which boosts catalytic activity. LSPR also greatly enhances the local electromagnetic field around the nanoparticle surface, thereby increasing the optical absorption cross-section and promoting efficient light harvesting. While plasmonic absorption is usually limited to certain resonant frequencies, advanced nanostructures can achieve a wider range of spectral absorption. Plasmonic effects are often seen in metallic nanoparticles and some semiconductor nanostructures, working together to enhance both photochemical and thermal processes (Agrawal et al., 2018).

3.2.2. Non-Plasmonic Photothermal Catalysis

Non-plasmonic photothermal catalysis is predominantly associated with semiconductor-based systems, wherein photoexcitation results in the formation of electron–hole pairs that facilitate catalytic reactions. In these configurations, thermal effects can enhance photocatalytic efficiency by improving the generation, separation, and mobility of charge carriers. Concurrently, light-induced heating can modify the physicochemical properties of thermocatalysts, such as the formation of surface defects or frustrated Lewis pairs, thereby augmenting catalytic performance. Although non-plasmonic methods are less extensively studied compared to plasmonic ones, they remain highly significant for practical applications (Wang et al., 2024).

In numerous contexts, visible and infrared light primarily functions to selectively heat catalytic sites, thereby enhancing energy efficiency by directing thermal energy precisely to the areas of greatest need. Unlike plasmonic systems, the potential for additional electronic synergies is often constrained, resulting in catalytic performance that may resemble that achieved under conventional thermal

conditions. Thermal properties, such as heat capacity and thermal conductivity, are crucial in determining the distribution of local temperatures and the overall efficiency of catalysis. Furthermore, the use of spectrally selective absorbers, materials that absorb strongly in the visible range while exhibiting low emissivity in the infrared, can significantly enhance photothermal performance by minimizing radiative losses sunlight-driven (Li et al., 2019).

3.3. Mechanisms for photothermal-driven catalysis

Photothermal catalysis functions through the concurrent involvement of light-induced charge carriers and thermally activated processes, leading to a synergistic enhancement of catalytic performance. This dual activation mechanism effectively addresses the limitations of traditional methods by integrating the high selectivity characteristic of photocatalysis with the elevated reaction rates associated with thermocatalysis.

Two primary mechanistic scenarios can be identified (Song et al., 2022):

- **Sequential mechanism**, where photocatalysis and thermocatalysis occur in distinct steps, with one half-reaction driven by photogenerated carriers and the other facilitated by thermal activation.
- **Synergistic mechanism**, where photochemical and thermal effects occur concurrently, leading to catalytic performance that exceeds the sum of individual contributions.

The synergistic interactions not only boost catalytic activity but also enhance product selectivity and catalyst stability. Additionally, photothermal activation allows for the use of materials that would otherwise remain inactive and opens up reaction pathways that are not possible under solely thermal or photochemical conditions. Thus, photothermal catalysis serves as a versatile platform for the development of advanced catalytic systems aimed at efficient CO_2 conversion (Xie et al., 2022, Zhang et al., 2015).

3.4. Systematic Approach for Photothermal Catalytic CO_2 Conversion Research

The development of photothermal catalysts is crucial for enhancing photocatalytic efficiency and optimizing solar energy utilization. In photothermal systems, catalysts absorb solar irradiation to facilitate chemical reactions, with a portion or the entirety of the absorbed energy being converted into heat. The performance of various photothermal catalysts is largely contingent upon the distribution of absorbed solar energy between photochemical and thermochemical pathways, which determines the overall catalytic efficiency. Consequently, integrating fundamental insights from both traditional photocatalysis and thermocatalysis offers an effective strategy for optimizing photothermal catalyst performance (Zhang et al., 2015). The design and optimization of photothermal catalysts are particularly critical for enhancing key performance metrics such as apparent quantum yield (AQY) and solar-to-hydrogen (STH) efficiency. Efficient light harvesting is directly correlated with the generation of photogenerated electron–hole pairs and the effective utilization of solar energy. In semiconductor-based systems, optical properties are primarily determined by bandgap energy, which dictates light absorption and charge excitation. Enhancing light absorption across a broader spectral range promotes charge carrier generation and, consequently, improves catalytic activity. A general workflow for evaluating photothermal catalytic CO_2 conversion performance is illustrated in Figure 3.

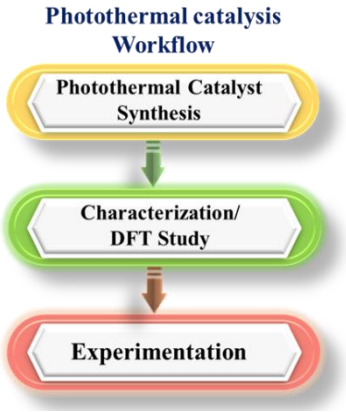

Figure 3. Basic workflow for photothermal CO_2 conversion research.

Thorough characterization of photothermal catalysts is crucial for elucidating catalytic mechanisms and informing the rational design of catalysts. Analytical techniques developed for conventional

photocatalysis and thermocatalysis are largely applicable to photothermal systems. Photothermal catalysis encompasses a series of interconnected processes occurring over multiple timescales, including photon absorption, charge carrier generation and separation, surface adsorption/desorption of reactants, and subsequent redox reactions on catalyst surfaces (Rehan et al., 2025b). The efficiency of the overall process is governed by the interplay of these fundamental steps, making it crucial to quantitatively analyze each stage.

Advanced characterization techniques offer valuable insights into crystal structure, morphology, composition, optical properties, and charge carrier dynamics, all of which significantly influence photothermal catalytic performance. Understanding the structure and charge transfer mechanisms in catalysts is both challenging and essential for the rational design and enhancement of solar energy utilization. The absorption spectrum governs light absorption and electron excitation, with these processes occurring on different timescales that collectively determine the overall photocatalytic efficiency. Each fundamental step must be quantitatively characterized through appropriate experimental methodologies to inform the "photothermal catalyst by design" concept. Electrochemical analyses further facilitate the investigation of band structure, charge transport, and interfacial processes. Nonetheless, conventional ex situ characterization methods, such as X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and X-ray diffraction (XRD), frequently fail to capture the true active state of catalysts under reaction conditions. Surface contamination and structural alterations during operation can obscure active sites and reaction intermediates. Consequently, in situ and operando techniques, conducted under controlled environments or actual working conditions, are increasingly essential for monitoring dynamic changes in catalyst structure, composition, and charge transfer processes in real time. These methodologies are crucial for bridging the gap between catalyst design and mechanistic understanding (Figure 4). Notably, AQY remains a key metric for evaluating photon-to-product conversion efficiency in both photocatalytic and photothermal systems.

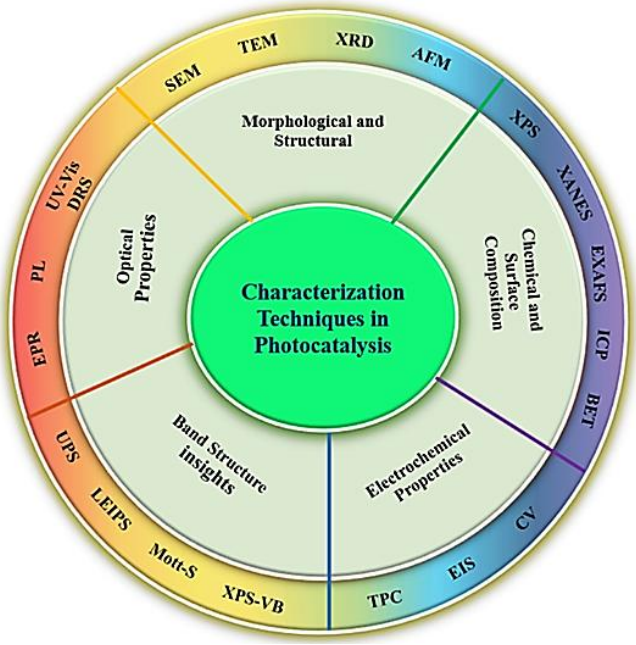

Figure 4. Characterization techniques used in photothermal catalysis for CO_2 conversion.

Ex situ methods are insufficient in accurately representing actual reaction conditions, as surface contamination can obscure active sites, and capturing the real-time evolution of phases, composition, and charge transfer remains challenging (Issa Hamoud et al., 2022). Traditional ex-situ characterization techniques, such as X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and X-ray diffraction (XRD), are limited to capturing the "inactive" state of a catalyst. This limitation highlights the necessity for in-situ techniques, which operate within controlled environments, and operando techniques, which function under actual working conditions, to observe transient intermediates. These methodologies effectively bridge the gap between structural design and catalytic mechanisms. Furthermore, the apparent quantum yield (AQY) is a critical metric that reflects the efficiency of photon-to-product conversion and is extensively utilized in photocatalytic and photothermal systems.

In addition to catalyst properties, reaction conditions such as catalyst loading, type and concentration

of sacrificial agents, agitation speed, pH, and reactor temperature significantly influence photothermal catalytic performance (Issa Hamoud et al., 2022). Although hybrid photocatalysts often exhibit enhanced activity, their application in colloidal systems is challenged by light attenuation effects and nanoparticle instability. Issues such as ligand desorption and nanoparticle aggregation can alter optical and thermophysical properties, reduce active surface area, and ultimately diminish catalytic efficiency (Issa Hamoud et al., 2022). For quantitative catalytic analysis, report activity in units such as $mmol.g^{-1}.h^{-1}$ for mass-normalized performance, $mmol \cdot m^{-2} \cdot h^{-1}$ to account for surface area effects, or $\mu mol.h^{-1}$ for absolute rates. Stability requires at least 10 hours of continuous operation (preferably 24+ hours) with periodic activity measurements, as shorter 1–2 hour tests fail to capture deactivation mechanisms like coking, sintering, or oxidation (Rehan et al., 2025c).

3.5. Photothermal catalysis for CO_2 conversion

Recent research has increasingly focused on the photothermal effect for various environmental and energy-related applications, including water desalination, steam production, air purification, and CO_2 reduction. A notable advantage of photothermal catalysis is its ability to effectively utilize the entire solar spectrum, particularly the low-energy infrared radiation, which is typically inactive in systems relying solely on photocatalysis. In gas-phase heterogeneous reactions, the localized heating at catalyst surfaces facilitates high reaction rates while maintaining relatively mild overall operating conditions. This unique feature allows photothermal catalysis to act as a bridge between photocatalysis and thermocatalysis, offering enhanced activity and selectivity (Ghoussoub et al., 2019). Consequently, photothermal methods have shown significant potential for converting CO_2 into valuable fuels and chemicals through various reaction pathways, as detailed in Table 2.

Table 2. CO_2 as a feedstock: known reaction pathways to fuels.

Photocatalysis	Chemical Equation	Reference(s)
Reverse Water Gas Shift	$CO_2 + H_2 \rightarrow H_2O + CO$	(Jia et al., 2017)
Methane Synthesis	$CO_2 + 2H_2O \rightarrow CH_4 + 2O_2$	(Wang et al., 2016)
Dry Reforming	$CO_2 + CH_4 \rightarrow 2H_2 + 2CO$	(Han et al., 2016)
Sabatier Reaction	$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$	(O'Brien et al., 2014)
Methanol Synthesis Route 1	$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$	(Zhang et al., 2017)
Methanol Synthesis Route 2	$CO_2 + 2H_2O \rightarrow CH_3OH + \frac{3}{2}O_2$	(Ghoussoub et al., 2019)

3.6. Key Reaction Routes in CO_2 Catalytic Conversion

Photothermal CO_2 conversion has gained prominence as a direct and efficient method for converting CO_2 into valuable fuels under relatively mild conditions. In these processes, the primary reductants are H_2O, H_2, and CH_4, which correspond to the pathways of artificial photosynthesis, hydrogenation, and dry reforming, respectively. This section examines the principal reaction pathways for CO_2 conversion through photothermal catalysis, focusing on these three reductants. From a chemical standpoint, CO_2 conversion processes can be categorized into non-reductive and reductive pathways. In non-reductive processes, the carbon atom maintains its $^{+4}$ oxidation state, leading to the production of chemicals such as urea or salicylic acid. In contrast, reductive processes involve converting CO_2 into fuels (e.g., CO, CH_4, CH_3OH), which requires overcoming substantial thermodynamic and kinetic challenges. Therefore, the use of efficient catalysts and high-energy reductants is crucial for facilitating these reactions. Among the reductants, H_2, CH_4, and H_2O are most frequently employed in photothermal CO_2 conversion, aligning with the hydrogenation, reforming, and artificial photosynthesis routes, respectively (Wang et al., 2024). Despite significant research efforts, these processes have yet to achieve large-scale commercial implementation.

3.6.1. CO_2 reduction with H_2

The hydrogenation of CO_2 utilizing renewable (green) hydrogen constitutes one of the most promising avenues for the production of sustainable fuels. The principal reactions involved in this process include CO_2 methanation, the reverse water–gas shift (RWGS), and the synthesis of methanol or higher alcohols (Yang et al., 2026).

- *CO_2 methanation:*

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O \quad \Delta H_{298\,K} = -164.9\ kJ\ mol^{-1} \tag{5}$$

This exothermic reaction is extensively investigated for its potential in energy storage within power-to-gas (P2G) systems. Catalysts based on nickel (Ni) and ruthenium (Ru) are among the most thoroughly examined due to their superior activity and stability (Yang et al., 2026).

• *Reverse water–gas shift (RWGS):*

$$CO_2 + H_2 \rightarrow CO + H_2O \qquad \Delta H_{298\,K} = 41.2\ kJ\ mol^{-1} \tag{6}$$

The reverse water-gas shift (RWGS) reaction generates carbon monoxide (CO), a crucial intermediate in syngas-based chemical synthesis. Catalysts based on copper (Cu) and iron (Fe) are frequently utilized due to their advantageous selectivity and cost-effectiveness (Yang et al., 2026).

• *Methanol synthesis:*

$$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O \qquad \Delta H_{298\,K} = -49.5\ kJ\ mol^{-1} \tag{7}$$

This reaction facilitates the direct conversion of CO_2 into a liquid fuel, rendering it highly appealing. Conventional copper-based catalysts, along with emerging oxide systems such as In_2O_3 and ZnO/ZrO_2, have been extensively studied (Yang et al., 2026). The synthesis of higher alcohols (e.g., ethanol) is generally accomplished through tandem processes involving the reverse water-gas shift (RWGS) reaction followed by syngas conversion.

3.6.2. CO_2 reduction with CH_4

The dry reforming of methane (DRM) utilizes CO_2 as an oxidant to react with CH_4, converting two greenhouse gases into valuable syngas.

$$CO_2 + CH_4 \rightarrow 2CO + 2H_2 \qquad \Delta H_{298\,k} = 247.3\ kJ/mol \tag{8}$$

The highly endothermic nature of this reaction renders it of considerable interest for both environmental remediation and energy-related applications. Nickel-based catalysts are regarded as the most promising candidates for industrial use due to their high catalytic activity and relatively low cost. However, challenges such as carbon deposition and catalyst deactivation persist (Yang et al., 2026).

Ni-based catalysts are widely reported as promising for photothermal CO_2 methanation due to their abundance and moderate activity. However, a critical examination reveals three key nuances: (1) most Ni-based studies require bulk temperatures above 300 °C to achieve meaningful conversion, questioning the true photothermal advantage over conventional thermocatalysis; (2) carbon deposition rates are rarely quantified via post-reaction thermogravimetric analysis, making stability claims difficult to validate; and (3) direct comparisons show Ru-based catalysts consistently outperform Ni by factors of 3–5 in activity and stability under identical conditions, albeit at higher cost. Thus, while Ni remains economically attractive, its photothermal applicability may be limited to coking-suppressive conditions (e.g., high H_2/CO_2 ratios, short reaction times).

3.6.3. CO_2 reduction with H_2O

Artificial photosynthesis involves the direct conversion of CO_2 and H_2O into solar fuels under light irradiation, mimicking natural photosynthesis.

$$CO_2 + H_2O \rightarrow CH_4 + CH_3OH \qquad \Delta H_{298\,k} = 247.3\ kJ/mol \tag{9}$$

This pathway facilitates the direct storage of solar energy within chemical bonds, representing an optimal sustainable approach for fuel production. Semiconductor oxides and perovskite-based materials have been extensively studied as potential catalysts for this process (Yang et al., 2026). Nevertheless, the reaction is both thermodynamically challenging and kinetically intricate, necessitating efficient light harvesting, charge separation, and multi-electron transfer processes. As demonstrated in Table 3, recent research has focused on photothermal catalytic CO_2 conversion systems for solar fuel production.

Table 3. Recent literature on photothermal catalytic CO_2 Conversion to fuels.

Fuel	Catalyst	CO_2/H_2O	Product Yield ($mmol.g^{-1}.h^{-1}$)	Reaction Conditions (Xe Lamp)	Ref.
CH_4	$Ru/Mg\text{-}CeO_2$	1:3	469, 60%	300 W, 400°C, 2.9 W/cm^2,	(Zhang et al., 2024)
	$Au/Ce_{0.95}Ru_{0.05}O_2$	1:3	473, 75%	300 W, 50°C	(Jiang et al., 2023)
	$Ru/MnO/Mn_3O_4$	1:4	166.7, 66.8%	300 W, 200°C, 2.5 W/cm^2	(Zhai et al., 2024)

	Cu_3Ni-MA	1:1	339.8	300 W, 1.4 W/cm^2	(Wang et al., 2025)
CH_3OH	RCC@InQaN	--	226.6	300 W	(Ye et al., 2024)
	CoPc/CNT	1:3	2.4	1000 W, 2.5 W/cm^2	(Ren et al., 2025)
	NiO@InNi/In_2O_3	1:1	42.97	300 W, 2.72 W/cm^2	(Zhang et al., 2025)
CO	Ni/C-In_2O_3	1:4	20.96, 33.26%	300 W	(Mo et al., 2025)
	Pt/TiNxOy	1:1	11.28, 2.76%	300 W, 280°C	(Zou et al., 2024)

4. Rational Design for Photothermal Catalysts

4.1. Photothermal Catalyst Design Criteria

To effectively design photothermal catalysts, it is essential to not only enhance traditional catalytic properties but also integrate features unique to photothermal processes. Important design considerations include: (i) the ability to absorb a wide range of solar wavelengths, (ii) high efficiency in converting light to heat, (iii) efficient heat transfer and retention at active sites, (iv) maintaining accessible active sites, and (v) the effective creation and movement of photoinduced charge carriers. Among these, the absorption of a broad spectrum of light and efficient conversion of photothermal energy are crucial, primarily influenced by the inherent properties and structural features of photothermal materials. Typical materials used are plasmonic metals, semiconductors with narrow bandgaps, and carbon-based nanomaterials. Their optical characteristics can be precisely adjusted by manipulating their size, shape, and composition, which enhances solar absorption and the generation of hot carriers. Managing heat is also a vital aspect of photothermal catalysis (Ramos‐Fernandez et al., 2025). To optimize reaction efficiency, the heat produced when light is absorbed must be efficiently transferred to or retained at the catalytically active sites, rather than being lost to the surrounding environment. This presents a design challenge: photothermal components generally need high thermal conductivity for effective heat transfer, while catalysts require low thermal conductivity to concentrate heat. To tackle this issue, methods such as coating catalysts with thermally insulating layers have been used to reduce heat loss and increase local temperature. Moreover, catalyst supports are crucial in regulating heat transport, enhancing dispersion, and boosting overall catalytic stability (Cai et al., 2020).

The presence and accessibility of active sites are crucial, as catalytic reactions take place at these surface points. Thus, when integrating photothermal components, it is important to avoid obstructing or deactivating these sites. In scenarios where the photothermal material also acts as the catalyst, methods such as expanding surface area, adding appropriate supports like metal oxides, and incorporating co-catalysts can significantly increase the density of active sites. Additionally, photoinduced charge carriers generated by photothermal materials, especially in plasmonic metals and semiconductors, can play an active role in catalytic processes. These carriers aid in essential steps such as reactant adsorption, bond activation, intermediate transformation, and product desorption. Therefore, carefully choosing materials with suitable band alignment and carrier energy levels is vital to ensure efficient charge transfer pathways, ultimately enhancing catalytic activity, selectivity, and stability. Besides these aspects, practical considerations like material compatibility, thermal and chemical stability under reaction conditions, and high surface area are also essential for the effective design of photothermal catalysts (Gao et al., 2022).

4.2. Catalyst architectural design

In line with the aforementioned design principles, a successful photothermal catalytic system generally consists of three key components: (i) the main catalyst that includes active sites, (ii) a photothermal material that absorbs light and generates heat, and (ii) a support material that improves dispersion and surface accessibility (Ghoussoub et al., 2019, Kho et al., 2017). Three typical architectural designs can be outlined as follows:

• *Dual-function (self-heating) catalysts*

In this configuration, the catalyst functions as both the active site and the photothermal absorber. The same material facilitates light absorption, heat production, and catalytic reactions. Although this design can achieve high efficiency, it often complicates the task of distinguishing between the contributions of photochemical and thermal effects due to the simultaneous occurrence of multiple processes (Gao et al.,

2022).

• *Support-mediated photothermal systems*

In this design, the support material acts as the photothermal absorber, producing heat that is then conveyed to the active catalytic sites. This division enhances the ability to control light absorption and catalytic efficiency (Ramos‐Fernandez et al., 2025).

• *Hybrid photothermal systems with discrete components*

In this design, a distinct photothermal material acts as the heating core, conveying heat to the catalyst via support. The support, in turn, offers active sites for the catalytic reaction. This strategy allows for the independent optimization of light absorption, heat management, and catalytic activity, providing greater flexibility in system design. Unlike dual-function systems, hybrid architectures offer improved controllability and tunability, as the light absorption and catalytic functions are spatially separated. This separation facilitates systematic optimization of individual components and a deeper understanding of the underlying mechanisms (Cai et al., 2021). It is crucial to recognize that these architectures serve as general design guidelines, and in practical systems, component functions may overlap. Additional elements, such as co-catalysts, are often added to further enhance performance and stability.

5. Reactor Design and Scale-up

Although there have been notable advancements in photothermal catalyst materials, such as plasmonic nanoparticles, oxygen vacancies, and metal–organic frameworks, scaling these laboratory achievements to industrial levels necessitates strategic reactor engineering. Moving from meticulously controlled milligram-scale reactions to continuous processes in large-scale facilities transforms the system from an "ideal medium" to a "real working fluid," and from static interfacial reactions to dynamic multiphase flow systems. This shift presents interconnected challenges, including diminishing light intensity over distance, uneven heat flux distribution, limitations in material transport, and the dynamic deactivation of catalysts. Collectively, these elements create intricate engineering challenges (Yang et al., 2026). The assessment of performance and the choice of pathways for thermal-catalytic CO_2 reduction are influenced not just by the catalyst's inherent characteristics but also by the reaction engineering environment in which it functions. The type of reactor establishes the macroscopic boundary conditions for the transfer of light, heat, and mass, which in turn significantly impacts the reaction's efficiency, selectivity, and even our comprehension of its mechanism. The assessment of performance and the choice of pathways for thermal-catalytic CO_2 reduction are influenced not just by the catalyst's inherent characteristics but also by the reaction engineering environment in which it functions. The type of reactor establishes the macroscopic boundary conditions for the transfer of light, heat, and mass, which in turn significantly impacts the reaction's efficiency, selectivity, and even our comprehension of its mechanism (Ramos‐Fernandez et al., 2025).

Photothermal catalysis utilizes a range of reactor types, such as fixed-bed reactors, slurry reactors, and structured reactors, which can operate in either batch or continuous modes. In a fixed-bed reactor, the catalyst is immobilized, allowing light to shine on it while feed gases pass through and interact with it. A slurry reactor is a multiphase system where the reactant gas is bubbled through a liquid containing dispersed solid catalyst particles that are illuminated during the reaction. Structured reactors, also known as monolithic reactors, have a catalyst coated on the walls of the monolith, ensuring high contact between the reactants, light, and catalyst surface. Additionally, some innovative designs inspired by traditional shell-and-tube heat exchangers have been developed (Ramos‐Fernandez et al., 2025). Batch and fixed-bed reactors are essential configurations that connect laboratory findings to practical engineering applications. Stirred high-pressure reactors enhance the removal of engineering transfer limitations by ensuring consistent mixing and temperature distribution, closely mimicking intrinsic reaction kinetics. Nonetheless, significant photon scattering losses and gas-liquid mass transfer control can cause the observed reaction rate to differ greatly from intrinsic kinetics, leading to reduced spatiotemporal yield. Fixed-bed reactors replicate the traditional industrial production model, acting as the main point for transitioning powder catalysts into shaping and engineering. A well-designed reactor can greatly improve catalyst utilization and the overall efficiency of the reaction (Bian et al., 2023, He et al., 2025).

6. Role of Machine Learning in Photothermal CO_2 Conversion Research

Historically, the transition from discovery to deployment has been obstructed by the necessity for resource-intensive empirical trials and computationally exhaustive first-principles simulations. The emergence of data-driven informatics, particularly through machine learning (ML), has revolutionized this domain, facilitating the rapid exploration of extensive compositional and structural spaces to pinpoint optically viable candidates. Recent advancements in the development of autonomous

laboratories that integrate ML with electronic-structure modeling and experimental feedback are underscored, along with notable challenges concerning data quality, model generalization, and interpretability. Traditionally, the discovery and optimization of photocatalysts have been reliant on labor-intensive experiments and demanding theoretical calculations. However, artificial intelligence (AI) and machine learning (ML) have introduced a transformative paradigm to expedite photocatalytic research. Photothermal CO_2 conversion is a complex, multi-variable system involving interdependent parameters such as catalyst composition, morphology, light wavelength and intensity, temperature, pressure, flow rate, and reactor geometry. Traditional trial-and-error approaches are increasingly inadequate for navigating this high-dimensional space. Recent research has demonstrated that learning has emerged as a powerful tool to accelerate discovery, optimize performance, and enable rational scale-up (Ali et al., 2025, Kotob et al., 2025). By handling vast datasets, identifying trends, and optimizing outcomes for sustainable building design, including performance prediction, material selection, and lifecycle assessment, AI has the potential to transform architectural practice. It enables a move away from gut-feeling decisions toward evidence-based design processes that better integrate environmental, social, and economic priorities (Sharma and Gupta, 2025).

In this domain, one of the key uses of machine learning (ML) is in the screening of catalysts and the optimization of their design. By leveraging experimental and computational datasets, ML algorithms can swiftly forecast catalyst performance indicators such as apparent quantum yield (AQY), CO selectivity, conversion rate, and solar-to-chemical (STH) efficiency. Additionally, ML techniques are increasingly employed to determine the relationships between structure, property, and performance. In the realm of photothermal catalysis, catalyst performance is influenced by a mix of optical properties (such as bandgap and absorption spectrum), thermal properties (such as conductivity and heat capacity), and electronic characteristics (including band alignment and charge mobility). Machine learning models can synthesize these multidimensional descriptors to uncover subtle design principles that are challenging to identify with traditional theoretical methods (Wen et al., 2025). Another significant function of ML is in elucidating reaction mechanisms and optimizing parameters. In CO_2 photothermal conversion systems, the outcomes of reactions are heavily dependent on operating conditions like temperature, light intensity, catalyst loading, and reactant composition. ML-based regression and optimization algorithms can effectively navigate this complex parameter space, facilitating the discovery of optimal reaction conditions that enhance selectivity and conversion efficiency. Furthermore, the combination of high-throughput materials discovery with ML-guided screening has greatly broadened the spectrum of potential materials, including plasmonic metals, semiconductor heterostructures, and carbon-based composites. When combined with density functional theory (DFT) and experimental datasets, ML models further improve predictive accuracy and speed up catalyst development cycles. Overall, incorporating ML into photothermal CO_2 conversion research provides a transformative approach to data-driven catalyst design, understanding mechanisms, and optimizing processes, ultimately hastening the advancement of efficient and scalable solar fuel technologies.

7. Conclusions and Outlook

Photothermal conversion of CO_2 has gained recognition as a highly effective approach for producing sustainable fuels and chemicals by combining the benefits of photocatalysis and thermocatalysis. By utilizing both solar photons and localized heat, photothermal systems achieve better use of the solar spectrum, faster reaction rates, and access to reaction pathways that are difficult to achieve with only thermal or photochemical methods. This review systematically outlines the core principles of photocatalysis, thermocatalysis, and their photothermal integration, focusing on the synergies between photonic and thermal processes, both plasmonic and non-plasmonic mechanisms, and essential CO_2 conversion methods such as hydrogenation, dry reforming, and artificial photosynthesis.

Significant advancements have been made in catalyst design, particularly in enhancing light absorption, photothermal conversion efficiency, engineering active sites, and managing charge carriers. Improvements in catalyst structures have led to more efficient separation and coordination of light harvesting, heat production, and catalytic functions. Recent progress in operando and in situ characterization techniques has provided insights into dynamic structural changes, interfacial charge transfer, and localized thermal effects during operation, bridging catalyst design and mechanistic understanding.

Despite advancements, photothermal CO_2 conversion remains nascent, facing fundamental and practical hurdles. These include unclear differentiation between thermal and nonthermal effects, limited understanding of interfacial coupling, inadequate stability during prolonged use, and challenges in measuring local reaction environments. Additionally, scalability is restricted by light penetration, heat management, catalyst deactivation, and reactor design constraints.

Future research should focus on creating mechanistic frameworks to separate and measure photonic

and thermal effects. Combining operando characterization with theoretical modeling and data-driven techniques, like machine learning, is expected to accelerate catalyst discovery and enhance reaction systems. Strategies integrating optical, electronic, and thermal properties across length scales will be crucial for high efficiency and selectivity.

Photothermal catalysis is an emerging and interdisciplinary field of research with significant potential to tackle global energy and environmental issues. Ongoing advancements in catalyst development, understanding of mechanisms, and reactor design are anticipated to lead to effective, durable, and scalable solar-powered CO_2 conversion technologies, ultimately aiding in the achievement of a carbon-neutral future.

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Mirza Abdullah Rehan: Conceptualization, data curation, conducted the literature search, methodology, and writing—original draft preparation.

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