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Breaking the efficiency–selectivity trade-off in CO_2 reduction through photochemical H_2 dissociation

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Carbon dioxide is a key molecule in the global carbon cycle. The molecular chemical inertness of CO_2, the complex thermodynamics and kinetics involved in the reduction process and the difficulty of controlling product selectivity in multi-electron transfer pathways are the main bottlenecks for its efficient conversion.[1] With the advancement of green chemistry concepts, utilizing renewable hydrogen energy to efficiently reduce carbon dioxide into high-value-added products is regarded as one of the promising pathways for sustainable development.

Homolytic dissociation of H_2 on metal nanoparticles produces neutral hydrogen atoms. However, this process typically requires high temperatures, and neutral hydrogen (H•) exhibits poor selectivity toward C_{2+} compounds in the CO_2 reduction reaction (Figure 1A1).[2] The heterolytic dissociation of H_2 can be promoted through multiple pathways, such as utilizing acid-base pairs on metal oxide surfaces (Figure 1A2) and the localized surface plasmon resonance (LSPR) effect of gold nanoparticles (Figure 1A3), as well as specific active sites like negatively charged, coordinatively unsaturated hydroxyl groups (Figure 1A4)[3] or the frustrated Lewis pairs (FLPs) (Figure 1A5)[4] dependent on the metal-support interface. However, efficient dissociation via these strategies still requires additional heating due to high thermodynamic energy barriers and slow kinetic rates. In summary, although the aforementioned studies have successfully achieved hydrogen dissociation and accelerated the reaction process, it remains challenging to avoid high-temperature conditions at room temperature, stably generate sufficient nucleophilic hydrogen species, and obtain the desired single product. Therefore, it is crucial to develop a method capable of H_2 heterolytic dissociation at ambient temperature while selectively reducing CO_2 to a single C_{2+} compound.

Recently, Wang et al. made a significant breakthrough in this field, reporting the successful photocatalytic heterolytic dissociation of H_2 at ambient temperature using an Au/TiO_2 system (Figure 1A6).[5] This process involves the formation of interfacial electric dipoles (IEDs) under light exposure, which drives the near-quantum-yield conversion of CO_2 into C_2H_6 with a yield of over 99%. Subsequently, a cascade photodehydrogenation reaction yields high-purity C_2H_4. The key to this research lies in precisely constructing a photocatalytic reaction interface with an integrated electric field. Specifically, a roughly 1 nm-thick TiO_x layer is generated in situ on the surface of Au nanoparticles during the photoinduced process, forming an atomic-level Au–O–Ti interface structure. Under UV excitation, electrons and holes generated from TiO_2 are captured at the metallic gold nanoparticles and the Au–O–Ti interface, respectively, forming spatially separated electron–hole pairs. This structure is functionally analogous to FLPs and constitutes potent IEDs that effectively promote charge separation. The localised electric dipole field strongly polarises H_2 molecules, driving their heterolytic dissociation to generate highly reactive $H^{\delta-}$ and $H^{\delta+}$ species. This yields strongly reducing hydrogen species without the need for heating. This novel catalyst structure overcomes the inherent electron recombination limitations of traditional Au/TiO_2 catalysts. The small size of Au nanoparticles increases the number of Au-TiO_2 interfaces per unit area, thereby enhancing the quantity of active sites. This not only provides active sites but also promotes the separation of photo-generated electron-hole pairs, thereby enhancing the local electric field strength.

Researchers revealed that the H/D exchange reaction rate on Au/TiO_2 was 30 times higher under 365 nm illumination than under dark conditions. However, under 525 nm illumination, the reaction activity nearly vanished. This suggests that light-induced charge separation is the main cause of H_2 dissociation rather than thermal effects. Furthermore, FTIR and ambient pressure XPS analyses conducted in an H_2 atmosphere revealed a 0.7 eV redshift in the characteristic binding energy of the $Au^{\delta+}$ peak. This confirms that photoexcited TiO_2 undergoes heterolytic dissociation of H_2 at the Au/TiO_2 interface, yielding $H^{\delta+}$ and $H^{\delta-}$ species. Additionally, thin-layer SiO_2 encapsulation experiments on Au nanoparticles or TiO_2 carriers demonstrated that the catalytically active sites are strictly confined to the Au/TiO_2 interface. Neither photogenerated electrons nor holes alone could effectively induce this dissociation, indicating the necessity of an interfacial synergistic effect. This provides strong support for a mechanism in which IEDs dominate H_2 dissociation.

In a flow photochemical apparatus, the optimised Au/TiO_2 catalyst achieved almost 100% CO_2 conversion under 365 nm illumination, with C_2H_6 selectivity of 99% and a production rate of 440 mmol h^{-1} m^{-2} (Figure 1B1). Reducing the size of the Au nanoparticles to 2 nm significantly increased the apparent quantum efficiency (AQE) for CO_2 conversion from 37.1% to 58.5%. This catalytic system demonstrated exceptional stability, operating continuously for over 210 h without any notable decline in performance. Furthermore, researchers have successfully extended this approach to a series of Au catalysts supported on visible light-responsive carriers (e.g. N-TiO_2, CeO_2 and In_2O_3). Under concentrated natural sunlight within the visible-light-dominated spectrum (350–1100 nm), the $Au_{2nm}/N–TiO_2$ catalyst achieves CO_2 conversion exceeding 99% at light intensities above 470 mW cm^{-2}, delivering a C_2H_6 formation rate of up to 792 mmol h^{-1} m^{-2} with a selectivity of ~90%. Coupling the CO_2 hydrogenation with ethane dehydrogenation constructed a cascading reaction system. This system stably produced ethylene at a production rate of 447 mmol h^{-1} m^{-2} with over 99% selectivity, and could operate continuously for up to 1500 h (Figure 1B2). This work holds promise for advancing CO_2 reduction from laboratory to practical applications, though operational selectivity, yield, and stability require further validation and enhancement.

Wang et al. have successfully developed a novel catalytic strategy that uses IEDs to achieve almost complete CO_2 conversion and highly selective C_{2+} product synthesis under mild conditions by driving H_2 heterolytic dissociation. A super-thin TiOx layer is formed on the surface of Au nanoparticles via photodeposition, precisely regulating the number of active sites to significantly enhance charge separation efficiency and efficiently generate reactive hydrogen species. Although Au is a noble metal, its loading in this catalyst remains at approximately 1.0 wt%, and its stable properties facilitate easy recycling without significantly increasing costs during subsequent industrialization. Compared to the best-reported results for photocatalytic CO_2 hydrogenation in the literature, this catalytic system achieves a significant breakthrough. Furthermore, a clever coupling strategy combines high selectivity with long-term stability to enable the efficient production of C_2H_4. Furthermore, this catalytic strategy has been successfully extended to visible light-responsive systems, broadening its applicability to solar-driven processes. When combined with a cascade strategy for the direct production of bulk chemicals, it shows great promise for industrial implementation. While Jin's work presented a promising new paradigm for CO_2 reduction that holds potential for industrial-scale implementation, several challenges remain. While the research can be extended to visible-light-responsive carriers (such as N-TiO_2), it still requires artificial white LEDs for efficient reaction driving, leading to low photoelectric conversion efficiency. In practical production, CO_2 and H_2 must be co-adsorbed at the $Au–TiO_2$ interface for reaction. Gas-solid mass transfer resistance often arises in fixed-bed or membrane reactors, particularly at high flow rates where reactants cannot fully contact active sites. High-intensity illumination induces localized heating at the nanoscale, potentially damaging the TiO_x shell or inducing side reactions. Future research should further optimize catalyst structures and enhance energy efficiency by increasing light intensity.

This work paves the way for a new strategy for the directed utilisation of CO_2, achieving the precise conversion of CO_2 to ethylene within the complex network of reactions involved in CO_2 reduction. By controlling photogenerated charge behaviour and constructing a unique active reaction interface,

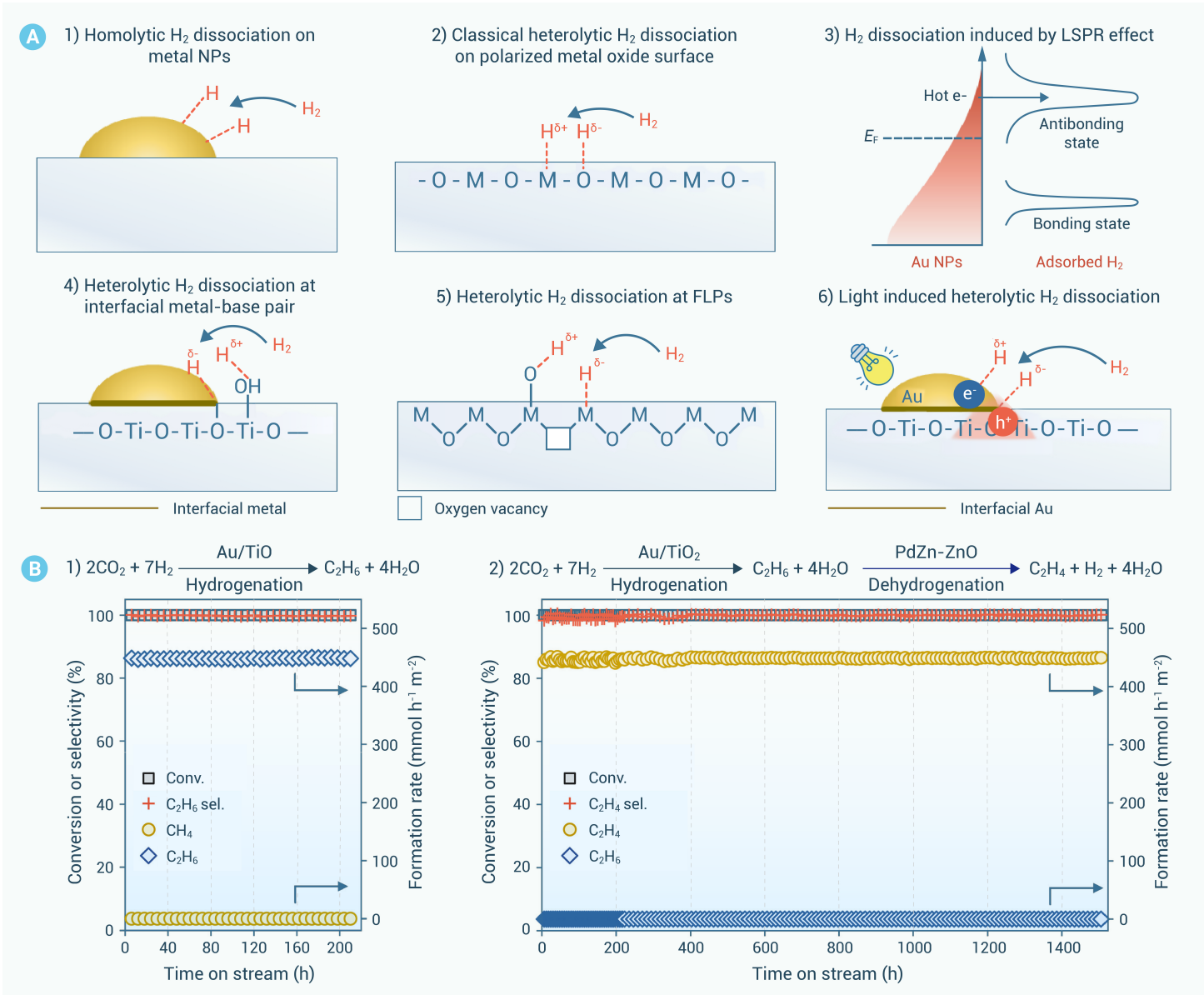

Figure 1. Hydrogen dissociation and CO_2 cascade reaction mechanism (A) Hydrogen dissociation mechanism, (B) Cascade reaction system for CO_2. Reproduced with permission.[5] Copyright 2025, AAAS.

reaction pathways, selectivity and stability that were previously unattainable in thermal catalytic systems are enabled. However, scaling this process for industrial applications and extending it to other catalytic processes, such as nitrogen activation and methane conversion, presents challenges. These include optimizing energy efficiency, ensuring long-term catalyst stability, and addressing the cost of materials like Au. As research continues to advance in the exploration and optimisation of photocatalytic materials and reaction processes, the prospect of using solar energy to convert CO_2 into valuable resources is becoming increasingly clear and feasible, paving the way for large-scale production of low-carbon chemicals and fuels. Furthermore, the core concept revealed in this work, namely the precise regulation of photogenerated charges to construct well-defined reaction interfaces, has implications far beyond CO_2 conversion. It also offers novel insights and references for achieving other crucial catalytic processes. This lays a solid foundation for the future development of cleaner, more efficient clean energy technologies, thereby powerfully advancing the long-term development of the global carbon circular economy and a sustainable society.

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AUTHOR CONTRIBUTIONS

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DECLARATION OF INTERESTS

The authors declare no competing interests.