

II–VI semiconductor nanoplatelets for photocatalysis: From structure regulation to mechanistic understanding and applications

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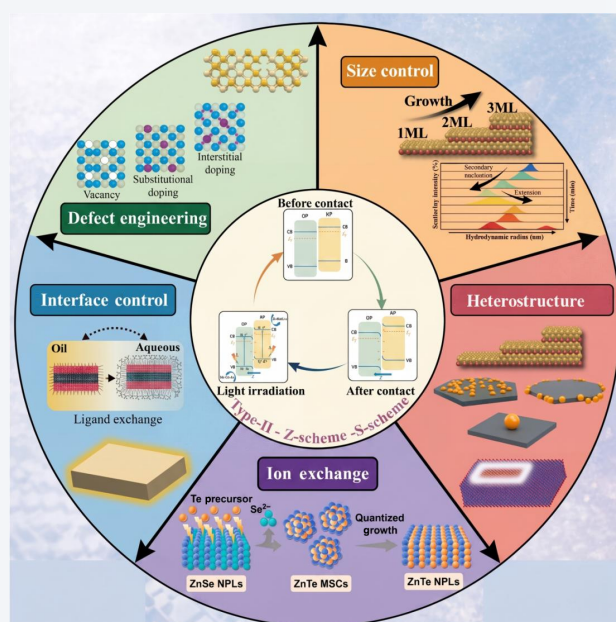
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ABSTRACT: II–VI semiconductor nanoplatelets have emerged as promising photocatalysts due to their tunable band structures, low cost, and unique two-dimensional geometry. The atomically confined thickness induces strong quantum confinement, enabling efficient charge separation, abundant surface-active sites, and precise structural regulation. These features make them attractive for solar-driven processes, including hydrogen evolution, CO₂ reduction, and pollutant degradation. This review summarizes recent advances in the controlled synthesis and structural regulation of II–VI nanoplatelets, focusing on thickness control, ligand engineering, defect modulation, heterostructure design, and ion exchange-driven transformations. The photocatalytic mechanisms are discussed by correlating structural characteristics with light absorption, charge dynamics, and surface reaction pathways. Representative applications in energy conversion and environmental remediation are highlighted. Finally, current challenges and future perspectives are outlined to guide the rational design of high-performance nanoplatelet-based photocatalysts. This work provides a framework for the rational design of efficient and stable nanoplatelet-based photocatalysts.

KEYWORDS: photocatalysis, semiconductor nanoplatelets, structure regulation, exciton dynamics, charge separation



1 Introduction

Amid escalating challenges related to energy scarcity, climate change, and environmental pollution, the development of green, efficient, and sustainable technologies for energy conversion and environmental remediation have become a central research priority. Photocatalysis, driven directly by solar energy, enables key reactions such as water splitting for producing hydrogen [1], CO₂ reduction [2], organic pollutants degradation [3], and high-value-added chemical synthesis [4] offering a promising route to address both energy and environmental issues. As the core component of

photocatalytic systems, semiconductor catalysts play a decisive role, where their electronic structure, light absorption capability, charge separation and transport efficiency, and surface reaction activity collectively determine overall performance. Therefore, the development of highly efficient, stable, and low-cost semiconductor photocatalysts is critical for advancing photocatalysis toward practical applications.

Fundamentally, photocatalysis relies on the generation of photogenerated electron-hole pairs upon light excitation of semiconductors, followed by their migration to the surface to drive redox reactions, thereby converting solar energy into chemical energy [5]. However, conventional bulk semiconductors generally suffer from rapid charge recombination, limited surface area, and insufficient visible-light response, which hinder their photocatalytic efficiency [6]. In recent years, two-dimensional (2D) nanomaterials have emerged as a promising class of photocatalysts due to their pronounced quantum confinement effects along the thickness

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direction and unique surface characteristics. Among them, II–VI semiconductor nanoplatelets (NPLs), such as ZnSe, CdS, CdSe, and ZnS, have attracted considerable attention owing to their excellent optical properties, tunable bandgaps and band structures, and relatively low synthesis cost [7–10]. On the one hand, their atomic- or nanoscale thickness induces strong quantum confinement, enabling precise regulation of electronic structures and facilitating efficient charge separation [11]. On the other hand, their large specific surface area and abundant exposed facets provide rich active sites and interfaces for surface reactions. Moreover, their compositional and structural tunability offers versatile platforms for performance optimization through heterostructure structure [12], surface engineering [9], and defect modulation [7].

In this context, this review focuses on II–VI semiconductor NPLs as a distinctive class of photocatalytic materials (Fig. 1). First, their unique structural and electronic properties arising from dimensional confinement are introduced to establish the fundamental basis for their photocatalytic behavior. Next, recent advances in synthesis and structural modulation strategies are systematically summarized, including control over size and thickness, ligand regulation, defect engineering, heterostructure construction and ion exchange-driven transformations, with an

emphasis on their effects on material properties. Subsequently, the key photocatalytic mechanisms are discussed, covering light absorption and exciton dynamics, charge separation and transport, surface reaction pathways, and structure–function relationships. Finally, recent progress in applications, including CO₂ reduction, photocatalytic hydrogen evolution, environmental remediation, and value-added chemical synthesis, is reviewed, followed by a discussion of current challenges and future perspectives. This review aims to provide insights into the rational design and controllable synthesis of efficient, stable, and low-cost II–VI nanoplatelet photocatalysts and to promote their further development in photocatalytic applications.

2 The unique electronic structure and structural properties of II–VI NPLs

With the rapid development of semiconductor materials, a wide range of novel systems with tailored structures and properties have been successfully synthesized. Among them, II–VI semiconductor NPLs have emerged as a particularly promising class of materials owing to their remarkable physicochemical properties and strong potential in photocatalytic applications. Compared with

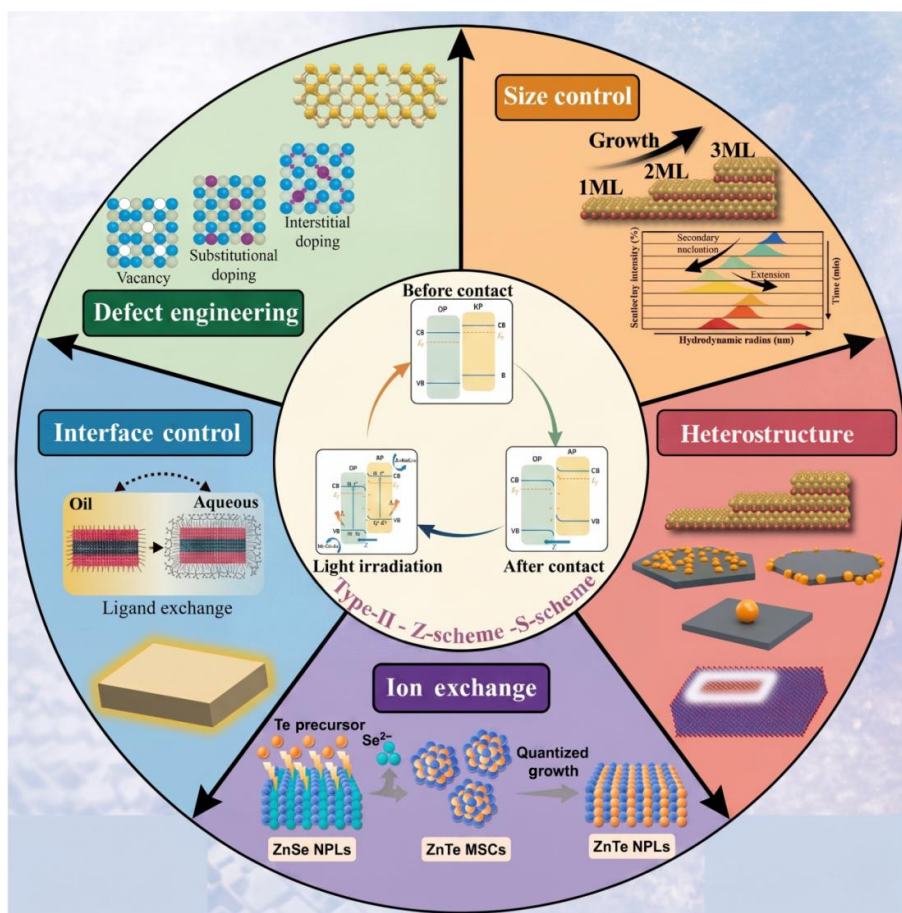


Figure 1 Schematic diagram of strategies for two-dimensional nanomaterials. These include size control, heterostructure fabrication, ion exchange, surface and interface engineering, and defect engineering. The figure also demonstrates the changes in the band structures of the photocatalytic systems under light irradiation. At the same time, the possible micro-mechanism of II–VI NPLs in the field of photocatalysis is discussed, including light absorption, charge separation and exciton dynamics, surface reaction path, and common conformation-effect relationships, which provides a theoretical basis for better understanding of photocatalytic reactions. In addition, on the basis of briefly reviewing the development process of photocatalysis of II–VI materials, this article further highlights the development potential of the material in the field of photocatalysis by combing in more detail the latest progress of the material in the three aspects of photocatalytic hydrogen production, carbon dioxide reduction, degradation of harmful substances and the synthesis of high value-added materials.

conventional bulk semiconductors, reducing dimensionality to the 2D limit not only alters the crystal structure but also fundamentally modifies the electronic properties through quantum confinement effects, thereby influencing their optical and electrical behaviors. In this section, the intrinsic characteristics of II–VI NPLs are discussed from both structural and electronic perspectives, providing a foundation for the subsequent discussions on synthetic regulation and photocatalytic mechanisms.

From a structural standpoint, bulk II–VI compounds typically adopt either cubic zinc blende or hexagonal wurtzite phases. However, when confined to the 2D limit, structural rearrangements can occur due to changes in geometric stability and long-range Coulomb interactions. For example, CdS and CdSe can transform from their bulk wurtzite structures into a tetragonal-triangular (TT) configuration in the monolayer form [13]. In addition, deviations from stoichiometry can further induce structural evolution in NPLs. Ma and co-workers demonstrated that partial removal of Se atoms from the surface of CdSe NPLs via electron beam irradiation altered the CdSe ratio from 1:1 to approximately 1:0.8, leading to the formation of an intermediate structure between wurtzite and zinc blende phases and ultimately triggering a phase transition [14]. These observations indicate that the crystal structure of II–VI NPLs in the ultrathin limit differs significantly from that of their bulk counterparts and is highly sensitive to factors such as stoichiometry and surface chemistry. Such structural variations play a critical role in determining their photocatalytic properties.

From an electronic perspective, dimensional reduction enhances quantum confinement along the thickness direction, leading to significant modifications in the electronic band structure [15]. As the dimensionality decreases from three to two dimensions, the density of states evolves from a continuous, parabolic distribution into a step-like profile, which holds true for all two-dimensional materials due to the universality of quantum theory, including those made of II–VI semiconductors [16]. They can be expressed mathematically as

$$N(E)_{\text{bulk}} = \frac{\sqrt{2}m^{3/2}E^{1/2}}{\pi^2\hbar^3} \quad (1)$$

$$N(E)_{2-D} = \frac{nm^*}{\pi\hbar^2} \quad n = 1, 2, 3 \quad (2)$$

where the function $N(E)$ is the density of states as a function of the electric field. This transition has profound implications for the optical and electronic properties of the material. One key consequence is the substantial increase in exciton binding energy in 2D semiconductors, arising from reduced dielectric screening and enhanced confinement effects [17]. As a result, exciton formation becomes more favorable compared to bulk systems [15]. For photocatalysis, this enhanced excitonic effect has both positive and negative implications. For catalytic reactions that require separate occurrence of oxidation and reduction half-reactions at distinct active sites on the catalyst surface like CO₂ reduction and nitrogen fixation, excitations must first dissociate into free electrons and holes. During this process, the strong Coulomb interaction between electrons and holes makes exciton dissociation into free charge carriers more difficult, which can limit their participation in surface redox reactions. In the absence of efficient separation pathways, excitons may undergo radiative or nonradiative recombination, thereby reducing the quantum efficiency of photocatalytic processes [18, 19]. But when surface chemical reactions are primarily

dependent on the transfer of excited-state energy rather than charge transfer, excitons more likely act as direct energy transfer media. Such reactions include photocatalytic disinfection, degradation of organic pollutants, and specific selective oxidation reactions [20]. Under this circumstance, the increased binding energy is often accompanied by prolonged exciton lifetimes, which can provide a longer time window for subsequent charge or energy transfer processes. Notably, recent studies have shown that excitons themselves can directly participate in photocatalytic reactions. For instance, Shen et al. reported that excitons can activate molecular oxygen via energy transfer to generate singlet oxygen (¹O₂), which subsequently undergoes further reduction without involving superoxide intermediates [21]. This mechanism highlights the unique role of excitons in 2D photocatalytic systems.

In addition to excitonic effects, dimensional confinement can also modify the band structure of semiconductors. The distinction between direct and indirect bandgaps arises from the relative positions of the conduction band minimum (CBM) and valence band maximum (VBM) in momentum (*k*) space. In direct bandgap semiconductors, the CBM and VBM are located at the same *k*-point (typically at the Brillouin zone center), allowing vertical electronic transitions without momentum change. In contrast, indirect bandgap semiconductors require phonon assistance for transitions between different *k*-points, resulting in less efficient light absorption and emission processes (Fig. 2) [22]. Importantly, reducing dimensionality can induce transitions from indirect to direct bandgaps. For example, Zhang et al. used angle-resolved photoemission spectroscopy (ARPES) to reveal that bulk and multilayer MoSe₂ exhibit indirect bandgaps, whereas monolayer MoSe₂ transitions to a direct bandgap structure [23]. Considering typical II–VI group semiconductors (including ZnS, ZnSe, CdS, CdSe, ZnTe, etc.) are usually direct bandgap materials in their stable zinc blende or wurtzite crystal structures [24], this transition of bandgaps lacks extensive experimental support for common II–VI group NPLs. However, understanding band-structure modulation in ultrathin NPLs still provides valuable support for the construction of photocatalytic structures using new two-dimensional II–VI semiconductor materials that may be discovered in the future. After all, the emergence of bandgaps is beneficial for enhancing light absorption and improving solar energy conversion efficiency, which is highly desirable for photocatalytic applications [25].

In summary, the unique properties of II–VI NPLs arise from the interplay of structural reconstruction and quantum confinement effects induced by dimensional reduction. These features endow them with distinct advantages in photocatalysis, including tunable electronic structures, enhanced light-matter interactions, and flexible surface chemistry. In addition, external modulation strategies—such as defect engineering, heterostructure design, and cocatalyst integration—can further tailor their structural and electronic characteristics. Consequently, current research efforts are largely focused on these aspects to fully exploit the photocatalytic potential of II–VI NPLs.

3 Synthetic strategy and structural regulation

The structural characteristics of II–VI NPLs are governed by a hierarchy of regulation strategies, including dimensional control, ligand-mediated surface engineering, compositional design, defect modulation, and post-synthetic transformations. Among these,

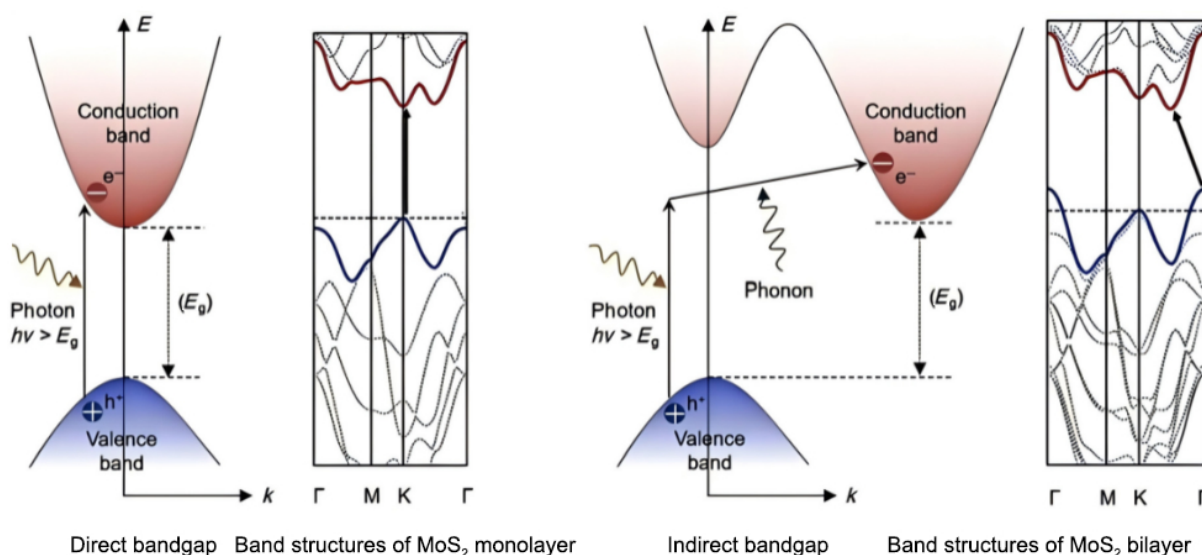


Figure 2 The computational energy band structure of molybdenum disulfide and two different band gap characteristics-direct excitant and indirect electronic transition. The solid arrow indicates the lowest energy jump. Reproduced with permission from Ref. [22], © The Royal Society of Chemistry 2023.

precise control over thickness and lateral dimensions is particularly critical, as they directly determine the optical and electronic properties of NPLs.

3.1 Control of thickness and lateral dimensions

II–VI NPLs typically exhibit characteristic doublet features in their absorption spectra, corresponding to excitonic transitions involving heavy-hole and light-hole bands. The sharp peak arises from the first electron-heavy-hole transition, while the broader peak originates from the electron-light-hole transition. Notably, the spectral positions of these features are strongly dependent on the thickness of the NPLs. As the number of atomic layers increases, both peaks exhibit a pronounced redshift, reflecting the reduction of quantum confinement with increasing thicknesses (Fig. 3(a)) [6]. In addition to thickness, lateral dimensions also play an important role in determining the optical properties of NPLs. Increasing the lateral size has been shown to enhance photoluminescence (PL) efficiency and suppress nonradiative recombination pathways [26]. Therefore, achieving independent and precise control over both thickness and lateral size is essential for tailoring the optoelectronic performance of II–VI NPLs.

The thickness of II–VI NPLs is primarily governed by precursor chemistry and ligand interactions during nucleation and growth. Akhmetova et al. systematically investigated the influence of different cadmium precursors on the growth behavior of CdTe NPLs [27]. When cadmium propionate or cadmium acetate was used, NPLs with thicknesses of 5–6 monolayers were rapidly formed after precursor injection. However, further thickening was not observed upon increasing the temperature. This behavior was attributed to the transformation of thinner NPLs into thermodynamically more stable thicker ones, with the transformation rate strongly dependent on temperature and precursor concentration. In contrast, when long-chain cadmium myristate was employed, its stronger stabilizing effect enabled the coexistence of NPLs with thicknesses ranging from 5 to 8 monolayers, accompanied by the formation of CdTe quantum dots (QDs).

Halide ligands also play a crucial role in thickness modulation. Meerbach et al. demonstrated that halide ions, particularly chloride,

can systematically reduce both the reaction enthalpy and surface energy of CdSe, thereby favoring the formation of thicker NPLs [28]. By tuning the halide content in the precursor solution, NPLs with different thicknesses could be obtained (Fig. 3(c)). Furthermore, Moghaddam proposed that halide ligands can induce a dissolution–recrystallization process from the NPLs edges toward the basal planes, enabling thickness growth in discrete steps of two monolayers [29]. Based on this mechanism, thickness-tunable homostructures were achieved through the combined regulation of halide and acetate ligands (Fig. 3(b)).

Compared to thickness control, studies on lateral size modulation remain relatively limited, although it plays an important role in influencing nonradiative recombination and overall optical performance. Bertrand et al. demonstrated that the aspect ratio of CdSe NPLs can be tuned by controlling the concentration of short-chain ligands that promote lateral growth [30]. In their study, the amount of cadmium acetate in the precursor solution was found to be a key parameter. The presence of crystallization water in cadmium acetate leads to the *in situ* generation of hydroxide ions during heating, which compete with acetate ligands for adsorption on the NPL surface. This competitive adsorption regulates anisotropic growth, thereby controlling the aspect ratio.

Alternatively, lateral size can be tuned through growth kinetics at the mesoscale. Tenney et al. investigated the time-dependent evolution of NPLs size during synthesis (Fig. 3(d)). Within the first 45 min, a large number of small NPLs were formed through secondary nucleation. At around 60 min, larger NPLs began to emerge. After one hour, a second nucleation burst occurred, while the lateral dimensions of large NPLs reached their maximum. Beyond this stage, the depletion of precursors limited further lateral growth (Fig. 3(e)). These results highlight the dynamic interplay between nucleation and growth processes in determining lateral size [31].

Based on these studies, a general understanding of dimensional control in II–VI NPLs can be established. Thickness evolution is primarily dictated by the interplay between cation precursors and surface ligands during nucleation and early-stage growth. In contrast, lateral dimensions and aspect ratios are governed by

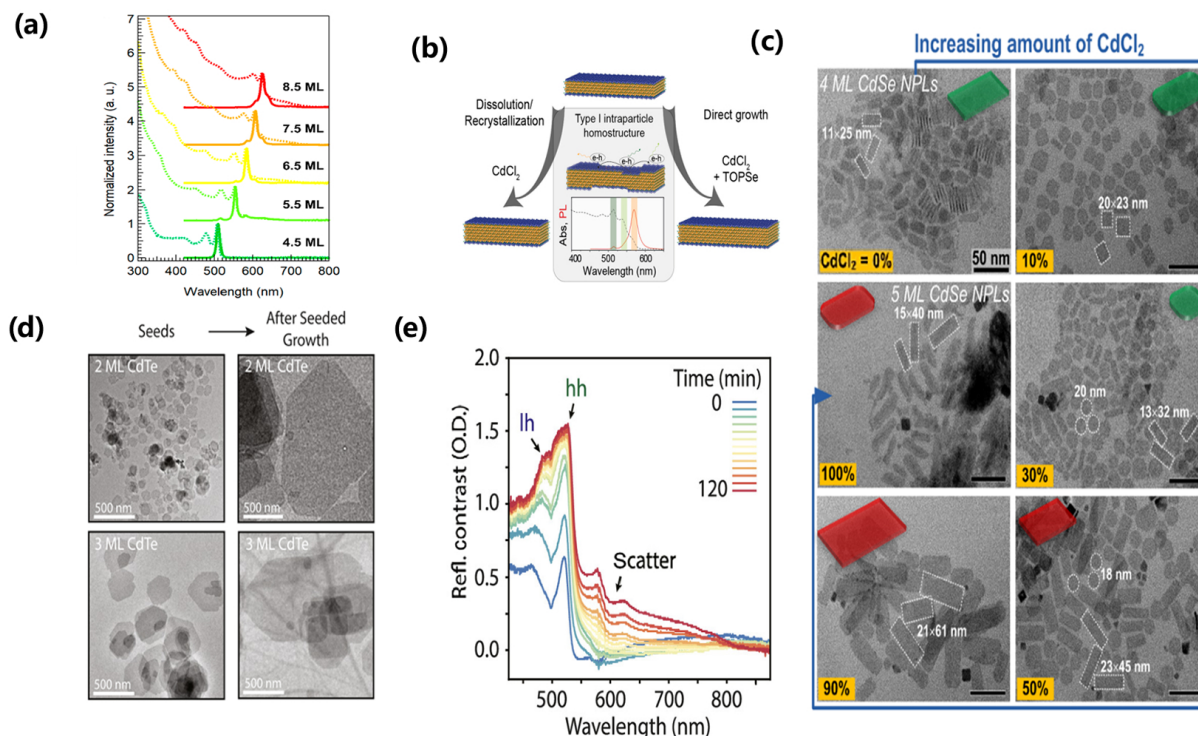


Figure 3 (a) The absorption (dots) and emission (curve) for 4–8 ML CdSe NPLs. Reproduced with permission with Ref. [6], © World Scientific Publishing Company 2025. (b) By introducing the metal halide precursor and chalcogenide precursor on the NPLs, the core/shell homo- and heterostructures are achieved. When an incomplete layer is grown, NPLs with steps are synthesized. Reproduced with permission with Ref. [29], © American Chemical Society 2021. (c) TEM images of CdSe NPLs obtained with different amounts of CdCl₂, showing the evolution of the size and the shape of the resulting particles. Reproduced with permission with Ref. [28], © American Chemical Society 2019. (d) TEM of 2 and 3 ML CdTe N-PL seeds before and after seeded growth. (e) Reflectance contrast collected *in situ* (data shown for every 10 min) for the duration of a seeded growth of 3 ML CdTe. Reproduced with permission with Ref. [31], © American Chemical Society 2022.

competitive ligand adsorption and precursor concentration, which regulate anisotropic growth kinetics. The formation of large-area NPLs further depends on multiple parameters, including temperature, injection rate, seed concentration, and growth time.

3.2 Ligand engineering and surface/interfacial control

As a representative class of two-dimensional materials, II–VI NPLs possess atomically flat surfaces that provide an ideal platform for surface and interfacial engineering. During their growth and post-synthetic processing, surface ligands are inevitably adsorbed onto the NPLs, where they not only stabilize colloidal dispersions but also regulate morphology, phase-transfer behavior, and optical properties through surface stress, ligand-ligand interactions, and ligand-environment interactions [32–34]. Consequently, ligand engineering plays a central role in tailoring the structural and functional characteristics of NPLs.

One important aspect of ligand engineering lies in its ability to modulate interparticle interactions and drive controlled assembly. Graf et al. investigated the stacking behavior of NPLs during slow solvent evaporation and identified multiple driving forces underlying this process [32]. By replacing conventional oleic acid/acetate ligands with 11-mercaptopundecanoic acid (MUA), NPLs were transferred into polar media, enabling a detailed analysis of stacking interactions. The assembly was found to be governed by a combination of van der Waals attractions between NPLs, interactions between ligands and the surrounding solvent, ligand-ligand interactions, and bridging effects mediated by MUA through its carboxyl and thiol groups. In a related study, Wang et al. utilized sodium dodecyl sulfate (SDS) ligand exchange combined with

phase transfer to process CdSe/CdZnS core/shell NPLs (Fig. 4(a)) [33]. Through emulsification and solvent evaporation, spherical suprastructures composed of NPLs were obtained, highlighting the role of surfactant-assisted confinement in directing NPLs assembly.

Beyond structural assembly, ligand engineering also enables precise control over optical activity and morphology. Lehouelleur et al. introduced chiral tartaric acid ligands onto NPLs surfaces and observed strong circular dichroism signals with dissymmetry factors exceeding 1×10^{-2} , accompanied by a notable sign inversion behavior (Fig. 4(b)) [35]. This phenomenon was attributed to changes in ligand binding configurations. Building on this, Po et al. developed a mechanical model to quantitatively describe ligand-induced structural deformation, demonstrating that surface ligands can induce curvature and even helical morphologies in NPLs [36]. By exchanging surface carboxylates with thiols of varying chain lengths, they established a correlation between ligand structure and NPLs curvature, enabling predictive control over shape evolution (Fig. 4(c)).

In addition to small-molecule ligands, polymer-based strategies provide further flexibility in tailoring surface and interfacial properties. Li et al. developed a layer-by-layer assembly approach to achieve uniform dispersion of NPLs within polymer matrices [37]. By selecting different polyelectrolytes, both the thickness and surface roughness of the resulting nanocomposites could be finely tuned. This method exploits the negatively charged surfaces of ligand-exchanged NPLs, allowing for alternating deposition with oppositely charged polymers (Fig. 4(d)). Similarly, Halim et al. demonstrated that amphiphilic polymer chains can be used to facilitate the phase transfer of individual NPLs [38]. By employing a

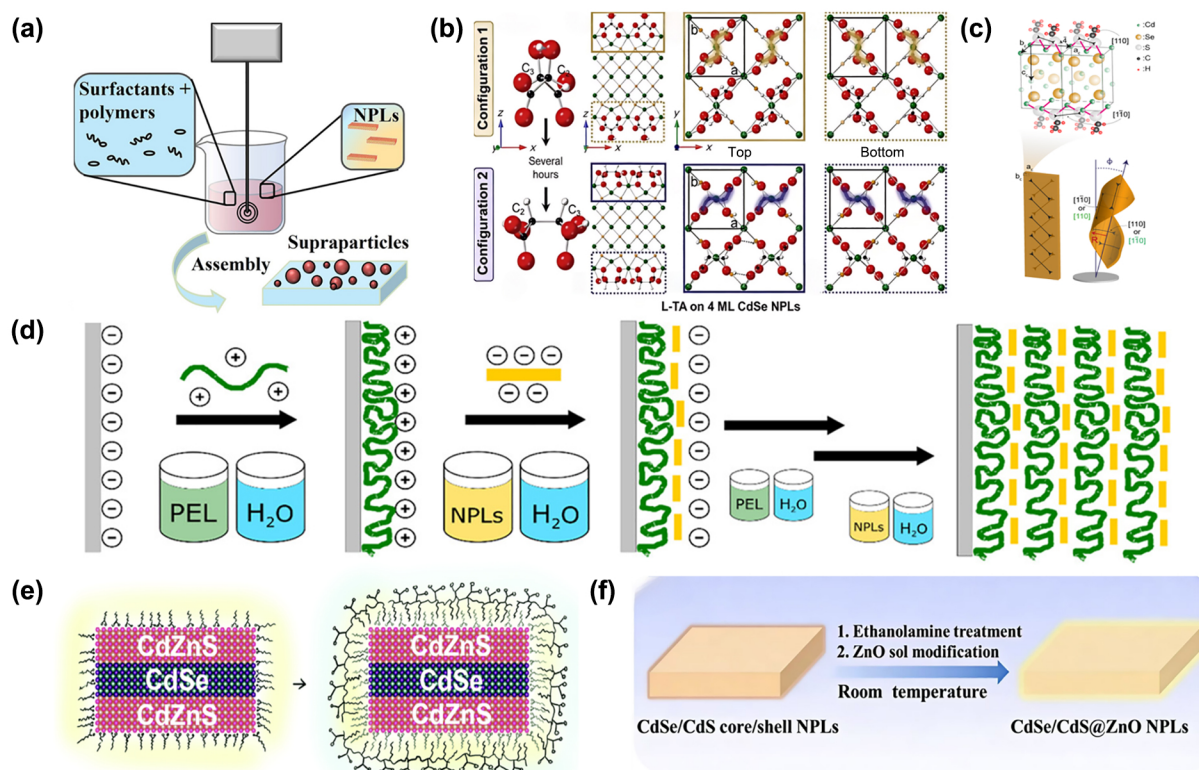


Figure 4 (a) Schematic illustration of NPLs self-assembly process via oil-in-water emulsion. Reproduced with permission from Ref. [33], © American Chemical Society 2026. (b) Possible binding of L-TA ligands on 4 ML of CdSe NPLs and the related projection of the NPLs in the [010] direction. In these two conformers of L-TA, the C–OH bonds are “parallel” and “perpendicular” to the NPLs plane. Reproduced with permission from Ref. [35], © American Chemical Society 2024. (c) CdSe/ZnS core-shell crystal structure in a 3 ML CdSe NPLs. The arrows illustrate the compressive stress brought by ethanethiolate ligands. Reproduced with permission from Ref. [36], © American Chemical Society 2022. (d) Scheme of the LbL dip-coating process. Layer-by-layer deposition of NPLs onto a polymer via electrostatic attraction between the charges on the NPLs surface ligands and the polymer. Reproduced with permission from Ref. [37], © American Chemical Society 2022. (e) Illustration of polymer coating. Hydrophobic regions are highlighted in yellow. Reproduced with permission from Ref. [38], © The Royal Society of Chemistry 2020. (f) Schematic demonstration of synthesis and post-treatment of CdSe/CdS@ZnO NPLs. Reproduced with permission from Ref. [34], © Elsevier B.V. 2019.

commonly available dodecyl-grafted polymer, they simplified the encapsulation process and formed a hydrophobic intermediate layer that enhances environmental stability, enabling NPLs to withstand harsh conditions such as low pH environments (Fig. 4(e)).

While polymer coatings improve stability and processability, inorganic surface modification can be more effective in enhancing charge transport and preserving intrinsic electronic properties. Bai et al. reported the coating of CdSe/CdS NPLs with colloidal ZnO, which simultaneously improved charge transport and passivated surface defects (Fig. 4(f)) [34]. In addition to preventing aggregation, the ZnO layer facilitates charge transfer by extracting electrons trapped at surface defect states and modulating Auger recombination processes, thereby improving overall charge transport efficiency.

Overall, ligand engineering and surface/interfacial control offer versatile approaches for tuning the morphology, anisotropy, optical properties, and stability of II–VI NPLs. However, despite significant advances in fundamental studies, their application in photocatalysis remains relatively limited, largely due to challenges associated with aggregation and structural instability under reaction conditions. Nevertheless, the ability of ligand and interface engineering to enhance optical stability and facilitate charge transport provides important guidance for improving photocatalytic performance, and further integration of these strategies with reaction-specific design is expected to unlock the full potential of II–VI NPLs.

3.3 Composition and heterostructure engineering

While ligand engineering and surface/interfacial control enable fine tuning of morphology, stability, and optical properties, the construction of heterostructures provides a more direct route to modulate electronic band alignment and improve charge separation at the nanoscale. Among the various strategies developed to enhance photocatalytic performance, heterostructure engineering is widely regarded as one of the most effective approaches, as it can suppress charge recombination and facilitate directional carrier transfer.

Core/shell heterostructures, in which one material serves as the core and another is grown epitaxially on its surface, represent a well-established design. Owing to the relatively low thermal stability of NPLs, their synthesis is typically carried out using low-temperature colloidal atomic layer deposition (c-ALD) [39]. This approach has so far been applied to the synthesis of different core/shell NPLs heterostructures of a CdSe/CdS [40] and CdSe/ZnS [41] type. However, heterostructures prepared via c-ALD often suffer from limited quantum efficiency and poor stability. To address these issues, Rossinelli et al. developed a hot-injection shell growth strategy that prevents the dissolution of the NPLs core prior to shell formation, enabling the deposition of thick CdS shells on CdSe NPLs (Fig. 5) [42]. Their study further revealed that the dispersion solvent plays a crucial role in determining core stability: CdSe NPLs undergo etching in oleylamine at 150 °C, whereas they remain

stable in octadecene (ODE) even at temperatures up to 240 °C. In addition, the introduction of $\text{Cd}(\text{OA})_2$ enhances the stability of the CdSe core through improved surface passivation by excess carboxylates.

In contrast to vertical shell growth, core/crown heterostructures are formed through lateral epitaxial growth around a NPLs core. This architecture allows spatial separation of different semiconductor domains within the same plane. A representative example was reported by Li et al., who used four-monolayer CdSe NPLs (comprising four Se layers and five Cd layers, with a thickness of approximately 1.8 nm) as the core and injected additional Cd and Te precursors into a CdSe-ODE solution to induce lateral growth of a CdTe crown with the same thickness [43]. By tuning the crown growth time, the lateral size of the CdTe domain could be precisely controlled, yielding a series of CdSe/CdTe core/crown NPLs. Energy-dispersive X-ray (EDX) mapping confirmed the spatial distribution of Se in the core, Te in the crown, and Cd throughout the entire structure. Beyond ultrathin cores, thicker NPLs have also been employed to construct core/crown heterostructures. For instance, Shamraienko et al. synthesized six- and seven-monolayer CdSe NPLs and used them as seeds to grow CdSe/CdS core/crown structures, with the lateral dimensions controlled by adjusting the injection amount and rate of sulfur-trioctylphosphine precursor (S-TOP) [44]. Notably, while

core/crown heterostructures have been extensively explored in photoluminescence studies, their application in photocatalysis remains relatively limited compared to core/shell systems.

Another emerging class is the dot-on-plate (2D/zero-dimensional (0D)) heterostructure, where quantum dots are either grown on or embedded within NPLs. Li et al. recently reported a general colloidal method for constructing such heterostructures with tunable spatial distributions [45]. Using wz-CdS and wz-ZnS NPLs with highly exposed {0002} facets as seeds, they demonstrated that precursor reactivity plays a key role in determining growth modes. When a less reactive selenium precursor (DPSe) was used, the reaction followed a thermodynamic pathway, leading to preferential growth of CdSe or ZnSe QDs on the side facets of NPLs. In contrast, a more reactive precursor (DBSe) resulted in kinetically controlled growth, yielding uniform deposition of quantum dots on the basal planes (Fig. 5(i)). Despite these advances, studies on dot-on-plate heterostructures remain relatively scarce, and their application in photocatalysis is still largely unexplored, representing an important direction for future research.

In addition to these representative configurations, various synthetic approaches—such as preheating, cation exchange, hot-injection, and one-pot methods—have also been employed to construct heterostructures [46]. Overall, composition and

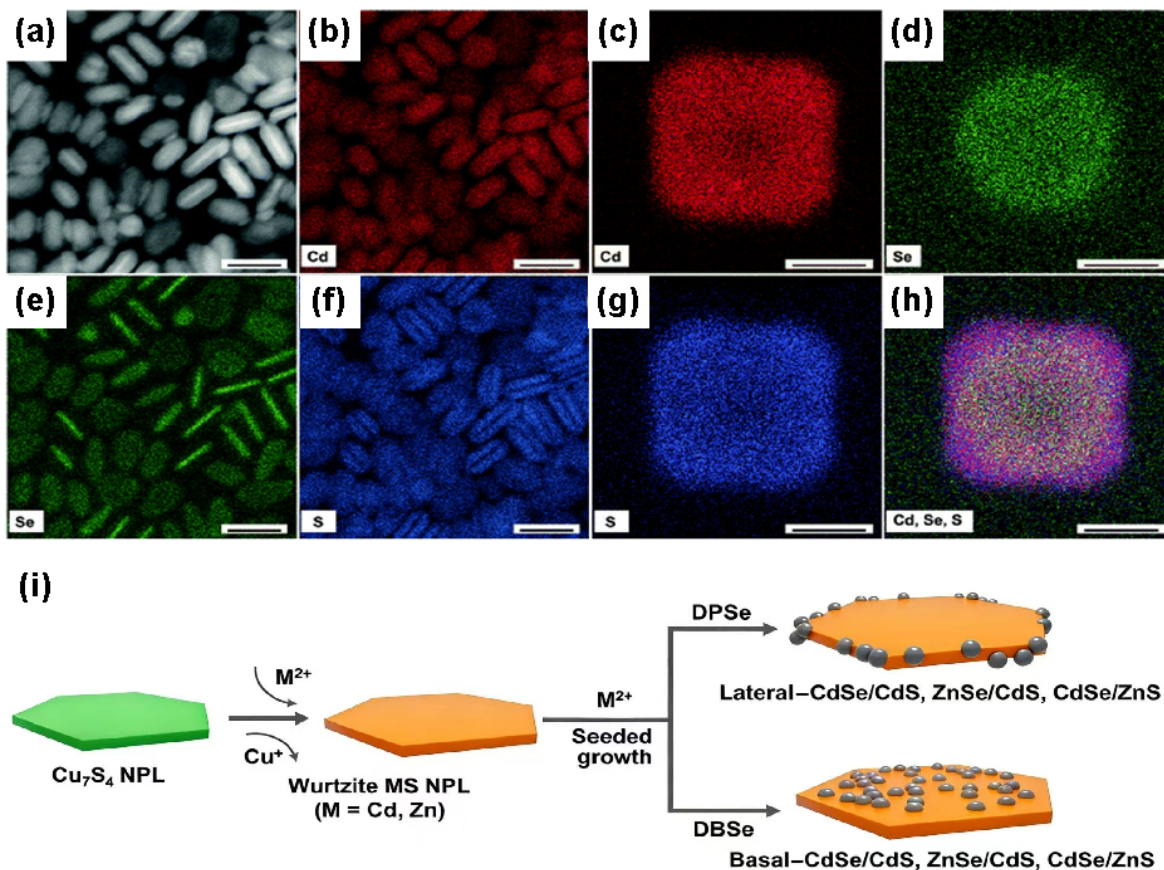


Figure 5 (a) STEM image of the synthesized CdSe/CdS core/shell heterostructure NPLs. (b)–(d) Corresponding EDX images showing the elemental distribution of Cd, Se, and S, respectively. These side-by-side stacked particles clearly reveal the core/shell structure of the material, with Se located in the core, S in the shell, and Cd distributed uniformly. (e)–(h) EDS images of Cd, Se, and S, as well as superimposed images of these elements in a single NPLs laid flat on the substrate. In (a)–(d) and (e)–(h), the black scale bars represent 20 and 10 nm, respectively. Reproduced with permission with Ref. [42], © The Royal Society of Chemistry 2017. (i) Schematic illustration of the synthesis of lateral-type or bottom-type CdSe/CdS, ZnSe/CdS, and CdSe/ZnS. Reproduced with permission with Ref. [45], © American Chemical Society 2025. DPSe: diphenyl diselenide; DBSe: dibenzyl diselenide.

heterostructure engineering provide versatile means to tailor band alignment and charge transfer pathways in II–VI NPLs. However, compared with their extensive use in optoelectronic applications, the integration of these heterostructures into photocatalytic systems is still in its early stages. Further exploration of structure-function relationships in reaction environments will be essential for unlocking their full potential in photocatalysis.

3.4 Defect engineering

Defect engineering provides an additional and powerful dimension for tailoring the electronic structure and carrier dynamics of II–VI NPLs beyond geometric and compositional control. While the optical properties and quantum confinement effects of these materials can be predictably tuned through thickness and lateral size, the deliberate introduction and regulation of defects enables further optimization of charge separation and surface reactivity. In this context, defect engineering represents a shift from minimizing imperfections to actively designing defects as functional elements that enhance photocatalytic performance.

In two-dimensional semiconductor NPLs, defects are typically classified into two categories: vacancies and dopants (Fig. 6(a)). Vacancies, defined as missing atoms at lattice sites, are among the most common point defects in catalytic semiconductors. In ultrathin systems, such vacancies can act as trapping centers for photogenerated electrons and holes, thereby suppressing carrier recombination [47]. At the same time, they can serve as active sites for the adsorption and activation of reactant molecules, significantly enhancing reaction efficiency. For example, Luo et al. introduced selenium vacancies into CdSe NPLs using the oxidizing and Lewis acidic reagent NOBF_4 , while preserving their original morphology and crystal structure [7]. These vacancy sites function as efficient electron traps, improving both charge separation and transfer processes, and consequently enhancing the photocatalytic response.

Similarly, Hao et al. prepared a ZnCdS/ZnS composite photocatalyst with a high concentration of zinc vacancies by treating $\text{ZnCdS}/\text{MOF-5}$ with a $\text{Na}_2\text{S}/\text{Na}_2\text{SO}_3$ solution under visible-light irradiation (Fig. 6(b)) [10]. Spectroscopic analyses indicated that these vacancies not only capture photogenerated electrons and suppress recombination, but also introduce defect states within the ZnS bandgap, extending light absorption into the visible region and significantly improving photocatalytic activity (Fig. 6(c)).

Another important class of defects arises from heteroatom doping. The incorporation of foreign ions into the host lattice, either through substitutional replacement or interstitial insertion, can induce charge redistribution and orbital hybridization, thereby modifying the Fermi level, introducing impurity states, and tuning the band structure [47]. Medda et al. investigated Cu^{2+} -doped CdSe NPLs using femtosecond transient absorption spectroscopy and observed pronounced photoluminescence quenching accompanied by extended carrier lifetimes [48]. The prolonged lifetime increases the probability of charge carriers participating in surface redox reactions, which is beneficial for photocatalysis. Further insights into doping mechanisms were provided by Ji et al., who developed a nucleation-controlled doping strategy based on magic-sized clusters to synthesize ZnSe quantum nanoribbons with a thickness of ~ 1.5 nm (Fig. 6(d)) [49]. Their results revealed that different dopant ions exhibit distinct incorporation behaviors: Mn^{2+} preferentially occupies substitutional sites, whereas Co^{2+} tends to occupy interstitial positions. This dependence of doping geometry on dopant identity has also been observed in CdSe systems, suggesting a general trend across II–VI semiconductors.

Beyond single-element doping, co-doping strategies offer a more versatile route for synergistic regulation of electronic structure and catalytic performance. Liu et al. reported a Co/N co-doped CdIn_2S_4 system in which dopants are incorporated through a pair-substitution mechanism (N replacing S and Co replacing In),

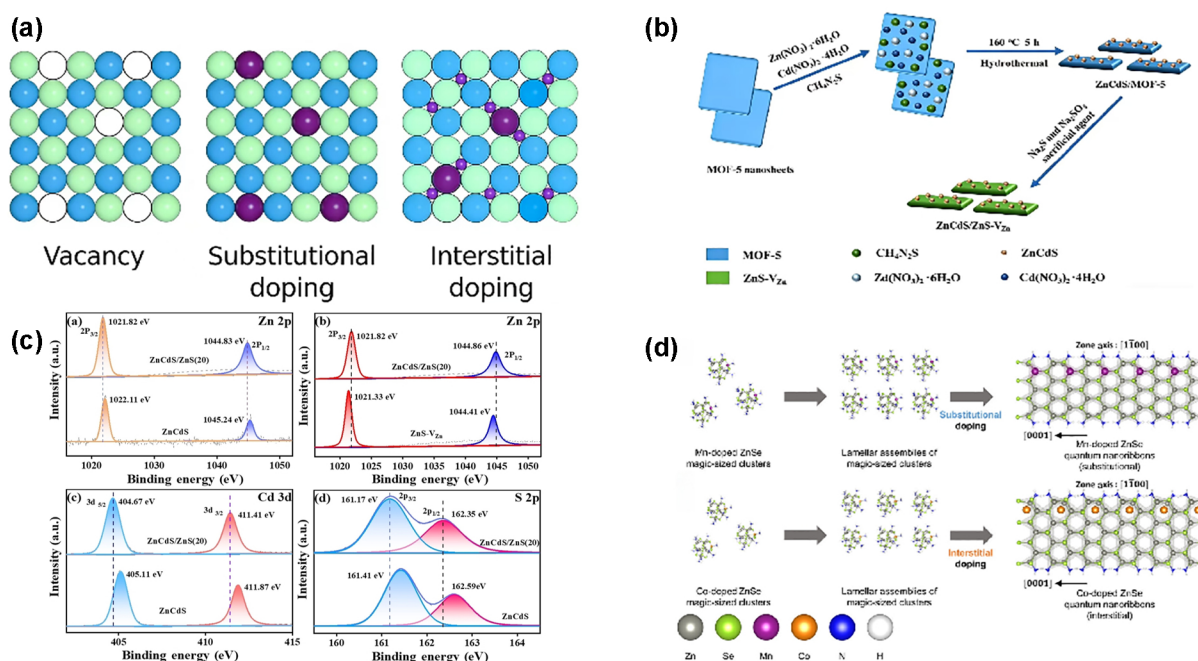


Figure 6 (a) Schematic diagram of different types of defects in defect engineering. (b) Schematic diagram of the preparation of ZnCdS/ZnS composite photocatalysts. (c) XPS spectra of Zn 2p, Cd 3p, and S 2p, corresponding to ZnCdS/ZnS , ZnCdS , and $\text{ZnS-}V_{\text{Zn}}$. Reproduced with permission from Ref. [10], © Wiley-VCH GmbH 2021. (d) Schematic illustration showing the nucleation-controlled doping process. Doping mechanism of Mn-doped and Co-doped ZnSe quantum nanoribbons. Gray, light green, purple, orange, blue, white, and green balls represent the Zn, Se, Mn, Co, N, H, and Cl atoms. Reproduced with permission from Ref. [49], © Ji, S. et al. 2024.

resulting in a stable doped lattice [50]. This configuration increases local electron density and introduces impurity levels that facilitate carrier transport. At the same time, co-doping reduces the bandgap (from 2.19 to 2.06 eV) and shifts the conduction band edge, thereby enhancing CO_2 adsorption and activation. This study highlights the potential of multi-element doping for achieving coordinated control over electronic structure, carrier dynamics, and photocatalytic activity.

Overall, defect engineering—including vacancy creation, heteroatom doping, and co-doping—provides versatile tools for modulating the electronic structure, carrier dynamics, and surface reactivity of II–VI NPLs. Despite significant progress, precise control over defect type, concentration, and spatial distribution remains challenging. Future efforts should focus on developing controllable and reproducible defect-engineering strategies, as well as establishing clear structure–function relationships under realistic reaction conditions, to fully exploit the potential of defect-engineered NPLs in photocatalysis.

3.5 Post-synthetic component transformation

In addition to direct synthesis and heterostructure construction, post-synthetic ion exchange has emerged as a powerful strategy for tailoring the composition and functionality of II–VI NPLs [51]. As a widely adopted approach in nanomaterials chemistry, ion exchange enables compositional transformation while largely

preserving the original morphology and crystal framework. Recent advances combining experimental studies with density functional theory (DFT) calculations have further deepened the mechanistic understanding of ion exchange processes at the nanoscale.

Anion exchange in II–VI NPLs presents significant challenges due to the larger ionic radius and slower diffusion kinetics of anions compared to cations. Direct replacement of lattice anions often leads to structural distortion or vacancy formation, thereby compromising material stability [52]. To address this issue, Wang and co-workers developed a template-assisted strategy using cadmium-based NPLs, in which a bilayer ligand environment stabilizes the structure and enables nearly damage-free anion exchange. Under ligand-rich conditions, the layered template promotes face-to-face stacking of NPLs, restricting ion exchange to occur preferentially through lateral polar facets. Kinetic studies and theoretical calculations revealed that guest anions first adsorb on Cd- or Se-terminated surfaces and subsequently diffuse into the lattice via a direct substitution mechanism (Fig. 7(a)).

In contrast to template-assisted systems, recent work on zinc-based NPLs has demonstrated large-area anion exchange under template-free conditions [8]. *In situ* ultraviolet–visible (UV–vis) spectroscopy revealed two distinct exchange pathways depending on ionic size mismatch. When the mismatch is small, facet-selective direct substitution dominates; when the mismatch is large, a cluster-mediated mechanism becomes operative (Fig. 7(b)). Further

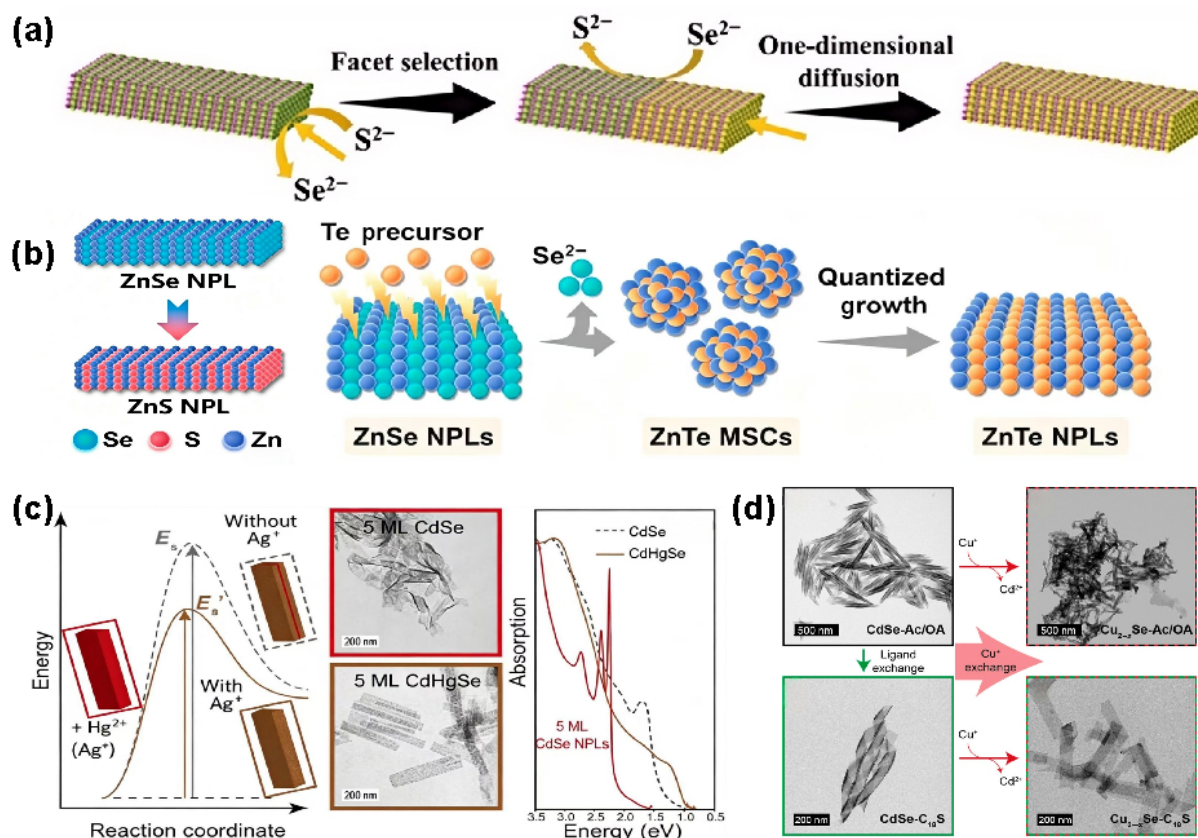


Figure 7 (a) The phenomenon of facet-selective anion exchange, whereby guest anions follow a one-dimensional diffusion pattern into the interior of the host NPLs. Reproduced with permission from Ref. [52], © American Chemical Society 2024. (b) Scheme of size mismatch effect drives MSCs formation rather than directed diffusion. Reproduced with permission from Ref. [8], © American Chemical Society 2025. (c) Schematic diagram of silver ion reduction cation exchange reaction energy, changes in the morphology of NPLs before and after the reaction and the corresponding changes in absorption peaks. Reproduced with permission from Ref. [53], © American Chemical Society 2024. (d) Morphological changes in CdSe NPLs with different ligands after copper ion exchange. Reproduced with permission from Ref. [54], © American Chemical Society 2023.

analysis showed that surface ligands play a critical role in this process by modulating steric hindrance and electronic interactions. Specifically, short-chain amines tend to form thinner and more ordered surface layers, facilitating exchange, whereas long-chain ligands increase surface coverage and suppress anion diffusion. These studies collectively provide fundamental insights into the mechanisms governing anion exchange and establish a framework for designing functional NPLs.

Compared with anion exchange, cation exchange is generally more accessible due to the smaller ionic radii and greater diversity of cation species. In a recent study, cation exchange was employed to synthesize thick $\text{Hg}_{1-x}\text{Cd}_x\text{Se}$ NPLs with tunable optical properties, including amplified spontaneous emission (Fig. 7(c)) [53]. Although Hg^{2+} is expected to bind more strongly with chalcogenides than Cd^{2+} , direct synthesis of mercury-based NPLs remains challenging. As a result, such systems are typically obtained via cation exchange from Cd-based NPLs, often limited to a few atomic layers due to kinetic constraints, leading to alloyed or core/shell-like structures. In this work, the introduction of Ag^+ as a catalyst enabled efficient Hg^{2+} incorporation into CdSe NPLs with thicknesses of 3–7 monolayers, effectively suppressing surface diffusion and promoting deeper lattice exchange.

Beyond isovalent cation exchange, heterovalent systems have also been explored. For example, Cu^+ -based cation exchange in II–VI NPLs has been achieved by carefully tuning ligand environments [54]. By controlling the chain length of thiol ligands, lattice distortion during exchange was minimized, resulting in Cu_{2-x}Se NPLs that retain their original morphology (Fig. 7(d)). In this system, CdSe NPLs were used as templates, and ligand exchange from carboxylates to thiolates enabled cation substitution without disrupting the two-dimensional structure, despite the presence of ligand-induced lateral distortions such as helical morphologies.

Overall, ion exchange offers a versatile and powerful post-synthetic route for modulating the composition, band structure, and surface properties of II–VI NPLs. Both anion and cation exchange processes provide valuable opportunities for tuning carrier transport, electronic structure, and active site distribution, which are critical for photocatalytic performance. More importantly, the interplay among ligand-lattice interactions, interfacial compatibility, and compositional gradients during ion exchange provides important design principles for constructing high-performance photocatalysts. Continued efforts toward precise control of exchange pathways and mechanistic understanding will be essential for fully exploiting the potential of ion-exchange-engineered NPLs.

4 Photocatalytic mechanisms in II–VI NPLs

The synthetic and structural modulation strategies discussed above enable precise control over the microscopic structure of II–VI NPLs, ultimately leading to improved photocatalytic performance. Photocatalysis is an inherently multistep process involving light absorption, charge carrier generation and transport, and surface redox reactions. Understanding the mechanisms governing each of these processes, as well as the intrinsic relationships between structure and performance, is essential for the rational design of efficient photocatalysts. In this section, the fundamental photocatalytic mechanisms of II–VI NPLs are discussed, with particular emphasis on light absorption and exciton dynamics, charge separation and transport, and their interplay with surface reactions.

4.1 Light absorption, exciton dynamics and charge separation

The photocatalytic performance of II–VI NPLs is closely related to their efficient light absorption and distinctive exciton dynamics, both of which originate from their two-dimensional structure and strong quantum confinement effects. Light absorption represents the initial step of photocatalysis. When photons with energies exceeding the bandgap (E_g) are absorbed, electrons are excited from the valence band to the conduction band, generating electron-hole pairs. Due to Coulomb interactions, these carriers tend to form bound quasiparticles known as excitons. The subsequent dynamics of excitons—including their formation, diffusion, dissociation, and recombination—play a central role in determining photocatalytic efficiency (Fig. 8) [55].

The light absorption behavior of semiconductors is fundamentally governed by their band structure. In II–VI NPLs, quantum confinement leads to an increase in bandgap energy, which provides a stronger thermodynamic driving force for redox reactions. However, this effect also narrows the spectral absorption range, often necessitating additional strategies, such as heterostructure construction, to extend light harvesting into the visible region [56]. Furthermore, as discussed in Section 2, the density of states in NPLs exhibits a step-like distribution, resulting in characteristic staircase-like absorption edges. When the exciton binding energy exceeds thermal energy (kT), sharp excitonic peaks corresponding to discrete electronic transitions can be observed in absorption spectra [15].

In low-dimensional systems, the conventional band theory alone is insufficient to describe optical processes, as it neglects electron-hole interactions. Therefore, the excitonic framework becomes essential [17]. Excitons can be classified into singlet and triplet states based on their spin configurations [57]. Upon photoexcitation, electrons are promoted to singlet excited states, leaving holes in the ground state and forming singlet excitons [58]. These singlet excitons may undergo intersystem crossing (ISC) to form triplet excitons with lower energy [59]. In photocatalytic systems, singlet excitons typically possess higher energy but shorter lifetimes, often undergoing rapid radiative or nonradiative recombination before participating in interfacial processes. In contrast, triplet excitons exhibit significantly longer lifetimes due to spin-forbidden transitions, providing more opportunities for diffusion to the catalyst surface and for engaging in charge or energy transfer processes [60]. These intrinsic properties of triplet excitons, which are completely distinct from those of singlet ones, are likely to undergo specific interactions with the in-plane-edge asymmetry of II–VI group semiconductor NPLs (e.g., CdS NPLs), thereby directly leading to the spatially observable difference in their utilization efficiency. For example, to CdS NPLs, the Cd-terminated surface and S-terminated surface exhibit distinct work functions and electron affinities, thereby inducing lateral energy band bending and a built-in electric field within the NPLs [61]. This will induce electrons to migrate toward the edges, while holes migrate toward the large basal plane. During this process, longer-lifetime triplet excitons are more likely to reach the edges, leading to an observable difference in the utilization efficiency of singlet excitons and triplet excitons between different sites. However, current inferences regarding the carrier migration direction and the triplet exciton dominating edge reactions remain hypothetical and lack sufficient literature support. Such hypotheses can potentially be validated by combining spatially resolved ultrafast spectroscopy and magneto-

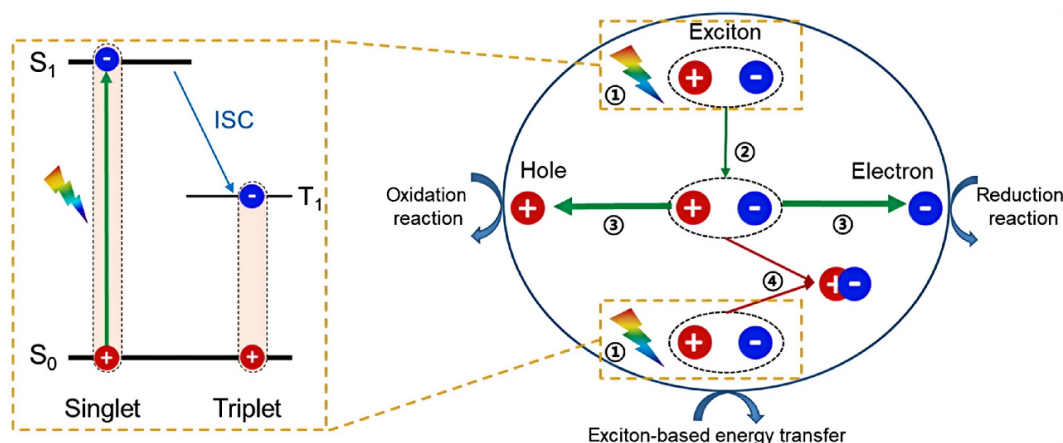


Figure 8 The left side of the schematic diagram shows the process of exciton migration from the singlet state to the triplet state, and the right side show the exciton dynamics in the photo(electro)catalytic process: path 1, exciton generation; path 2, exciton diffusion; path 3, exciton dissociation; path 4, exciton recombination; ISC: intersystem crossing. Reproduced with permission with Ref. [55], © Elsevier Inc. 2021.

optical spectroscopy, which constitutes a valuable research direction.

Depending on the analysis above, promoting singlet to triplet states is beneficial to photocatalytic performance. However, under the electric dipole approximation, optical transitions must obey the spin selection rule ($\Delta S = 0$), which prohibits direct transitions between states of different spin multiplicities. As a result, singlet-to-triplet conversion relies on spin-orbit coupling (SOC), which enables partial mixing of spin states [62]. Recent studies have further suggested that spin-vibronic coupling can dynamically modulate SOC strength through specific vibrational modes, allowing efficient ISC even in systems without heavy atoms [63]. In addition, reducing the singlet-triplet energy gap (ΔE_{ST}) can further accelerate ISC processes. These insights provide important guidelines for the design of photocatalytic materials with enhanced exciton utilization.

After the singlet and triplet excitons are formed, both of them begin to refine themselves and dissociate into electrons and holes via several mechanisms. These include attaching to electron or hole acceptors in a photocatalytic material, impurities [64], defect sites, or even external electric fields [65]. The resulting free carriers then migrate to the surface, where they participate in reduction and oxidation reactions, respectively, initiating the photocatalytic process [55]. However, exciton recombination remains a major loss pathway. This process occurs either through direct electron-hole recombination or through Auger processes involving exciton-exciton annihilation [66]. In singlet exciton annihilation, one exciton relaxes to the ground state while transferring energy to another, which is promoted to a higher excited state before dissipating energy via phonons [67]. In triplet exciton annihilation, two triplet excitons interact to generate a higher-energy singlet exciton and a ground-state species [68]. Both pathways reduce the population of active excitons, thereby limiting photocatalytic efficiency [69]. Therefore, when constructing a photocatalytic system, strategies including engineering surface defects and vacancies and constructing heterojunctions are generally employed to suppress exciton annihilation. For instance, Pt modification on the surface of CdS enables the rapid conversion of bound excitons into free carriers and their injection into Pt within an extremely short timescale. In the subsequent process, the built-in electric field provided by the Schottky junction and the low overpotential property of Pt as an electron sink can both efficiently extract and

rapidly consume electrons, thereby maximizing the inhibition of exciton annihilation and carrier recombination during the photocatalytic process [70].

4.2 Surface reaction pathways

After photoexcitation and charge separation, photogenerated electrons and holes migrate to the catalyst surface, where they participate in redox reactions that ultimately determine photocatalytic activity, selectivity, and product distribution. While all photocatalytic processes originate from semiconductor activation under light irradiation, the subsequent reaction pathways vary depending on the nature of the reactants. Typical photocatalytic processes include hydrogen evolution, CO₂ reduction, pollutant degradation, and the synthesis of value-added chemicals [71].

In photocatalytic hydrogen evolution, the reduction of protons by photogenerated electrons is often kinetically limited, requiring efficient charge separation and accumulation at catalytically active sites. In II–VI NPLs, the ultrathin geometry facilitates rapid carrier transport, while spatially separated reaction sites further enhance charge utilization. For example, in CdS NPLs-Pt heterostructures, photogenerated holes rapidly migrate to the basal plane, whereas electrons diffuse toward the edges (Fig. 9(a)). These electrons are transferred to Pt nanoparticles within ~ 8.8 ps, where they reduce H⁺ to H₂ [72]. The behavior of holes is strongly dependent on the reaction environment: Under alkaline conditions, OH⁻ acts as the primary hole scavenger, generating $\cdot$ OH radicals that react with ethanol and enable nearly unity internal quantum efficiency; under acidic conditions, L-cysteine serves as the hole acceptor, although competing recombination processes may reduce efficiency (Fig. 9(b)). The intrinsic spatial separation of oxidation and reduction sites between basal planes and edges prolongs the lifetime of charge-separated states and suppresses recombination. A similar mechanism is observed in Au/Pt-modified CdSe/CdS core/crown NPLs, where electrons are selectively transferred to metal domains (Pt at S-terminated edges and Au at the CdSe core), which act as electron sinks and catalytic sites for hydrogen evolution [72]. Spectroscopic studies confirm that the metal-semiconductor interface provides an efficient pathway for charge separation, and that the spatial distribution of metal domains governs electron collection efficiency and overall catalytic performance. Furthermore, the selective metal deposition at given sites

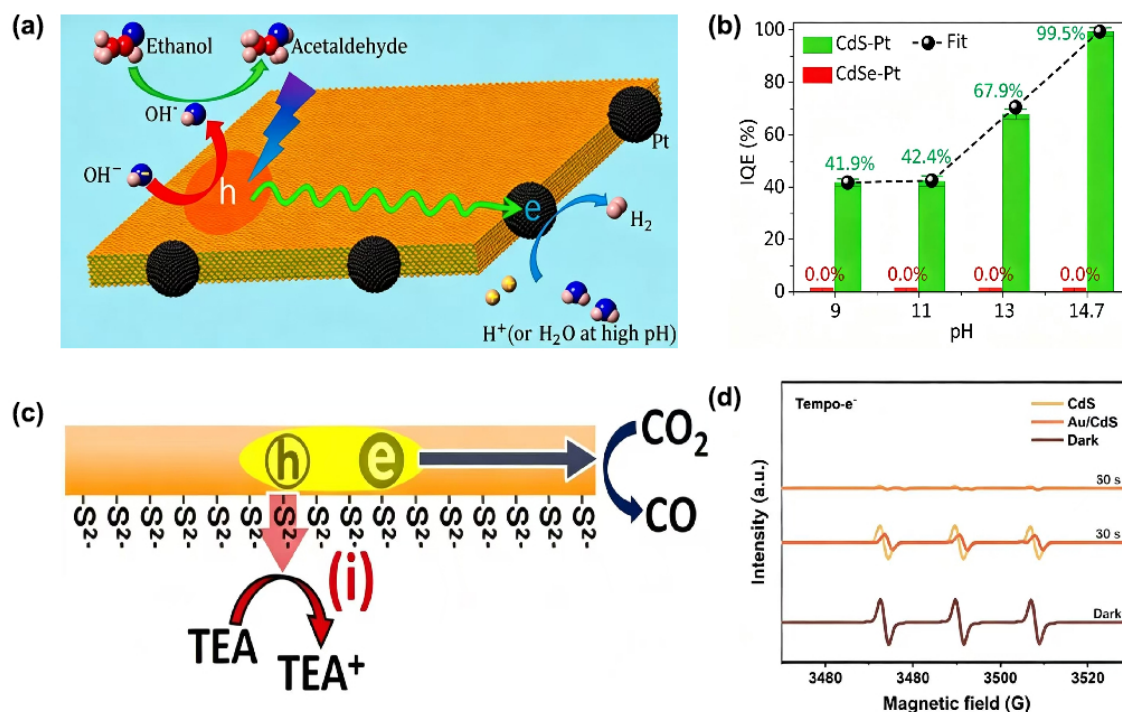


Figure 9 (a) Schematic illustration of a major step forward to highly efficient photodriven hydrogen production in the CdS NPL-Pt heterostructure. Reproduced with permission with Ref. [72], © American Chemical Society 2018. (b) pH-dependent internal quantum efficiency (IQE) of photodriven hydrogen production for CdS NPL-Pt (green bars) and CdSe NPL-Pt (red bars). Reproduced with permission with Ref. [72], © American Chemical Society 2018. (c) Schematic of the hole consumption pathway in the excited state of CdS NPL-Pt NPLs during the photocatalytic CO_2 reduction reaction. Holes in the excited state of CdS-S^{2-} NPLs are consumed via oxidation of TEA. Reproduced with permission with Ref. [61], © American Chemical Society 2022. (d) Comparison of the electron paramagnetic resonance spectra of the active hydrogen species induced by CdS NPLs and Au/CdS NPLs. Reproduced with permission with Ref. [9], © American Chemical Society 2025.

determines the efficiency of charge collection and thus the hydrogen evolution photocatalytic activity [73].

In Au/Pt-modified CdSe/CdS core/shell NPLs, after photo-generation, electrons drift towards the selectively deposited metal domains, which are Pt at the S-terminated edges and Au in the core region. These metals trap the electrons and become sites for hydrogen evolution by reducing H^+ to H_2 . Meanwhile, holes are neutralized by the sacrificial agents, which can be an ascorbic or formic acid. Quenching of the photoluminescence and transient absorption studies demonstrate that the selective metal-semiconductor interface determines the path for charge separation. Furthermore, the selective metal deposition at given sites determines the efficiency of charge collection and thus the hydrogen evolution photocatalytic activity [74].

For photocatalytic CO_2 reduction, the activation of the chemically inert CO_2 molecule is the primary challenge. Upon adsorption on the catalyst surface, the linear CO_2 molecule transforms into a bent configuration, lowering its lowest unoccupied molecular orbital (LUMO) energy and increasing its reactivity. The subsequent reaction proceeds through multistep electron and proton transfer processes, including C=O bond cleavage and C-H bond formation. However, the complexity of surface reactions and the presence of multiple competing pathways often lead to poor selectivity [75]. To address this issue, controlling the spatial distribution of active sites has emerged as an effective strategy. In S^{2-} -terminated CdS NPLs (CdS-S^{2-} NSs), photogenerated electrons migrate to edge sites to reduce adsorbed CO_2 , while holes accumulate on the basal plane to oxidize the sacrificial agent triethylamine (TEA) (Fig. 9(c)) [61]. This spatial separation of reduction and oxidation pathways not only suppresses

electron-hole recombination but also shortens the diffusion distance of holes, resulting in highly selective CO production (99%) with a generation rate of $2.13 \text{ mol} \cdot \text{g}^{-1} \cdot \text{h}^{-1}$ in the absence of cocatalysts. These results highlight that regulating the spatial orientation of surface reaction pathways is critical for overcoming the selectivity limitations in CO_2 reduction.

In photocatalytic degradation processes, photogenerated electrons and holes react with O_2 and H_2O to generate reactive oxygen species (ROS), such as hydroxyl radicals ($\cdot\text{OH}$) and superoxide radicals ($\cdot\text{O}_2^-$), which subsequently oxidize and decompose organic pollutants [76]. Although the overall mechanism is similar across systems, the detailed pathways depend on the type of pollutant. For instance, plastic waste can be directly utilized as a hole scavenger after appropriate pretreatment [5], whereas dye molecules are typically degraded indirectly via ROS-mediated oxidation in solution [77].

Photocatalytic synthesis of value-added chemicals follows similar principles but requires more precise control over reaction pathways and selectivity. In nitrogen fixation, although certain systems such as BiVO_4 -based heterostructures have been explored, the underlying mechanisms remain insufficiently understood [78], for example, have been investigated, but the understanding of the precise mechanisms has yet to be established [79]. In contrast, hydrogen peroxide production is relatively well established, typically proceeding via oxygen reduction reaction (ORR) and water oxidation reaction (WOR), with the two-electron ORR pathway being the most widely adopted [80].

More complex transformations further illustrate the importance of interfacial design. In an Au/CdS NPLs system, strong Au-S interactions suppress sulfur loss and promote charge separation. Au

nanoparticles act as electron trapping sites, facilitating electron transfer from CdS and lowering the dissociation barrier of D_2O to generate active deuterium species. Meanwhile, Au activates adsorbed C=N bonds, enabling the selective synthesis of α -deuterated amines (Fig. 9(d)) [9]. This mechanism shares common features with nitrogen fixation and ORR processes, particularly in terms of electron utilization and the role of surface-active sites.

4.3 Structure-function correlation and modulation

Building upon the surface reaction pathways discussed in Section 4.2, it becomes clear that photocatalytic performance is ultimately governed by how efficiently photogenerated carriers are generated, separated, transported, and utilized at reactive interfaces. Structural regulation of II–VI NPLs therefore serves as a means to directly manipulate these key steps. Establishing clear correlations between structural design and photocatalytic function is essential for the rational development of high-performance systems. In this section, three representative modulation strategies—heterostructure engineering, cocatalyst integration, and the synergistic combination of surface and defect engineering—are discussed to elucidate how structural features dictate photocatalytic behavior.

4.3.1 Heterostructure-induced charge separation

Constructing heterostructures is one of the most effective strategies for bridging performance limitations in semiconductor photocatalysts. A heterostructure can be defined as an interface between two semiconductors with different band structures. This yields a spatial band alignment and leads to a variation of the conduction band to valence band (CB–VB) alignment [81]. A spatial band alignment in heterostructure formation results from the migration of the photo-generated carriers between the two semiconductors in the presence of the built-in electric field [82].

Traditional heterojunctions are generally classified into Type I (Fig. 10(a)), Type II (Fig. 10(b)), and Type III configurations

(Fig. 10(c)). Among these, Type II heterojunctions are most widely utilized in photocatalysis due to their staggered band alignment, which promotes spatial separation of photogenerated electrons and holes. However, this separation often comes at the cost of reduced redox potential, as both electrons and holes reside at energetically less favorable levels after transfer.

To overcome this limitation, Z-scheme heterostructures have been developed. Depending on whether electron mediators (e.g., Ag or Au) are involved, Z-scheme systems can be categorized into indirect (Fig. 10(d)) and direct configurations (Fig. 10(e)). In these systems, electrons with weaker reduction ability recombine with holes of lower oxidation potential, preserving the highly reductive electrons and highly oxidative holes in the respective semiconductors. This mechanism allows efficient charge separation without sacrificing redox power [81, 83].

More recently, the S-scheme heterojunction has been proposed as an evolution of the Z-scheme concept (Fig. 10(f)) [84]. Due to differences in Fermi levels between oxidation and reduction photocatalysts, electrons spontaneously transfer across the interface until equilibrium is reached, establishing an internal electric field and band bending. Under illumination, this built-in field drives recombination of low-energy carriers while retaining high-energy electrons and holes in their respective bands. As a result, S-scheme systems simultaneously achieve efficient charge separation and strong redox capability, making them particularly attractive for advanced photocatalytic applications [85].

4.3.2 Cocatalyst-assisted surface kinetics

While heterostructures primarily regulate charge separation, cocatalysts play a critical role in accelerating surface reaction kinetics. By providing active sites and facilitating charge transfer, cocatalysts directly influence the efficiency of interfacial redox processes.

Pure metal cocatalysts, including both noble and non-noble

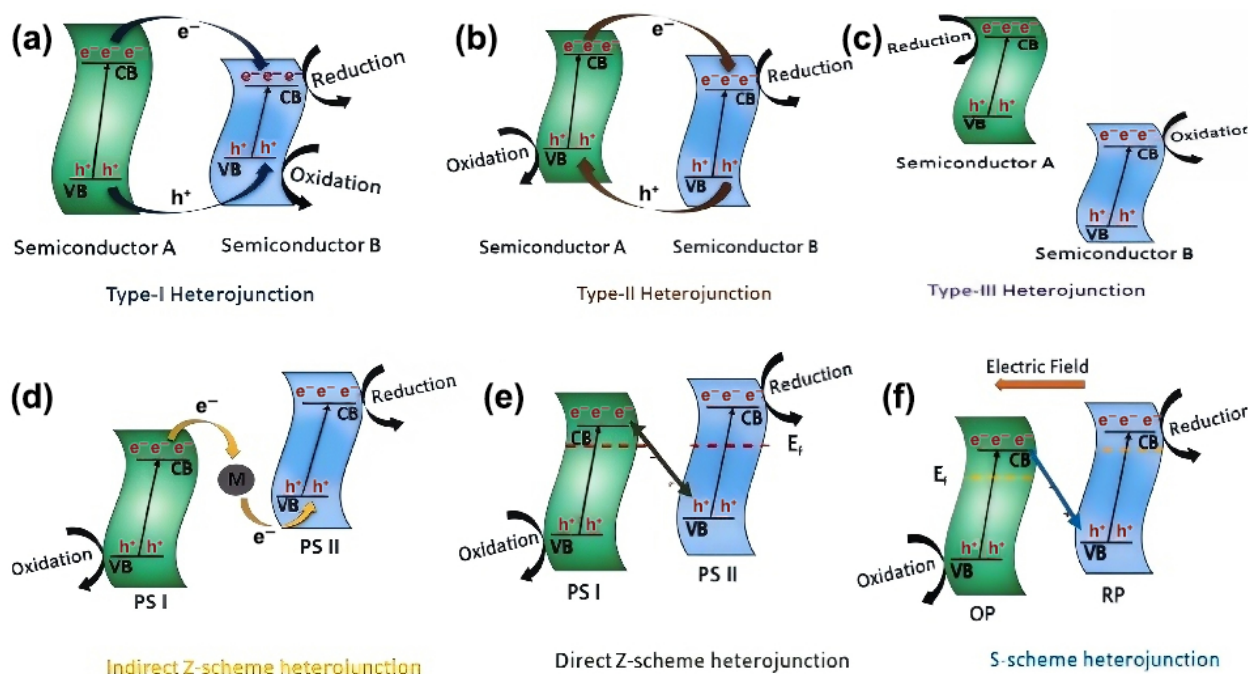


Figure 10 Schematic of the mobility of charge carriers in 6 different junctions of heterojunctions. (a) Type I heterojunction. (b) Type II heterojunction. (c) Type III heterojunction. (d) Indirect Z-type heterojunction. (e) Direct Z-type heterojunction. (f) S-type Heterojunctions. Reproduced with permission with Ref. [81], © Elsevier B.V. 2024.

metals, are widely used in II–VI semiconductor systems. Noble metals such as Pt, Au, Ag, and Pd are particularly effective due to their ability to form Schottky junctions with semiconductors, which promotes electron transfer from the semiconductor to the metal and suppresses carrier recombination [86], help in the efficient separation of the photo-induced electron-hole pairs [87], and modify the active sites of the photocatalyst's surface [88] or fill the active sites [89], which improves the photocatalytic activity of the photocatalysts.

Beyond noble metals, non-precious metals such as Cu, Co, Ni, Fe, and Sn have attracted increasing attention due to their lower cost, higher stability, and resistance to photodegradation [71]. Previous studies have shown that noble-metal cocatalysts such as Au, Ag, Pd, and Pt can promote interfacial charge transfer and suppress electron-hole recombination, thereby enhancing photocatalytic activity under light irradiation [90]. Furthermore, Wang et al. described the transformation of grade changes in precious metals for photocatalytic processes from the type of structures. Wang et al. detailed the modifications that were made to the photocatalytic process using different structures of gold that helped to enhance the reduction of metals such as CO_2 and CH_3OH [91].

Precious metals co-catalysts could also have lower selectivity and undergo early deactivation. Non-precious metals are more economical, stable and less susceptible to photodegradation. So, photocatalysts that have modified II–VI semiconductor materials as co-catalysts that are non-precious metals are favored [92]. For instance, the *in situ* introduction of cocatalysts into Cd/CdS systems significantly enhances photocurrent and hydrogen evolution rates, achieving activities up to 16 times higher than pristine CdS [93]. Cu-Ni bimetallic cocatalysts on CdS NPLs exhibit high apparent quantum yields (21.5% at 400 nm and 12.1% at 520 nm) and hydrogen production rates of $28.19 \text{ mmol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ [94].

Overall, cocatalysts improve photocatalytic performance through multiple mechanisms, including facilitating charge separation, lowering reaction energy barriers, modifying surface electronic structures, and providing abundant active sites. These effects collectively enhance both efficiency and selectivity of photocatalytic processes. However, different metal catalysts can show completely different reaction selectivity on the same semiconductor, which is rooted in the difference in the microscopic properties of the interface. An in-depth understanding of these differences is the key to realizing the rational design of the catalyst. The following takes the Au/CdS and Pt/CdSe systems as examples, and analyzes the four possible factors that determine selectivity.

First, the Schottky potential barrier can regulate the reduction ability of photoelectrons injected into metal. The function of Au ($\sim 5.1 \text{ eV}$) and the affinity energy of CdS electrons ($\sim 4.2 \text{ eV}$) form a moderate potential barrier of about 0.9 eV . After the photoelectron is injected from CdS to Au, the Fermi energy level of Au is shifted up, which is enough to activate the π^* orbit of the C=N bond, but not enough to efficiently reduce the potential of H^+ . The π^* orbital adsorbed on C=N on Au/CdS is closer to the Fermi energy level, and electrons give priority to filling the orbit, thus promoting the activation of C=N bonds. The function of Pt is higher ($\sim 5.6 \text{ eV}$), forming a higher potential barrier of about 1.4 eV . Electrons are highly enriched on the surface of Pt. In addition, Pt itself has excellent H adsorption energy, so H^+ reduction to H_2 becomes the dominant reaction.

Secondly, the interface bonding characteristics not only affect the

charge transfer efficiency, but also modify the electronic state of the metal through chemical action. XPS shows that S 2p in Au/CdS is displaced to high binding energy, confirming the formation of strong Au–S covalent bonds, which stabilizes the CdS surface and inhibits S loss on the one hand. On the other hand, it regulates the electronic structure of Au to make it more inclined to interact with C=N bonds. In contrast, Pt in Pt/CdSe/CdS is only anchored to the edge of CdS through Pt–S bonds. XPS does not observe obvious changes in the electron state of Pt, and Pt still maintains its inherent high hydrogenation activity.

In addition, the spatial distribution, size and shape of the catalyst determine whether the substrate can approach the active site. Transmissive electron microscope and elemental distribution diagram show that Au nanoparticles are evenly dispersed on the entire surface of CdS NPLs, and imine substrates can be freely approached; while Pt is only distributed on the edge of CdSe/CdS NPLs in the form of a “pearl necklace” and is surrounded by CdSe core and dense organic ligand layers, which may only allow small molecules such as H_3O^+ diffuse to the surface of Pt and cannot bind large-sized organic molecules.

Finally, the local cation environment further strengthens the selective differentiation. Au/CdS surface ligands are effectively replaced under reaction conditions ($\text{MeCN}/\text{D}_2\text{O}/\text{Na}_2\text{SO}_3$), exposing a clean Au site; while Pt/CdSe/CdS requires the use of 11-mercapto-undecanoic acid (MUA) to transfer to the aquatic phase, and MUA forms a dense single layer on the Pt surface, only H^+ is allowed to pass, and rejects hydrophobic or large-volume C=N substrates.

The synergy of the above four influencing factors interprets the catalyst design principle of “structure determines function” and provides a generalized regulatory paradigm for the future design of photocatalysts for specific reduction reactions (CO_2 reduction, N_2 reduction, etc.).

4.3.3 Synergistic effects of surface and defect engineering

Surface and defect engineering represent complementary strategies for regulating photocatalytic performance at different scales. Surface engineering primarily modifies the chemical environment and interfacial properties without altering the crystal lattice, whereas defect engineering introduces atomic-scale structural perturbations that directly influence electronic structure and carrier dynamics.

Both approaches contribute to the formation and optimization of active sites. Surface engineering enables macroscopic control over active site distribution and interfacial environments, while defect engineering regulates active sites at the atomic and electronic levels. For example, sulfur vacancies in II–VI NPLs generate unsaturated metal coordination sites, enhancing local electron density and improving adsorption of reactant molecules [95, 96]. Similarly, nitrogen doping introduces shallow donor states that enhance visible-light absorption and increase the density of active sites [97].

Importantly, surface and defect engineering exhibit strong synergistic effects in regulating carrier behavior. Surface modifications can construct efficient charge transport pathways and promote spatial separation of carriers, while defect states act as trapping centers that prolong carrier lifetimes and facilitate their migration to reactive sites [98, 99]. The balance between these effects is critical for optimizing quantum efficiency and carrier utilization.

This synergy also extends to key steps in surface reactions, including adsorption, activation, and desorption. Surface engineering enhances the chemical environment for reactant

adsorption and provides accessible reaction sites, whereas defect engineering lowers activation barriers and stabilizes reaction intermediates. For instance, in CO₂ reduction, defect-induced charge localization can reduce reaction energy barriers and stabilize key intermediates, thereby improving catalytic efficiency [95]. Together, these complementary effects highlight the importance of integrating surface and defect engineering for the rational design of high-performance photocatalysts.

5 II–VI NPLs as photocatalysts in the field

Building upon the structural characteristics, synthetic strategies, and photocatalytic mechanisms discussed in the previous sections, the practical applications of II–VI NPLs represent a critical step toward evaluating their functional relevance in real systems. Benefiting from their atomically controlled thickness, tunable electronic structures, and large surface-to-volume ratios, II–VI NPLs have emerged as a versatile platform for a wide range of photocatalytic processes. In particular, their unique combination of efficient charge separation, spatially resolved reaction sites, and tunable surface chemistry enables enhanced performance in hydrogen evolution, CO₂ reduction, and organic transformation reactions.

5.1 Development of II–VI material in photocatalysis

Photocatalysis has long been regarded as a promising strategy for converting solar energy into chemical energy under mild conditions. Since the seminal work by Fujishima and Honda in 1972, demonstrating water splitting on TiO₂ electrodes [100], the field has evolved toward increasingly complex and efficient material systems. Shortly thereafter, Halmann reported photocatalytic CO₂ reduction using GaP electrodes [101], extending photocatalysis from hydrogen production to carbon conversion.

In the early stages, research primarily focused on wide-bandgap oxide semiconductors such as TiO₂. Although these materials exhibit excellent stability, their limited absorption in the visible region significantly restricts solar energy utilization [102]. This limitation motivated the exploration of alternative semiconductor systems with narrower bandgaps. A key milestone was achieved when Inoue et al. demonstrated that CdS-based materials could reduce CO₂ into organic molecules under UV irradiation [103], marking the introduction of II–VI semiconductors into photocatalysis.

Subsequent studies further highlighted their potential. Grätzel and co-workers demonstrated photocatalytic hydrogen evolution using CdS powders combined with cocatalysts [104], while Reber and Meier showed that ZnS could achieve high hydrogen evolution efficiency even in the absence of noble metals [105]. Compared with oxide semiconductors, II–VI materials exhibit more favorable band structures and broader visible-light absorption, making them attractive candidates for solar energy conversion.

With the development of nanoscience, the focus gradually shifted from bulk materials to low-dimensional systems. In particular, the discovery that CdSe nanostructures exhibit photocatalytic activity under visible light, whereas bulk CdSe remains inactive [106], underscored the importance of dimensionality. Two-dimensional II–VI NPLs, with their ultrathin geometry, offer several intrinsic advantages: shortened carrier diffusion distances, increased density of exposed active sites, and tunable band structures via quantum confinement. These characteristics have driven extensive research into their application in photocatalysis.

In recent years, advances in colloidal synthesis, heterostructure engineering, and compositional tuning have significantly improved the performance of II–VI NPLs. Importantly, the research focus has evolved from demonstrating basic functionality to optimizing efficiency, stability, and selectivity. For example, in hydrogen evolution systems, efforts have focused on accelerating reaction kinetics and suppressing photocorrosion, while in CO₂ reduction, controlling reaction pathways and product selectivity has become a central challenge [107].

5.2 Photocatalytic hydrogen evolution

The hydrogen evolution reaction (HER) is fundamentally limited by slow reaction kinetics, requiring efficient accumulation and utilization of photogenerated electrons at catalytic sites. In II–VI NPLs, the ultrathin structure facilitates rapid carrier transport, while spatial separation of reduction and oxidation sites can effectively suppress recombination. However, these materials are also susceptible to photocorrosion under prolonged illumination, making stability a critical issue.

To address these challenges, cocatalyst loading has been widely adopted as an effective strategy [71]. Noble metals such as Au and Pt can act as electron sinks, facilitating charge separation and accelerating proton reduction. For instance, Wang et al. demonstrated that Au nanoparticles integrated with CdS significantly enhance charge separation efficiency and photocatalytic activity [9]. Similarly, Pt-decorated CdSe NPLs exhibit efficient interfacial charge transfer, achieving an apparent quantum efficiency of $19.3\% \pm 1.4\%$ (Table 1), which is approximately five times higher than that of unmodified systems [74].

Beyond simple cocatalyst loading, the structure and composition of cocatalysts play a crucial role in determining catalytic performance. Qiao et al. constructed a MoO₃/Mo₂C composite cocatalyst anchored on CdS NPLs via an *in situ* carbonization strategy [108]. The resulting system exhibits a hydrogen evolution rate of $18.43 \text{ mmol} \cdot \text{g}^{-1} \cdot \text{h}^{-1}$ and maintains excellent stability over extended operation (90 h) (Table 1), highlighting the importance of interfacial engineering.

In addition to cocatalysts, heterostructure design provides another effective route for improving HER performance. For example, Cu–Ni bimetallic nanoparticles integrated with CdS form ternary heterostructures that significantly enhance hydrogen evolution rates, reaching $28.19 \text{ mmol} \cdot \text{g}^{-1} \cdot \text{h}^{-1}$ —approximately 88 times higher than pure CdS (Table 1) [94]. Similarly, CdS/ZnS 1D/2D heterojunctions prepared via sonochemical methods exhibit both high activity and long-term stability, demonstrating sustained hydrogen production over 58 h (Table 1) [109]. These results collectively indicate that combining cocatalyst engineering with heterostructure design is essential for optimizing both efficiency and durability in hydrogen evolution systems.

5.3 Photocatalytic CO₂ reduction

Photocatalytic CO₂ reduction involves the conversion of CO₂ into value-added chemicals, such as CO, CH₄, CH₃OH, and HCOOH, driven by solar or artificial light irradiation. This process not only enables the transformation of light energy into chemical energy, but also offers advantages including low energy consumption and environmental compatibility, making it a promising route toward sustainable carbon utilization and carbon neutrality. However, the high thermodynamic stability and linear molecular structure of CO₂

Table 1 Comparison of photocatalytic hydrogen production performance of 2D II–VI NPLs under different modification strategies

Catalyst system	Modification strategy	Cocatalyst/hetero-junction component	Light source	Hydrogen production rate (mmol·g ⁻¹ ·h ⁻¹)	Apparent quantum efficiency	Stability	References
CdSe/CdS	Precious metal substrate	Pt	Xe arc-lamp	—	19.3% ± 1.4%(–)	—	[74]
Cu-Ni/CdS	Non-precious metal substrate	Cu-Ni alloy	300W Xe lamp ($\lambda \geq 420\text{nm}$)	28.19	21.5% (400 nm)	—	[94]
MoO ₃ /Mo ₂ C-C-CdS	Non-precious metal substrate	MoO ₃ /Mo ₂ C-C	300W Xe lamp ($\lambda \geq 420\text{ nm}$)	18.43	14.13%(–)	90 h of stable operation	[108]
Pt-ZnIn ₂ S ₄	Single-atom loading	Pt single-atom	300W Xe lamp ($\lambda \geq 420\text{ nm}$)	17.5	50.4% (420nm)	50 h of stable operation	[110]
Cd(OH) ₂ /CdS	Heterogeneous structure construction	Cd(OH) ₂	300W Xe lamp ($\lambda \geq 420\text{ nm}$)	3.48	5.73% (400 nm)	80% (4 operation)	[111]
CdS/ZnS	Heterogeneous structure construction	ZnS	300W Xe lamp ($\lambda \geq 400\text{ nm}$)	14.02	2.76% (400 nm)	58 h of stable operation	[109]
WO ₃ @ ZnIn ₂ S ₄	Heterogeneous structure construction	ZnIn ₂ S ₄	300 W Xe lamp	8.5	3.61% (420 nm)	4 cycles without attenuation	[112]
PtNF@Ni(OH) ₂ /CdS	Heterogeneous structure construction	Pt NF@Ni(OH) ₂	300 W Xe lamp ($\lambda \geq 420\text{ nm}$)	44.05	58.9% (420 nm)	89.9% of activity remained after 4 cycles	[113]
Eu-doped ZnO@GO	Heterogeneous structure construction	Eu GO	300 W Xe lamp ($\lambda \geq 420\text{ nm}$)	0.2558	6.47% (420 nm)	—	[114]
CdS/MoS ₂	Heterogeneous structure construction	MoS ₂	300 W Xe lamp ($\lambda \geq 420\text{ nm}$)	15.5	14.7% (420 nm)	5 cycles without attenuation	[115]
CdS/Ni(OH) ₂	Heterogeneous structure construction	Ni(OH) ₂	300 W Xe lamp ($\lambda \geq 420\text{ nm}$)	20.14	8.7% (420 nm)	90% of activity remained after 4 cycles	[116]
CdS/Fe ₂ O ₃	Heterogeneous structure construction	Fe ₂ O ₃	300 W Xe lamp ($\lambda \geq 420\text{ nm}$)	1.806	13.7% (420 nm)	90% of activity remained after 4 cycles	[117]

render its activation under mild conditions inherently challenging. As a result, photocatalytic CO₂ reduction is generally limited by three key processes: light absorption, charge carrier generation and transport, and surface reaction kinetics [75].

Conventional photocatalysts often suffer from limited visible-light absorption, rapid recombination of photogenerated electron-hole pairs, and insufficient CO₂ activation capability. In contrast, two-dimensional II–VI NPLs provide a unique platform to address these challenges synergistically. Their atomic-scale thickness significantly shortens carrier migration distances, thereby suppressing bulk recombination, while their large specific surface area offers abundant active sites for CO₂ adsorption and activation. Consequently, structural design has become a central strategy for optimizing carrier separation, enhancing CO₂ activation, and improving product selectivity in these systems.

A key factor limiting CO₂ reduction efficiency is the recombination of photogenerated carriers. In this context, spatial separation of redox sites in two-dimensional structures has proven particularly effective. Wang et al. exploited the intrinsic anisotropic surface characteristics of CdS NPLs to construct a photocatalytic system in which S²⁻-terminated basal planes and edge sites serve distinct roles. Upon light irradiation, photogenerated electrons migrate to edge sites, which function as reduction centers, while holes accumulate on the basal plane, acting as oxidation centers. This spatial separation of redox sites effectively suppresses carrier recombination and enhances charge utilization efficiency. As a

result, the system achieves a CO production rate of 2.13 mol·g⁻¹·h⁻¹ under AM 1.5G illumination, with an apparent quantum efficiency of 42.1% and a CO selectivity of 99%. These results clearly demonstrate that precise spatial regulation of reaction sites in two-dimensional NPLs is an effective strategy for improving photocatalytic performance [61].

Beyond carrier separation, efficient activation of CO₂ molecules is another critical challenge. Defect engineering has emerged as a powerful approach to address this issue. For instance, Luo et al. introduced surface Se vacancies into CdSe NPLs, leading to a significant enhancement in catalytic performance (Fig. 11(a)). The CO production rate reaches 2557.5 μmol·g⁻¹·h⁻¹, approximately four times higher than that of defect-free samples, while maintaining stability over a continuous 5-hour reaction. Mechanistic studies reveal that these surface vacancies not only act as electron trapping centers, enhancing the localization of photogenerated electrons, but also serve as active sites for CO₂ adsorption and activation (Fig. 11(b)), thereby improving overall reaction efficiency [7].

In addition to defect engineering, tuning the electronic structure through doping plays a crucial role in regulating product selectivity and energy conversion efficiency. Liu et al. reported a Co/N co-doped CdIn₂S₄ system prepared via a dual-element doping strategy. The resulting material exhibits a CO production rate of 92.17 μmol·g⁻¹·h⁻¹, which is 69.30, 59.46, and 2.55 times higher than those of pristine CdIn₂S₄, Co-doped CdIn₂S₄, and N-doped CdIn₂S₄, respectively. *In situ* infrared spectroscopy identified the formation

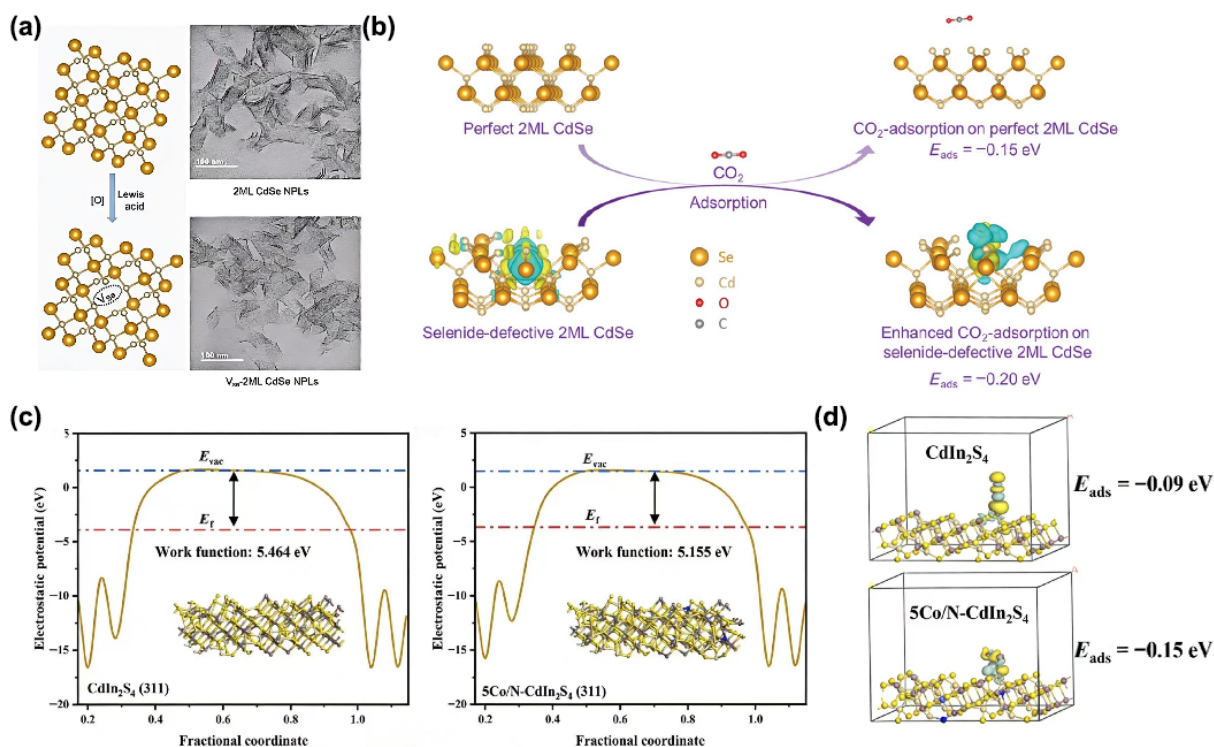


Figure 11 (a) Schematic introduction of the preparation of 2ML CdSe NPLs with Se vacancies (V_{Se} -2ML CdSe NPL) utilizing the synergistic effect of oxidation and Lewis acidity through post-treatment on 2ML CdSe NPLs. TEM images investigate morphology maintenance of as-prepared 2ML CdSe NPLs and V_{Se} -2ML CdSe NPLs with Se vacancies, respectively. (b) Comparison of CO_2 adsorption energies between perfect 2MLCdSe and V_{Se} -2ML CdSe NPLs. Reproduced with permission from Ref. [7], © Luo, H. H. et al. 2025. (c) The calculated work function of the (311) plane of $CdIn_2S_4$ and 5Co/N- $CdIn_2S_4$. (d) Differential charge density and adsorption energy of CO_2 over $CdIn_2S_4$ and 5Co/N- $CdIn_2S_4$. Reproduced with permission from Ref. [50], © Elsevier B.V. 2025.

of key $COOH^*$ intermediates, providing direct evidence of the reaction pathway. The enhanced performance is attributed to the synergistic effects of bandgap narrowing, a negative shift of the conduction band, and the introduction of impurity energy levels, which collectively optimize the electronic structure and promote both activity and selectivity (Figs. 11(c) and 11(d)) [50].

However, although the above research has made significant progress in high-performance phenomena and preliminary mechanism analysis, a series of rigorous verification standards must be met to truly establish the reliability of catalytic performance and reaction attribution.

The most basic one is $^{13}CO_2$ isotope tracer and whole product carbon balance analysis. Residual sacrificial agents or environmental carbon pollution in the system are very prone to produce false positives. Only by isotopic labeling that the C atoms in the product come from the incoming CO_2 can CO , CH_4 and other products be reliably attributed to the photocatalytic CO_2 reduction process. At the same time, researchers often focus only on the carbon conservation analysis of the main products and ignore the by-products, which is likely to cause a seriously low carbon recovery rate. Only by accurately quantifying all the detected products so that the molar output of carbon elements tends to be consistent with the consumption of CO_2 , can we verify the reliability of the experimental data and clarify the complete reaction path. In addition, the reaction path after the reactant is adsorbed on the surface of the catalyst must be evaluated for stability under continuous lighting conditions. Most of the high-efficiency data is collected under short-term light, but II–VI NPLs themselves have a tendency for ligands to be easy to dissolve and surface

reconstruction, and the catalytic active site may undergo great changes in tens of minutes. Therefore, we cannot determine whether the morphology and structure of the reacted NPLs are the same as those of the unreacted NPLs. We must monitor the product distribution and the activity decay of the NPLs under continuous long-term light. And the same batch of NPLs should be systematically characterized before and after catalysis, including X-ray diffraction and X-ray photoelectron energy spectrum, etc., to clarify the actual changes in the crystal phase, morphology, ligand and other parameters of NPLs before and after reaction.

However, these macro-level verifications cannot answer the fundamental question of “how the reaction occurs”. To truly clarify the core mechanism of how CO_2 molecules are adsorbed, activated and gradually transformed into products on the surface of NPLs, it is necessary to promote the deep mutual verification of the above macro verification and *in situ* characterization. With the help of *in situ* infrared spectrum, *in situ* Raman spectrum or *in situ* electron paramagnetic resonance, the fingerprint signals of $COOH$, $HCOO$, $^*CO$ and other key intermediates are captured in real time under reaction conditions, and their appearance is associated with attenuation kinetics and product generation rate. Then, with the help of density functional theory calculation, the full-path Gibbs free energy ladder diagram of interaction with the experimental intermediate is drawn at the level of energy and activation energy barrier. Only in this way can we realize the progress from the product to the generation path.

In summary, future research should take $^{13}CO_2$ tracer, whole product carbon balance, stability evaluation under long-term continuous light, and strict structural characterization before and

after catalysis as the basic requirements, and further carry out collaborative research on *in situ* spectroscopy and theoretical calculation on this premise. Only by establishing such a set of self-coherent machine theory proof closed loop, can the high-performance phenomena of CdS NPL and other model systems be expected to be transformed.

5.4 Photocatalytic organic transformations and environmental remediation

Semiconductor photocatalysis is fundamentally based on the excitation of electrons from the valence band to the conduction band under light irradiation, generating electron-hole pairs that subsequently migrate to the surface to drive redox reactions. In water-splitting systems, however, the overall efficiency is often limited by the sluggish kinetics of the four-electron oxygen evolution reaction, which is driven by photogenerated holes (Table 2) [118]. To overcome this limitation, sacrificial agents are frequently introduced to replace the water oxidation half-reaction, thereby improving overall catalytic efficiency. Based on this strategy, current research can be broadly divided into two categories: photocatalytic synthesis of high-value-added chemicals using organic substrates, and environmental remediation processes in which hazardous waste serves as a sacrificial agent and is simultaneously degraded.

II–VI NPLs have demonstrated remarkable activity and selectivity in photocatalytic organic transformations. For instance, in 2020, the visible-light-driven conversion of α -hydroxy acids into amino acids was achieved using CdS NPLs as photocatalysts (Fig. 12(a)). Mechanistic studies revealed that photogenerated holes first oxidize lactic acid into pyruvic acid, which subsequently reacts with ammonia to form an imine intermediate, followed by reduction via photogenerated electrons and protons to yield alanine [119]. Although subsequent studies indicated that the presence of OH^- under alkaline conditions inhibits the direct conversion of glucose to amino acids due to surface deactivation of CdS, this work provides important insights into the potential of II–VI NPLs for synthesizing high-value-added molecules.

Building upon this mechanism, Li et al. further improved the reaction efficiency by introducing single-atom Ru onto CdS NPLs (Fig. 12(b)). The enhanced catalytic activity of the Ru/CdS system is attributed to the activation of key functional groups (CH-OH and methyl- CH-OH) in lactate molecules, as well as the role of atomically dispersed Ru sites in facilitating electron accumulation

and transport. These effects collectively improve charge separation efficiency and reaction kinetics. As a result, the optimized Ru/CdS single-atom catalyst exhibits a significantly higher alanine formation rate compared with both Ru nanoparticle-modified systems and conventional thermocatalytic Ru catalysts [120].

Further studies have expanded the understanding of reaction pathways through different catalytic systems. Wang et al. reported the selective synthesis of α -deuterated amines using Au cluster-modified CdS NPLs, employing heavy water (D_2O) as the deuterium source (Fig. 12(c)). The results demonstrate that Au clusters not only promote charge separation but also suppress sulfur loss and oxidation via strong Au-S interactions [9]. Meanwhile, Miao et al. utilized Pd-coated CdS assemblies (formed from NPLs) to achieve stepwise dehydrogenation of lactic acid. In this system, Pd sites effectively activate α -hydroxy bonds, enabling the selective formation of pyruvate (Fig. 12(d)) [121]. These studies highlight that tailoring the structure of metal active sites and interfacial electronic properties provides a powerful approach for controlling reaction pathways and enhancing product selectivity.

In addition to organic synthesis, II–VI NPLs also exhibit excellent performance in environmental remediation processes, where hazardous waste is utilized as a sacrificial agent. In 2024, Liu et al. constructed a 2D/2D CdS-CuInSe₂ S-scheme heterojunction system, in which PET microplastics were introduced as sacrificial agents and successfully converted into small-molecule products such as formic acid, ethanol, acetic acid, and ethylene glycol [56]. Although excessive loading of CuInSe₂ (e.g. 20%) led to reduced photocatalytic activity due to light-shielding effects, the optimized system still achieved hydrogen production rates 7.5 times higher than pure CdS while enabling efficient microplastic degradation.

Subsequently, Zeng et al. developed a CdSe-CuInSe₂ 2D/0D composite system by integrating CuInSe₂ into layered CdSe NPLs. The coupling between components is driven by strong electrostatic interactions, which not only increases the density of surface active sites but also establishes efficient charge transport pathways, thereby promoting carrier separation. As a result, the system achieves nearly complete degradation of Rhodamine B ($5 \text{ mg}\cdot\text{L}^{-1}$) even at relatively high concentrations. Furthermore, this study provides additional insights into photocatalytic mechanisms under oxygen-rich conditions [122].

Although the photocatalytic applications of II–VI semiconductor NPLs have mainly focused on H_2 evolution, CO_2 reduction, pollutant degradation, and selective organic transformations,

Table 2 Comparison of the performance of II–VI nanolayers in the degradation of harmful substances and the synthesis of high-value-added products under different modifications

Catalyst system	Modification strategy	Cocatalyst/hetero-junction component	Specific use	Light source	Reaction system	Degradation/synthesis efficiency ($\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$)	Stability	References
ZnO/TiO ₂	Heterogeneous structure construction	TiO ₂	RhB degradation	UV light ($\lambda < 365\text{nm}$)	RhB aqueous solution	3.375	5 cycles without attenuation	[123]
ZnO/CoTe	Heterogeneous structure construction	CoTe	Dye degradation	Sunlight	MB or MR dye aqueous solution	MB:624MR:732	96.7% of activity remained after 5 cycles	[124]
ZnO/COF	Heterogeneous structure construction	COF	Synthesis of hydrogen peroxide	Solar simulator	O ₂ -saturated EtOH/H ₂ O solution	2443	4 cycles without attenuation	[125]
CdS/CuInSe ₂	Heterogeneous structure construction	CuInSe ₂	Microplastic degradation	Visible light	PET alkaline hydrolysate (pH > 14)	—	4 cycles without attenuation	[118]

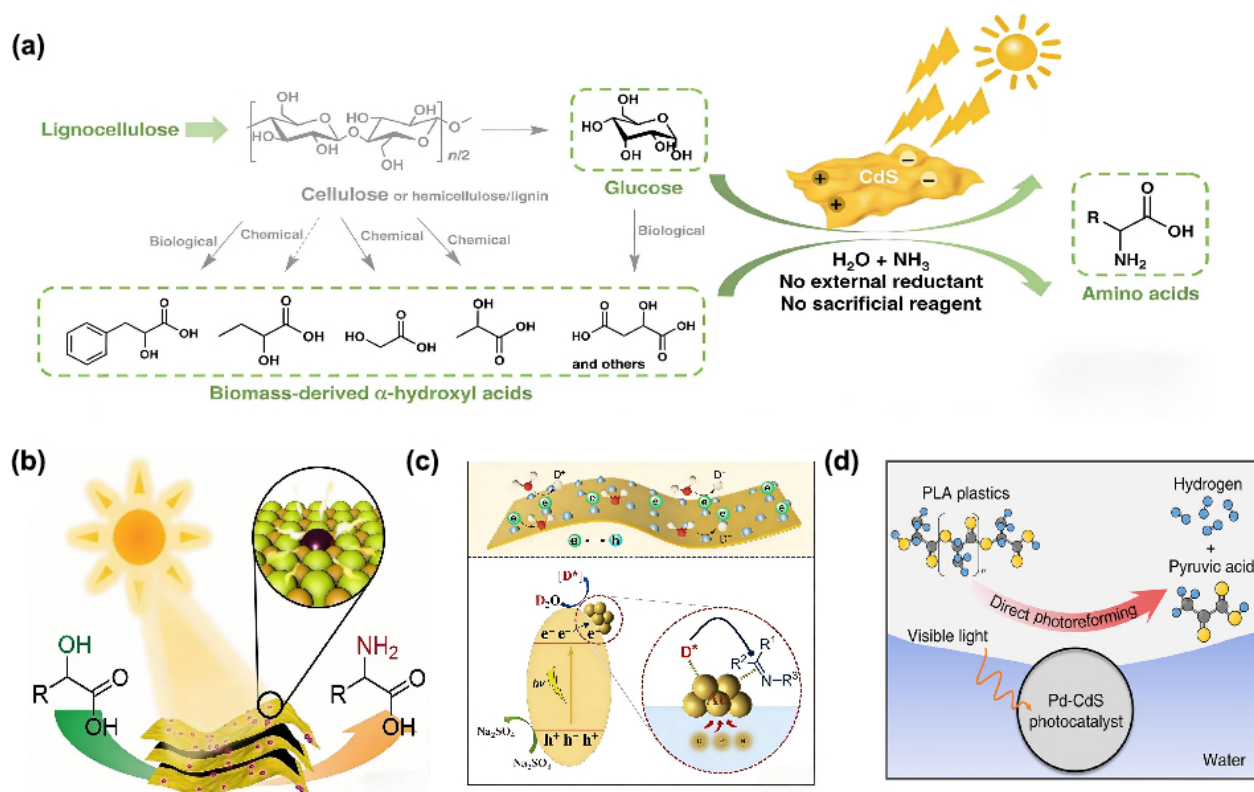


Figure 12 (a) Schematic of photocatalytic amination of glucose or biomass-derived α -hydroxyl acids to amino acids. Reproduced with permission from Ref. [119], © Song, S. et al. 2020. (b) Schematic diagram of rutilium-modified CdS NPLs with hydroxylic acid to obtain amino acids under photocatalytic conditions. Reproduced with permission from Ref. [120], © Wiley-VCH GmbH 2024. (c) Schematic of gold cluster-modified cadmium sulfide NPLs catalyzing the reduction of imines. Reproduced with permission from Ref. [9], © American Chemical Society 2025. (d) Schematic of Pd-CdS catalyzing the conversion of microplastics to pyruvate. Reproduced with permission from Ref. [121], © American Chemical Society 2024.

photocatalytic nitrogen fixation represents another potentially important but much less explored direction. To date, reports on N_2 reduction using II–VI semiconductor NPLs remain scarce, with only limited examples involving CdS-based NPLs or nanocrystal systems. Nevertheless, the structural features of II–VI NPLs may be beneficial for photocatalytic N_2 reduction. Their atomically thin geometry can shorten charge-migration distances and facilitate the separation and utilization of photogenerated carriers, while abundant surface sites, edge atoms, and vacancy defects may provide potential adsorption and activation sites for N_2 molecules. In particular, defect engineering, such as sulfur or selenium vacancies, could modulate the local electronic structure and promote N_2 activation, although such effects need to be carefully distinguished from enhanced competing hydrogen evolution. Future studies should therefore focus on the rational construction of active sites, coupling with suitable cocatalysts, suppressing proton reduction, and employing rigorous control experiments, to confirm the origin of generated NH_3 . Given the current scarcity of literature, photocatalytic nitrogen fixation based on II–VI NPLs remains an open and promising research direction rather than a mature application field.

6 Challenges and outlook

This review has systematically summarized recent advances in two-dimensional II–VI semiconductor NPLs for photocatalytic applications, covering their structural characteristics, synthetic strategies, photocatalytic mechanisms, and practical

implementations. Owing to their unique two-dimensional geometry and tunable electronic structures, II–VI NPLs have emerged as a highly promising class of photocatalysts, exhibiting distinct advantages in charge separation, surface reactivity, and structure–function tunability.

At the structural level, dimensional confinement endows these materials with strong quantum confinement effects, high specific surface areas, and tailorable electronic structures, making them particularly suitable for photocatalytic applications. From the perspective of synthetic regulation, a range of strategies—including thickness and lateral size control, defect engineering, ligand and interfacial modulation, heterostructure construction, and post-synthetic compositional transformation—have been developed to precisely tailor optical properties, carrier dynamics, surface chemistry, and band structures. At the mechanistic level, the fundamental processes of light absorption, exciton dynamics, charge separation, and surface reaction pathways have been systematically elucidated, establishing a clear relationship between structural design and photocatalytic performance. At the application level, modified II–VI NPLs have demonstrated excellent performance in CO_2 reduction, hydrogen evolution, pollutant degradation, and value-added chemical synthesis, highlighting their practical potential in energy conversion and environmental remediation.

Despite these advances, several critical challenges remain that hinder further development and practical implementation.

(1) Challenges in synthetic control

From a synthetic perspective, the preparation of high-quality

II–VI NPLs remains nontrivial. Current methods are largely dominated by hot-injection and colloidal growth techniques, which are highly sensitive to experimental parameters such as ligand selection, precursor concentration, and reaction temperature. The lack of precise control over these parameters often leads to limited reproducibility and variability in product quality.

To address this issue, emerging approaches based on artificial intelligence offer promising solutions. On the one hand, data-driven models can establish correlations between synthesis conditions and material properties, enabling predictive design and optimization of NPLs structures. On the other hand, high-throughput and automated experimentation can systematically explore parameter spaces with improved efficiency and reduced human error, thereby accelerating the discovery of optimal synthesis conditions.

More importantly, the application of AI/ML in this field should not be restricted to synthetic optimization. Given that this review also addresses exciton dynamics, interfacial charge separation, and photocatalytic mechanisms, future AI/ML studies could incorporate performance-relevant descriptors such as exciton lifetime, charge-transfer time at the NPL/cocatalyst interface, CO₂ adsorption energy, COOH* intermediate stability, and interfacial coupling strength. This broader data-driven framework may provide new opportunities for both mechanistic understanding and the prediction of photocatalytic performance.

(2) Challenges in mechanistic understanding

From a mechanistic standpoint, two key issues remain unresolved. Despite the substantial progress in the synthesis of II–VI NPLs, their growth mechanisms remain far from fully clarified. Recent mechanistic studies have suggested that the formation of CdSe-based ultrathin nanocrystals may involve layered assembly of nanoclusters within bilayer templates [126], transformation of magic-size II–VI nanoclusters into planar colloidal nanocrystals [127], and precursor-reactivity-dependent growth pathways revealed by *in situ* X-ray scattering [128]. In addition, direct observation of non-stoichiometry-induced phase transformation in two-dimensional CdSe NPLs has highlighted the possible role of surface reconstruction and phase evolution in these ultrathin systems [14]. These findings indicate that the nucleation, lateral growth, and structural evolution of II–VI NPLs are highly complex, and further in *operando* studies combined with theoretical calculations are still required to establish a unified mechanistic understanding.

Second, the microscopic understanding of photocatalytic surface reactions is still limited. In particular, for CO₂ reduction, the detailed reaction pathways and energy profiles following adsorption on catalyst surfaces are not yet fully understood. Addressing this challenge requires the integration of advanced *in situ* characterization techniques with theoretical calculations, enabling direct observation and quantitative analysis of reaction intermediates and energy evolution at the atomic scale.

(3) Challenges in structure–function integration

Although a variety of structural modulation strategies have been developed, their application remains unbalanced. On the one hand, heterostructure engineering and cocatalyst integration have been extensively explored in II–VI quantum dot systems, but their implementation in NPLs systems is still relatively limited due to the constraints imposed by two-dimensional geometries. On the other hand, strategies unique to NPLs—such as precise thickness control, lateral size tuning, and ligand engineering—have been primarily

studied in the context of fundamental physicochemical properties, with comparatively fewer reports linking these approaches directly to photocatalytic applications. Future research should therefore focus on bridging this gap by integrating structural control strategies with specific photocatalytic reaction systems. In particular, combining size regulation, ligand engineering, heterostructure design, and cocatalyst optimization within a unified framework could enable synergistic enhancement of photocatalytic performance.

Overall, while two-dimensional II–VI NPLs have demonstrated significant potential in photocatalysis, further progress requires coordinated advances in synthesis, mechanistic understanding, and structural design. Looking forward, the integration of multidisciplinary approaches—including artificial intelligence-assisted material design, *in situ/operando* characterization, and theoretical modeling—will play a crucial role in advancing this field. These efforts are expected to enable more precise control over material structure, deeper understanding of photocatalytic mechanisms, and more efficient translation from model systems to practical applications. Ultimately, the rational design and scalable fabrication of II–VI nanoplatelet-based photocatalysts will contribute to the development of sustainable solutions for energy conversion and environmental remediation, positioning these materials as key components in future photocatalytic technologies.

Data availability

No primary research results, software or code have been included and no new data were generated or analyzed as part of this review.

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Declaration of competing interest

There are no conflicts to declare.

Author contributions statement

H. M.: Conceptualization, data curation, formal analysis, investigation, writing – original draft, writing – review and editing. Y. B.: Conceptualization, investigation, writing – review and editing. H. J.: Conceptualization, data curation, formal analysis, writing – original draft. D. Y.: Writing – review and editing. W. Y.: Conceptualization, formal analysis, funding acquisition, investigation, project administration, supervision, validation, writing – review and editing. All authors contributed to the discussion, and gave approval to the final version of the manuscript.

Use of AI statement

None.

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