

Steering interfacial charge transfer via 2D-1D MoPS₃-CdS heterojunctions for highly efficient visible-light-driven uranium(VI) remediation

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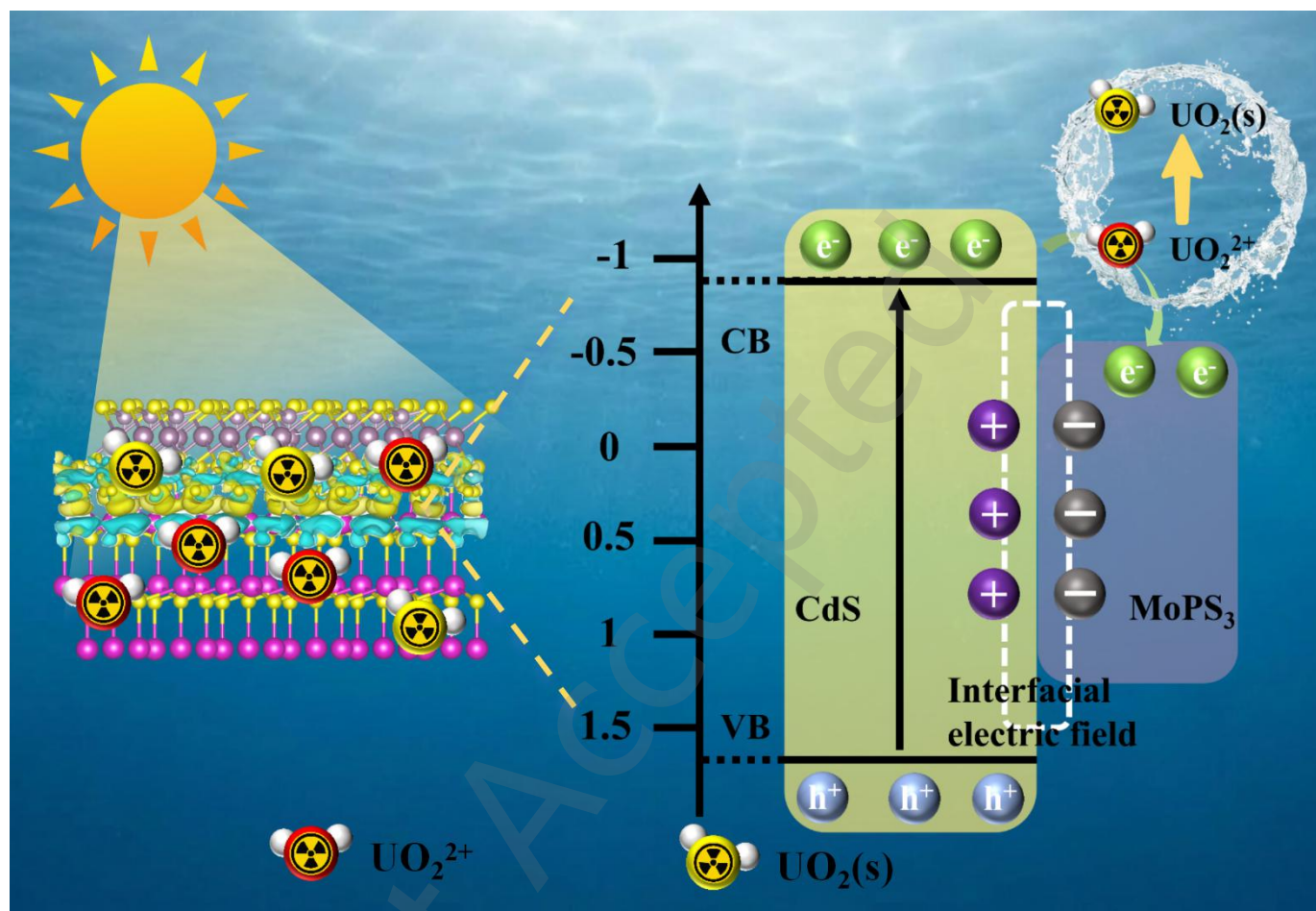
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Construction of a MoPS_3 - CdS heterointerface enables directional photogenerated electron transfer and efficient charge separation, thereby promoting rapid visible-light-driven reduction of aqueous U(VI) to insoluble UO_2 .

Steering interfacial charge transfer via 2D-1D MoPS₃-CdS heterojunctions for highly efficient visible-light-driven uranium(VI) remediation

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ABSTRACT: Addressing the urgent demand for the remediation of uranium-contaminated wastewater, the development of highly efficient and stable photocatalysts capable of reducing soluble U(VI) to insoluble U(IV) is of critical significance. Herein, a stable 2D-1D MoPS₃-CdS heterostructure was fabricated via an interfacial assembly strategy. The optimized 3% MoPS₃-CdS heterojunction achieved 99.3% U(VI) removal within 15 min, exhibiting exceptional reaction kinetics, robust tolerance to coexisting ions, and excellent cycling stability. Radical-trapping experiments and electron spin resonance (ESR) measurements revealed that photogenerated electrons and superoxide radicals ($\bullet\text{O}_2^-$) serve as the primary active species driving U(VI) reduction. The enhanced photocatalytic performance is attributed to efficient interfacial charge transfer and spatial charge separation. This mechanism was further supported by fs-TAS measurements and DFT calculations, which revealed pronounced interfacial charge redistribution and provided insights into the charge-transfer characteristics of the Schottky-type heterojunction. This work provides a robust design principle for engineering Schottky-type heterojunctions toward high-performance photocatalytic uranium remediation.

KEYWORDS: photocatalysis; uranium(VI) remediation; 2D-1D heterojunction; MoPS₃ nanosheets; interfacial charge transfer

1 Introduction

As a primary fuel for nuclear energy, uranium plays a vital role in global power production; however, its extraction, processing, and post-treatment often result in significant radioactive contamination[1]. Hexavalent uranium (U(VI)), due to its high solubility and mobility, is a prevalent environmental pollutant that requires urgent and effective removal[2]. As a result, efficient strategies for uranium remediation are urgently explored to address the related environmental pollution and nuclear waste issues. Common methods for U(VI) removal include electrochemical reduction [3], adsorption[4, 5], and photocatalysis[6]. Electrochemical reduction requires an external electrical input, whereas conventional adsorption mainly transfers U(VI) from the aqueous phase to a solid adsorbent, necessitating subsequent separation and disposal of the uranium-loaded adsorbent. In contrast, photocatalytic reduction uses light energy to convert soluble U(VI) into less soluble U(IV), providing a potentially energy-efficient route in which solar energy drives pollutant reduction[7]. These features make photocatalysis an attractive strategy for remediating uranium-contaminated wastewater. Upon light irradiation, photocatalysts facilitate the removal of uranyl ions from aqueous

solutions by reducing soluble U(VI) to insoluble tetravalent uranium (U(IV))[8]. Nevertheless, the practical efficiency of photocatalytic U(VI) reduction remains severely hindered by rapid charge recombination and insufficient catalytic activity; therefore, designing highly efficient photocatalytic systems is of great significance.

CdS is widely investigated as a potential photocatalyst due to its strong visible light-absorption capability and favorable band structure [9-11]. As a typical semiconductor, CdS possesses a narrow bandgap and suitable redox potentials for U(VI) reduction. However, its performance is restricted by issues such as photocorrosion and rapid photogenerated carrier recombination[12]. Constructing heterojunctions has proven to be an effective strategy to address these limitations by promoting charge separation [13-15]. Among these, two-dimensional (2D) nanostructure cocatalysts have emerged as highly versatile building blocks for constructing photocatalytic heterojunctions due to their large specific surface areas, abundant active sites, and superior charge-transfer properties[16]. For instance, Lu et al. leveraged these advantages to develop a CdS@NiCr-LDH, which achieved a 99.8% U(VI) removal efficiency under visible-light[17].

Particularly, layered transition metal phosphosulphides (MPS₃, where M = Fe, Co, Ni, Pd, Mo) exhibit intrinsic photocatalytic activity stemming from their favorable optical and electrical properties. Moreover, MPS₃ cocatalysts are known for forming heterostructures with tunable band alignment, enhancing catalytic activity through interfacial engineering and in-situ structural reconstruction [18-20]. Previous studies have revealed that MoPS₃ possesses unique electronic structures and excellent carrier transport capability, which facilitate interfacial charge redistribution, making MoPS₃ a promising component for constructing charge-transfer interfaces with Schottky-type interfacial electronic characteristics [21, 22]. However, the application of MoPS₃-based cocatalysts in photocatalytic uranium reduction remains unexplored. Benefiting from its excellent electrical conductivity and abundant active sites, MoPS₃ is expected to facilitate interfacial electron transfer, thereby overcoming the intrinsic limitations of CdS[23].

Herein, a novel MoPS₃-CdS heterostructure was rationally engineered to establish an efficient interfacial charge transfer highway for the rapid photocatalytic reduction of U(VI). The optimized 2D-1D MoPS₃-CdS heterostructure exhibited exceptional catalytic kinetics, achieving a U(VI) removal efficiency of 99.3% within 15 min, which was a dramatic enhancement that far surpasses pristine CdS. Furthermore, it demonstrated remarkable structural robustness, retaining 95% of its initial activity after five consecutive cycles. By combining PEC tests, fs-TAS, and DFT, we clarified the mechanism. Specifically, the strong interfacial electronic coupling induces interfacial electron redistribution between MoPS₃ nanosheets and CdS nanorods, supporting directional interfacial charge transfer with Schottky-type interfacial electronic characteristics. This work not only proposes a highly feasible strategy for developing MoPS₃-based heterojunctions but also offers profound mechanistic insights into efficient uranium extraction from radioactive wastewater.

2. Experimental

2.1. Synthesis of MoPS₃

MoPS₃ bulk crystal was synthesized via CVT using iodine as a transport agent[22]. Stoichiometric quantities of molybdenum powder (1.441 g, 99.99%), red phosphorus (0.467 g, 99.99%), sulfur sheets (1.446 g, 99.9995%), and iodine (0.072 g, 99.8%) were homogenized by grinding in an agate mortar, sealed under high vacuum ($\leq 10^{-3}$ Torr) in a quartz ampoule, and reacted at 700 °C for 120 hours with controlled ramp/cool rates. The product was ground, washed with ethanol, filtered (0.22 µm PTFE), and vacuum-dried.

2.2. Synthesis of CdS

Cd(CH₃COO)₂·2H₂O (2 mmol) and CH₄N₂S (4 mmol) were first introduced into 50 mL of C₂H₈N₂ under ultrasonic treatment, followed by magnetic stirring for 1 h to form a uniform precursor solution. The mixture was then transferred into a 100 mL Teflon-lined stainless-steel autoclave and subjected to a solvothermal reaction at 180 °C for 16 h. The resulting product was isolated via centrifugation, washed three times with Milli-Q water and absolute ethanol, and finally dried under vacuum at 60 °C for 6 h to yield CdS nanorods.

2.3. Synthesis of MoPS₃-CdS heterojunction

The MoPS₃-CdS heterostructures were fabricated through a post-synthetic solution-assisted interfacial assembly strategy, as shown in Figure 1a. CdS and MoPS₃ powders with various mass ratios (1:99, 3:97, 5:95, and 8:92) were dispersed in 30 mL of ethanol and continuously stirred for 24 h to promote intimate interfacial contact. Subsequently, the suspensions were centrifuged at 9000 rpm for 3 min, and the collected products were vacuum-dried at 60 °C for 6 h. The resulting MoPS₃-CdS heterostructure samples were labeled as 1%MoPS₃-CdS, 3%MoPS₃-CdS, 5%MoPS₃-CdS, and 8%MoPS₃-CdS, respectively.

2.4. Photocatalytic U(VI) Reduction

The photocatalytic experiment was conducted under a 300 W Xe lamp equipped with a 420 nm cutoff filter. 20 mg of the synthesized material was added to 80 mL of U(VI) solution with an initial concentration of 50 ppm, and the pH of the mixture was adjusted using NaOH or HCl. The suspension was stirred in the dark for 40 min to achieve adsorption equilibrium, followed by visible light irradiation. During irradiation, cooling water is used to maintain the reaction temperature at 25 °C. At designated time intervals, 1.5 mL samples were withdrawn and filtered through a 0.22 µm syringe filter. The concentration of U(VI) in the filtrate was quantified using inductively coupled plasma atomic emission spectroscopy (ICP-AES) to determine the removal efficiency (R%) according to the following formula:

$$R(\%) = \frac{C_0 - C_t}{C_0} \times 100\%$$

where C₀ and C_t (ppm) represent the initial and residual concentrations of U(VI), respectively.

3 Results

3.1. Structure and Morphology

The crystal structures of CdS, MoPS₃, and MoPS₃-CdS heterostructure were characterized by XRD (Figure 1b). The diffraction peaks of pristine CdS can be well indexed to hexagonal wurtzite crystal structure of CdS (PDF# 41-1049)[24]. The diffraction peaks of MoPS₃ are consistent with the layered MoPS₃ structure, with peak positions different from those of MnPS₃ and FePS₃ due to the distinct crystal structures and lattice parameters of Mo-based phosphosulfides. For MoPS₃-CdS heterojunction with low MoPS₃ loadings (such as 3% MoPS₃-CdS), the XRD patterns are dominated by CdS reflections without significant peak shifts, indicating the formation of an integrated MoPS₃-CdS heterostructure rather than lattice doping. With increasing MoPS₃ content, the characteristic MoPS₃ peaks at around 40.6° and 58.7° become gradually discernible, confirming the successful integration of MoPS₃ with CdS. The interfacial electronic characteristics of the heterostructure are further investigated by subsequent analyses.

FTIR spectra of MoPS₃, CdS and MoPS₃-CdS heterostructure are shown in Figure 1c. All samples display a broad absorption band at 3200-3500 cm⁻¹ and a band around 1600 cm⁻¹, which are attributed to surface -OH groups and adsorbed water. The characteristic vibrations of metal-sulfur bonds (Cd-S and Mo-S) are observed in the low-wavenumber region (400-600 cm⁻¹), while the bands at 700-800 cm⁻¹ correspond to P-S vibrations[25]. These characteristic bands are well retained in the heterojunction without the appearance of new peaks, indicating the retention of main vibrational features of the original components.

As shown in Figure 1d and Figure S1, the textural properties of CdS and 3%MoPS₃-CdS were investigated by Brunner-Emmet-Teller (BET) analysis. Both samples exhibit typical type IV isotherms with H3 hysteresis loops, indicative of mesoporous structures mainly originating from slit-like pores formed by particle aggregation. Pristine CdS presents a specific surface area (SBET) of 22.04 m²/g, with a pore size distribution centered at approximately 32.74 nm. 3%MoPS₃-CdS Schottky-type heterojunction material shows a slightly reduced SBET of 21.22 m²/g, accompanied by a marginal decrease in average pore size to 31.99 nm. This reduction might be attributed to the interfacial coupling between MoPS₃ and CdS, which leads to partial pore filling and a more compact stacking structure. The smaller surface area could reduce the number of accessible surface active sites, but this effect is minor relative to the much higher photocatalytic activity. The mesoporous characteristics and adsorption-desorption profiles remain largely unchanged after MoPS₃ incorporation, indicating that the pore properties of CdS are well retained. The preserved mesoporous features are favorable for reactant diffusion and exposure of accessible catalytic sites[26].

To evaluate the charge separation characteristics of the different samples, photoelectrochemical measurements was carried out. The light-harvesting properties of CdS, MoPS₃, and MoPS₃-CdS heterostructure were investigated by UV-vis diffuse reflectance spectroscopy (DRS), as shown in Figure 1e. Pristine MoPS₃ exhibits strong absorption in the ultraviolet region; however, its relatively weak visible-light absorption and inefficient utilization of photogenerated charge carriers result in negligible photocatalytic activity toward U(VI) reduction. Figure 1f indicates that MoPS₃ possesses a band gap of approximately 1.67 eV. In contrast, pure CdS displays an absorption edge around 520 nm, corresponding to a band gap energy of approximately 2.39 eV. The MoPS₃-CdS heterostructure shows enhanced absorption throughout the visible-light region compared with pristine CdS. Moreover, a slight red shift of the absorption edge is observed, indicating interfacial interactions between CdS and MoPS₃[27]. The extended photoresponse range and enhanced visible-light harvesting capability are expected to facilitate more efficient photon utilization, thereby contributing to the improved photocatalytic U(VI) reduction performance of the heterostructure.

XPS analysis was performed to investigate the surface elemental composition and chemical states of CdS, MoPS₃, and MoPS₃-CdS. The survey spectrum of the MoPS₃-CdS composite confirms the presence of Mo, P, S, and Cd elements (Figure S2), indicating the successful integration of MoPS₃ and CdS. All binding energies were calibrated using the C 1s peak at 284.8 eV. As illustrated in Figure 1g, pristine CdS exhibits two characteristic peaks centered at 404.75 and 411.50 eV, which are assigned to Cd 3d_{5/2} and Cd 3d_{3/2}, respectively[28]. After coupling with MoPS₃, both peaks shift toward higher binding energies in the MoPS₃-CdS heterostructure, appearing at 405.12 and 411.86 eV indicating a modified chemical environment of Cd species after heterointerface formation. The Mo 3d spectrum of pristine MoPS₃ (Figure 1h) exhibits two characteristic peaks at 230.45 and 233.60 eV, corresponding to Mo 3d_{5/2} and Mo 3d_{3/2}, respectively. Besides, the prominent peak centered at 226.32 eV is assigned to the S 2s state. After coupling with CdS, these peaks shift to higher binding energies, with the Mo 3d peaks appearing at 232.00 and 235.15 eV, while the S 2s peak moves to 225.79 eV, further confirming the altered chemical environment of Mo and S species caused by interfacial coupling between MoPS₃ and CdS. In addition, the P 2p spectrum of MoPS₃ (Figure 1i) presents characteristic peaks at 129.80 and 130.65 eV, which can be attributed to P 2p_{3/2} and P 2p_{1/2}, respectively[22]. Additionally, the peak at 133.7 eV can be attributed to surface PO_x species that may be generated by mild oxidation. A comparison with MoPS₃ shows that the peaks of MoPS₃-CdS shifted to 130.00 and 130.85 eV, respectively. The high-resolution S 2p spectrum of CdS (Figure 1j) exhibits two characteristic components at 161.16 and 162.44 eV, corresponding to the spin-orbit splitting of S 2p_{3/2} and S 2p_{1/2} [29]. The S peaks of MoPS₃ are located at 161.16 and 162.44 eV, representing the S 2p_{3/2} and S 2p_{1/2}. The S 2p spectrum in MoPS₃-CdS shifts towards higher binding energies relative to pure CdS and MoPS₃. In addition, an extra peak at 226.32 eV is observed, which is assigned to S 2s[30]. Overall, the shifts of Cd, Mo, P, and S core-level peaks in the MoPS₃-CdS heterostructure reveal significant changes in the chemical environments of the constituent elements, demonstrating strong interfacial coupling between CdS and MoPS₃[31, 32].

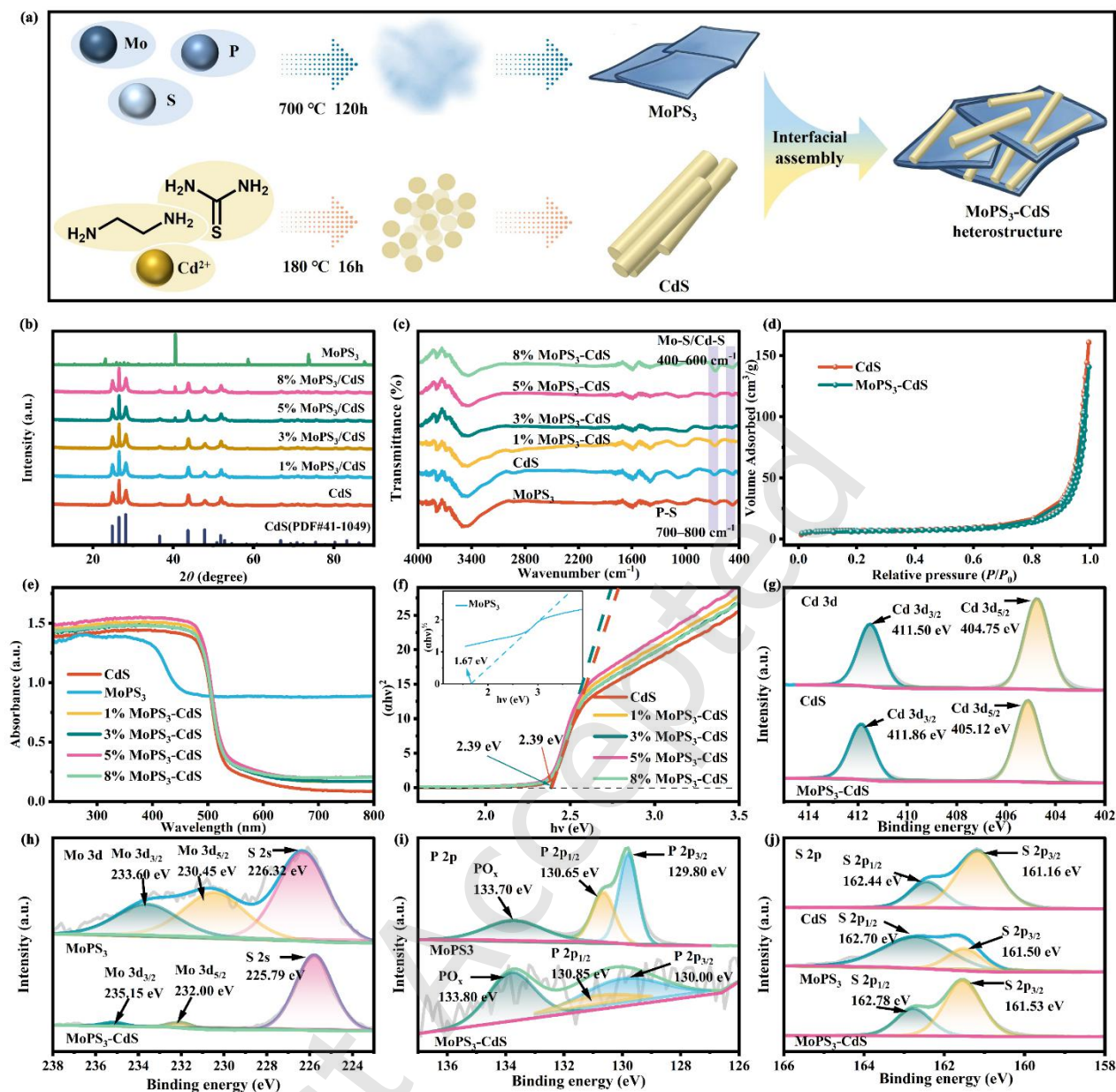


Figure 1. Schematic illustration of the preparation procedure for MoPS₃-CdS (a). XRD patterns (b), FTIR spectra (c), N₂ adsorption-desorption isotherms (d), UV-vis DRS (e), Tauc plots (f) of CdS, MoPS₃, and MoPS₃-CdS. (g-j) High-resolution XPS spectra of Cd 3d, Mo 3d, S 2p for CdS, MoPS₃, and MoPS₃-CdS.

In situ XPS spectroscopy was further employed to investigate the light-induced charge redistribution in the MoPS₃-CdS heterostructure. As shown in Figure 2, the Cd 3d and S 2p core levels shift toward higher binding energies under light irradiation, suggesting a decrease in the local electron density around Cd and S in CdS upon illumination[33, 34]. Although the Mo 3d signals of MoPS₃ exhibited relatively weak variations

due to the low MoPS₃ content and limited signal-to-noise ratio, the observed shifts of the Cd 3d and S 2p core levels provide evidence of light-induced interfacial charge redistribution in the MoPS₃-CdS heterostructure. The corresponding P 2p spectra are provided in Figure S3.

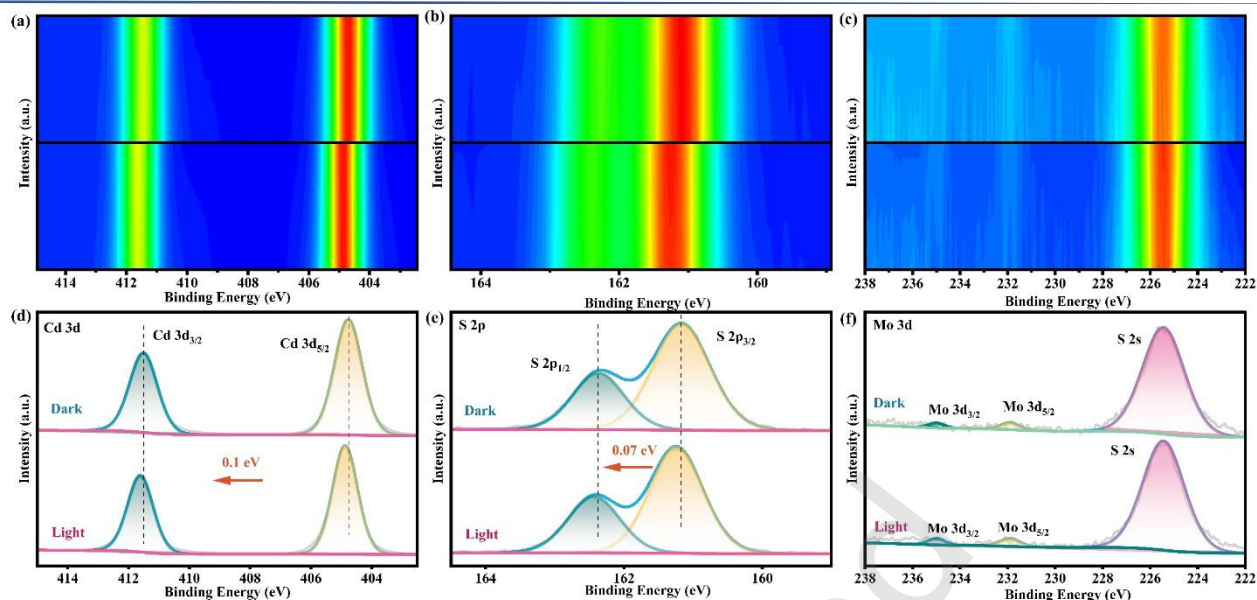


Figure 2. In situ XPS measurements before and after light irradiation. The in situ high-resolution XPS spectrum of (a), (d) Cd 3d, (b), (e) S 2p, (c), (f) Mo 3d in MoPS₃-CdS.

The surface morphology, microstructure, and elemental compositions of CdS, MoPS₃, and MoPS₃-CdS were investigated by scanning electron microscopy (SEM), transmission electron microscopy (TEM), high-resolution TEM (HRTEM), and energy-dispersive X-ray spectroscopy (EDS) mapping. As shown in Figure 3a, CdS exhibits a well-defined one-dimensional nanorod morphology with relatively uniform dispersion. The corresponding TEM image (Figure 3b) further confirms the rod-like structure of CdS. Moreover, the HRTEM image (Figure 3c) displays clear lattice fringes with an interplanar spacing of 0.358 nm, which can be indexed to the (100) plane of hexagonal wurtzite CdS. In contrast, MoPS₃ presents a typical two-dimensional sheet-like morphology (Figure 3d). The TEM image (Figure 3e) further reveals the layered structure of MoPS₃, while the HRTEM image (Figure 3f) shows distinct lattice fringes with a d-spacing of 0.32 nm, corresponding to the (110) plane of MoPS₃. After the integration of CdS and MoPS₃, the morphology and interfacial structure of the composite were further examined. As shown in Figure 3g,

CdS nanorods are uniformly distributed on the surface of layered MoPS₃, forming a well-coupled 2D-1D hybrid architecture. The TEM image (Figure 3h) further confirms the intimate contact between CdS nanorods and MoPS₃ nanosheets. Furthermore, the HRTEM image (Figure 3i) exhibits two sets of clear lattice fringes with interplanar spacings of 0.358 and 0.320 nm, corresponding to the (100) plane of CdS and the (110) plane of MoPS₃, respectively. These results confirm the successful integration of CdS and MoPS₃ with a closely coupled interface, providing a structural basis for the subsequent interfacial electronic interaction between MoPS₃ and CdS[22]. EDS elemental mapping results (Figure 3j) reveal the homogeneous distribution of Mo, P, S, and Cd elements throughout the MoPS₃-CdS composite, confirming the successful combination of CdS and layered MoPS₃. Combined with the HRTEM results, these findings demonstrate the formation of a closely integrated 2D-1D MoPS₃-CdS heterostructure, which provides a favorable structural platform for interfacial charge transfer[35].

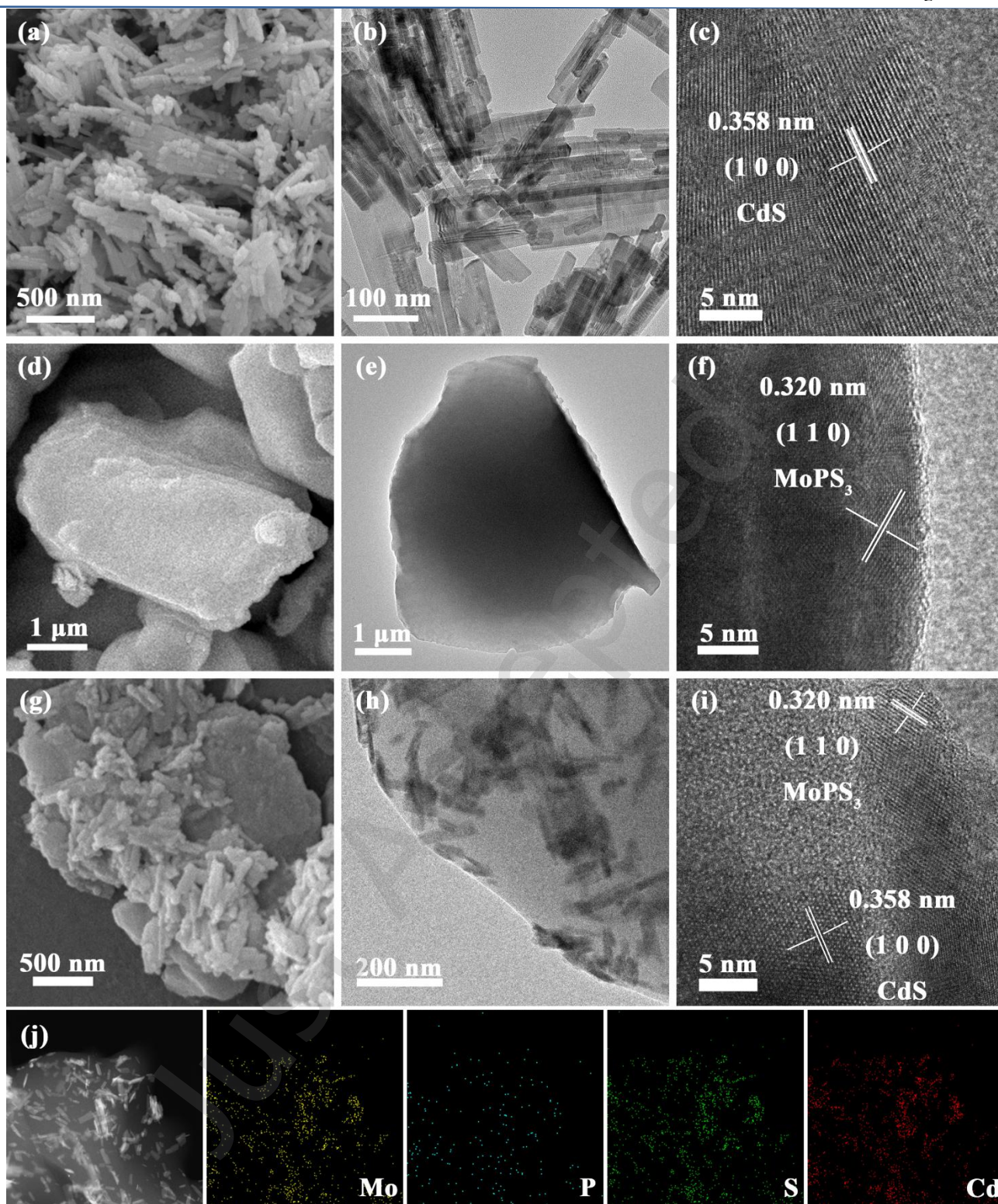


Figure 3. SEM, TEM, and HRTEM characterization of CdS (a-c), MoPS₃ (d-f), and MoPS₃-CdS (g-i), respectively. (j) Corresponding EDS elemental mapping images of the MoPS₃-CdS heterojunction.

3. 2. Photocatalytic performance analysis

Figure 4a illustrates the photocatalytic U(VI) removal performance of CdS-based samples under visible-light irradiation. The MoPS₃-CdS heterostructures exhibit obvious U(VI) adsorption capacities under dark conditions. Compared to MoPS₃, CdS exhibits a more pronounced adsorption effect, capable of removing approximately 30% of hexavalent uranium within 40 min. For the 3% MoPS₃-CdS composite, 28.1% of U(VI) was removed after 40 min of dark adsorption, followed by rapid removal to 98.0% within 5 min and 99.3% within 15

min under visible-light irradiation, confirming the dominant contribution of photocatalytic reduction. Compared to single-component materials, the MoPS₃-CdS heterostructures exhibit superior photocatalytic reduction performance under visible light. Additionally, the negligible photocatalytic U(VI) reduction activity of pristine MoPS₃ may be attributed to its narrow band gap, which leads to rapid recombination of photogenerated charge carriers, thereby limiting the availability of active electrons for U(VI) reduction[36]. The MoPS₃-CdS heterostructure exhibit obviously higher U(VI) removal rates

than pure CdS and MoPS₃ under light irradiation. Among the MoPS₃-CdS heterostructures, the sample with 3%MoPS₃ loading exhibits optimal U(VI) reduction performance, achieving 99.3% removal within 15 min. At lower MoPS₃ loadings, fewer MoPS₃-CdS interfaces may limit interfacial charge redistribution and electron transfer. Nevertheless, further increasing the MoPS₃ loading leads to a decline in photocatalytic performance. Excessive coverage of the CdS surface by MoPS₃ may weaken visible-light harvesting and consequently decrease the generation of photoinduced charge carriers[37]. At 3% loading, sufficient heterointerfaces promote charge separation while maintaining accessible CdS surfaces. Therefore, the 3% MoPS₃-CdS composite was selected as the optimal sample for characterization and mechanistic investigations. The enhanced photocatalytic activity is likely associated with the incorporation of MoPS₃, which promotes interfacial electron migration and suppresses the rapid recombination of charge carriers[38]. As shown in Figure 4b and Figure S4, the U(VI) reduction kinetics are fitted using a pseudo-first-order model to obtain the rate constant (*k*). For the 3%MoPS₃-CdS heterostructure, the calculated *k* value (0.6493 min⁻¹) is 12.4 times higher than that of pristine CdS (0.0524 min⁻¹) and 811.6 times higher than that of pristine MoPS₃ (0.0008 min⁻¹). Remarkably, this is a performance which is comparable to or superior to many reported photocatalysts (Figure 4c, Table S1).

The solution pH is a critical factor influencing the photocatalytic reduction of U(VI) by regulating the heterostructure's surface charge, uranium speciation, and interfacial charge-transfer behavior. As shown in Figure 4d, the photocatalytic reduction efficiency exhibits a strong dependence on solution pH, following an initial increase and subsequent decrease within the tested pH range of 3-8. The optimal performance is achieved at pH = 6, suggesting that a suitable acidic environment is beneficial for U(VI) adsorption and photocatalytic reduction. To further understand the pH-dependent behavior, the zeta potential of 3%MoPS₃-CdS was measured at different pH values. The zeta potential profiles (Figure 4e) reveal that the catalyst surface remains positively charged at pH values of 3-6, whereas the surface charge gradually becomes negative above pH = 6. This surface-charge transition affects the interaction between the catalyst surface and different uranium species, thereby contributing to the observed pH-dependent photocatalytic activity[39]. Visual MINTEQ simulations were performed to evaluate the pH-dependent speciation of U(VI) (Figure S5). In the low-pH range (3-5), the catalyst surface is positively charged, while U(VI) exists mainly as cationic species such as UO₂²⁺. Although electrostatic attraction is favorable, the high H⁺ concentration competes for surface active sites and thus restricts both the adsorption and reduction of U(VI)[40]. Near pH = 6, the surface becomes more negatively charged, promoting electrostatic interaction with positively charged uranyl hydroxyl complexes (mainly (UO₂)₃(OH)₅⁺ according to the U(VI) speciation diagram) and reducing H⁺ competition, thereby achieving the highest photocatalytic activity[41]. At higher pH (7-8), the surface of the MoPS₃-CdS heterostructure becomes increasingly negatively charged, which coincides with the formation of neutral or anionic U(VI) hydroxy complexes, reducing electrostatic attraction and thus lowering the reduction efficiency. Consequently, pH = 6 was identified as the optimal operating parameter for subsequent experiments.

As shown in Figure 4f, the photocatalytic U(VI) removal

performance of 3%MoPS₃-CdS heterostructure was evaluated across an initial concentration range of 20-200 ppm. Notably, this heterostructure retains a U(VI) removal efficiency of over 81% when the initial concentration ranges from 20-200 ppm. The effect of the 3%MoPS₃-CdS heterostructure dosage on U(VI) reduction was investigated. As shown in Figure 4g, the removal efficiency of U(VI) increases with the photocatalyst dosage and stabilizes at a near-complete removal rate at a dosage of 20 mg (0.25 g/L). Due to the minimal performance difference between the 20 mg and 25 mg dosages, and considering practical operational and economic factors, all subsequent experiments were conducted using a 20 mg dosage.

Considering the complexity of practical uranium-containing systems, the effects of common coexisting ions on photocatalytic U(VI) reduction were further investigated. Typical cations (Na⁺, Mg²⁺, Zn²⁺, Pb²⁺, K⁺, Ni²⁺, and Co²⁺) and anions (NO₃⁻, NO₂⁻, and Cl⁻) were separately added into the reaction system. As illustrated in Figure 4h, the photocatalytic reduction performance of MoPS₃-CdS heterostructure materials toward U(VI) was only slightly affected by the presence of most coexisting ions. Compared with the control experiment, which achieved a U(VI) reduction efficiency of approximately 99.3%, the removal efficiencies in the presence of these ions remained above 95%. Nevertheless, the slight inhibition observed in the presence of Co²⁺ can be attributed to its redox-active nature and partially filled 3d orbitals, which enable Co²⁺ to act as a competitive electron acceptor under light irradiation. The photocatalytic performance was also examined under more complex water conditions using a mixed-ion system containing representative cations (Na⁺, Ca²⁺, and Mg²⁺) and anions (Cl⁻, NO₃⁻, and SO₄²⁻). As summarized in Table S2, the 3% MoPS₃-CdS photocatalyst achieved approximately 79% U(VI) removal after 15 min of visible-light irradiation in the presence of these coexisting ions. Although this efficiency is lower than that in the control system without coexisting ions, U(VI) removal remains substantial, indicating that the photocatalyst retains considerable activity in a multi-ion aqueous environment. These results further support the applicability of the MoPS₃-CdS heterostructure under complex aqueous conditions. The recyclability of 3%MoPS₃-CdS was further evaluated through repeated photocatalytic U(VI) reduction experiments. As presented in Figure 4i, the photocatalyst retained over 95% uranium removal efficiency after five consecutive cycles, demonstrating its excellent stability and reusability. The minor performance attenuation may be due to the gradual accumulation of reduced U(IV) products on the catalyst surface, which partially occupies the active sites over repeated cycles[42]. Considering the typical photocorrosion of CdS, the Cd²⁺ leaching after 60 min of photocatalytic reaction was further quantified, as shown in Figure S6. Under air, pristine CdS lost approximately 90% of its Cd as Cd²⁺, whereas the 3% MoPS₃-CdS composite showed much less leaching, about 40%. Under an Ar atmosphere, Cd²⁺ leaching from 3% MoPS₃-CdS was further suppressed to approximately 2.1%, indicating that dissolved O₂ promotes Cd dissolution. The U(VI) reduction performance under air and Ar was also compared. Only a slight improvement was observed under Ar, with U(VI) removal increasing from 98.0% to 98.9% after 5 min and from 99.3% to 100% after 15 min as shown in Figure S7. Overall, MoPS₃ incorporation greatly improves the resistance of CdS to Cd²⁺ dissolution during photocatalysis.

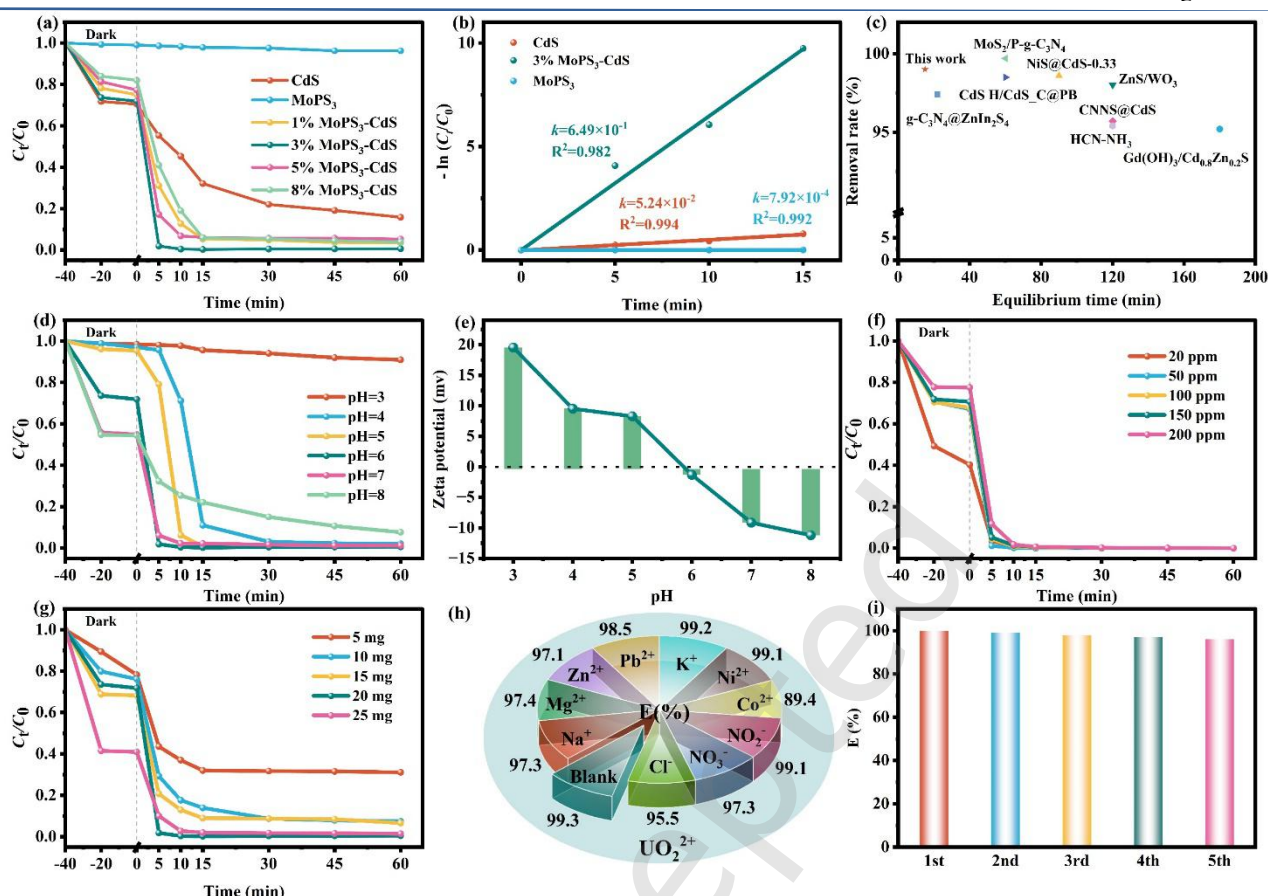


Figure 4. (a) Photocatalytic reduction performance, (b) Pseudo-first-order kinetic fitting curves, (c) Comparison of U(VI) reduction performance of MoPS₃-CdS with previously reported photocatalysts. Data sources are listed in Table S1 with corresponding references. (d) Effect of pH on the photocatalytic reduction of U(VI) (C_0 (U(VI)) = 50 ppm, $m/V = 0.25$ g/L, $t = 60$ min); (e) Zeta potentials of the 3%MoPS₃-CdS heterostructure; (f) Effect of initial U(VI) concentration; (g) Effect of catalyst dosage; (h) Effect of coexisting ions (1 mmol) for 3%MoPS₃-CdS; (i) Cycling stability of the 3%MoPS₃-CdS heterostructure.

3.3 Photocatalytic mechanisms

To elucidate the interaction mechanism between MoPS₃-CdS and uranium species, a series of characterizations including XRD, FT-IR, SEM, TEM, and XPS were performed. The XRD patterns of MoPS₃-CdS before and after photocatalytic U(VI) reduction are highly similar (Figure 5a), with no obvious change observed in the characteristic diffraction peaks of CdS and MoPS₃. This result suggests that the heterostructure maintains good structural stability during the photocatalytic reaction. Meanwhile, no additional diffraction peaks attributable to crystalline uranium-containing phases were observed after the reaction. This may be due to the relatively low amount of uranium species, along with their high dispersion or low crystallinity, which makes the corresponding diffraction peaks difficult to detect. Therefore, the absence of uranium-related diffraction peaks does not exclude the formation of uranium-containing products. The FT-IR spectra of 3%MoPS₃-CdS heterostructure before and after the reaction are presented in Figure 5b. Compared to the original heterostructure material, the photocatalytically treated heterostructure exhibits a new absorption band at approximately 904 cm^{-1} , which can be assigned to the characteristic vibrations of the O=U=O bond[43]. The emergence of these bands indicates the presence of uranium-containing species on the catalyst surface after photocatalytic reaction, suggesting effective interaction between uranium species and the heterostructure material. The XPS analysis results of the chemical state of uranium in the MoPS₃-CdS heterostructure after photocatalytic reaction are shown in Figure 5c, and two new characteristic peaks corresponding to the U 4f orbital are clearly observed. The peaks at 381.27 and 392.20 eV are assigned to U(VI) 4f_{7/2} and 4f_{5/2}, respectively,

while those located at 380.14 and 391.02 eV are attributed to U(IV)[44]. XPS analysis of the recovered catalyst indicates that approximately 38% of surface uranium species exist in the U(IV) state after photocatalytic reaction, confirming the occurrence of U(VI) reduction. The survey scan of 3%MoPS₃-CdS heterostructure after reaction is highly consistent with that of the pristine sample, which verifies uranium immobilization as well as structural stability of the heterostructure.

The HRTEM image of the 3%MoPS₃-CdS-U material (Figure 5d) reveals clear lattice fringes with interplanar spacings of 0.336 nm and 0.273 nm, which can be assigned to the (002) plane of hexagonal CdS and the (200) plane of UO₂, respectively. The appearance of the UO₂ lattice fringe indicates the reduction of U(VI) to U(IV) during the photocatalytic process. Furthermore, the EDS mapping results (Figure 5e) show that Cd, S, Mo, P, and U are distributed throughout the composite, reflecting the dispersion of uranium species on the catalyst surface. Free radical trapping experiments were performed to identify the primary active substances involved in the photocatalytic process on 3%MoPS₃-CdS. In these experiments, isopropyl alcohol (IPA), methanol (CH₃OH), p-benzoquinone (p-BQ), and ferric chloride (FeCl₃) served as sacrificial agents for hydroxyl radicals ($\bullet\text{OH}$), holes (h^+), superoxide radicals ($\bullet\text{O}_2^-$), and electrons (e^-), respectively[45]. As presented in Fig. 5f, the photocatalytic U(VI) reduction efficiency of 3%MoPS₃-CdS is markedly suppressed in the presence of p-BQ and FeCl₃, suggesting that $\bullet\text{O}_2^-$ and electrons play dominant roles during the photocatalytic process.

Electron paramagnetic resonance (EPR) spectroscopy was employed to investigate the generation of reactive species and the behavior of photogenerated electrons. 5,5-Dimethyl-1-

pyrroline N-oxide (DMPO) was used as a spin-trapping agent to identify oxygen-centered radicals, including $\bullet\text{O}_2^-$ and $\bullet\text{OH}$. The changes in electron-related EPR signals were further analyzed to evaluate the behavior of photogenerated electrons during the photocatalytic process. The EPR spectra were recorded under dark conditions and after visible-light irradiation for 10 min.

As shown in Figure 5g-i, no characteristic EPR signals corresponding to $\bullet\text{OH}$ or $\bullet\text{O}_2^-$ radicals were detected for the 3% MoPS₃-CdS Schottky-type heterojunction under dark conditions, whereas a strong electron-related signal was detected. Upon visible-light irradiation for 10 min, the EPR signal of $\bullet\text{O}_2^-$ increased markedly, while the electron signal exhibited a significant decrease. This electron-related signal is tentatively associated with localized or trapped photogenerated electrons. In

contrast, the signal intensity of $\bullet\text{OH}$ did not show any significant change after exposure to light. The decrease in the electron-related signal accompanied by the emergence of the $\bullet\text{O}_2^-$ signal is consistent with the participation of photogenerated electrons in dissolved O₂ reduction [46]. This interpretation is further supported by the atmosphere-control experiments, where U(VI) removal was slightly enhanced under Ar compared with air, suggesting that dissolved O₂ competes with U(VI) for a fraction of the photogenerated electrons. Collectively, these results suggest that photogenerated electrons are effectively involved in the reduction of dissolved O₂ to generate $\bullet\text{O}_2^-$ radicals [47], whereas $\bullet\text{OH}$ radicals play a negligible role in the photocatalytic process.

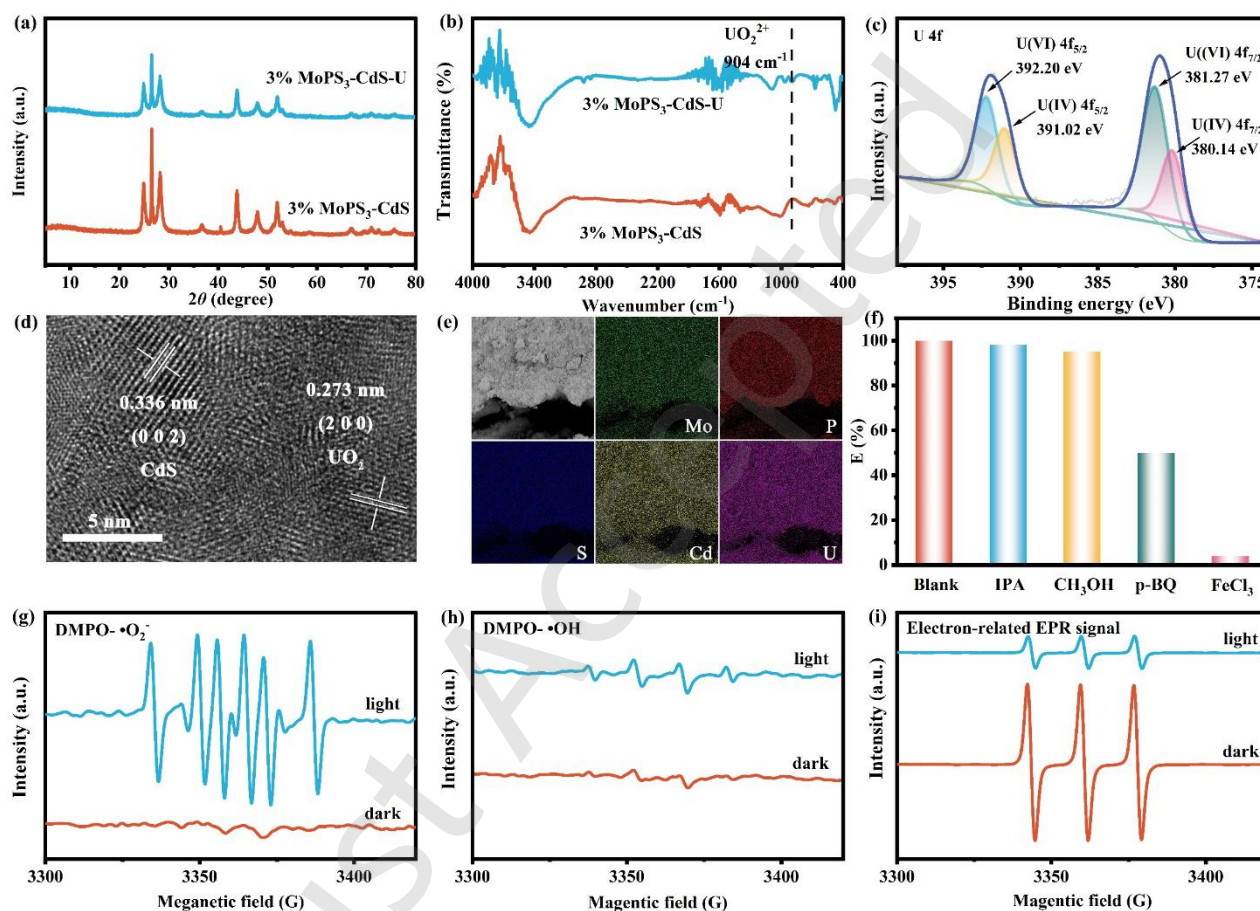


Figure 5. (a) XRD patterns of 3%MoPS₃-CdS-U; (b) FTIR spectra of 3%MoPS₃-CdS-U and 3%MoPS₃-CdS; (c) High-resolution XPS spectra of U 4f for 3%MoPS₃-CdS-U; (d) HRTEM, and (e) EDS mapping of 3%MoPS₃-CdS-U; (f) Effect of different scavengers on the photocatalytic reduction of U(VI). EPR spectra of (g) $\bullet\text{O}_2^-$, (h) $\bullet\text{OH}$ and (i) electron-related signals for the MoPS₃-CdS heterostructure under dark and light irradiation conditions.

To evaluate the efficiency of charge separation and transfer, photoelectrochemical measurements were carried out. The transient photocurrent profiles of MoPS₃, CdS, and MoPS₃-CdS under periodic visible-light illumination are presented in Figure 6a. Compared with pristine MoPS₃ and CdS, the MoPS₃-CdS composite delivers a much stronger photocurrent response, implying more efficient interfacial charge migration within the heterostructure[48, 49]. EIS measurements were conducted to evaluate the interfacial electron-transfer behavior of the photocatalysts. In the Nyquist plots, a reduced semicircle diameter generally reflects lower charge-transfer resistance and faster carrier transport. As shown in Figure 6b, MoPS₃ exhibits a lower charge-transfer resistance, attributed to its superior electrical conductivity and efficient carrier transport capability. Additionally, the smaller radius of MoPS₃-CdS compared to CdS suggests that the loading of MoPS₃ nanosheets enhances photogenerated charge separation efficiency. The PL spectra

(Figure 6c) show that the emission intensity of the heterostructure is significantly lower than that of pure CdS. This pronounced difference indicates that the introduction of MoPS₃ may effectively suppress the recombination of photogenerated electron-hole pairs, thereby promoting charge separation in the heterostructure[50].

The semiconductor characteristics and band structures of CdS and MoPS₃ were investigated by Mott-Schottky analysis and X-ray photoelectron spectroscopy (XPS) valence band spectra. As shown in Figure S8, both CdS and MoPS₃ exhibit positive slopes in the Mott-Schottky plots, indicating their n-type semiconductor characteristics[51]. The flat-band potentials of CdS and MoPS₃ are estimated to be approximately -0.84 and -0.52 V (vs. NHE), respectively. For n-type semiconductors, the flat-band potential can be regarded as an approximation of the conduction band edge. Furthermore, the valence band (VB) positions determined from XPS valence band spectra (Figure S9)

are 1.55 and 1.15 V for CdS and MoPS₃, respectively. Combining the bandgap values obtained from UV-vis diffuse reflectance spectra, the corresponding conduction band positions of CdS and MoPS₃ can be determined. The calculated conduction bands of both components are sufficiently negative compared with the reduction potentials of $\text{UO}_2^{2+}/\text{UO}_2$ (+0.411 V) and $\text{UO}_2^{2+}/\text{U}^{4+}$ (+0.267 V), demonstrating the thermodynamic feasibility of U(VI) photoreduction. These results reveal the suitable band alignment between CdS and MoPS₃, providing a favorable basis for interfacial charge migration in the 2D-1D MoPS₃-CdS heterostructure.

Femtosecond transient absorption (fs-TAS) spectroscopy was employed to track the photogenerated carrier dynamics of CdS and 3%MoPS₃-CdS under 400 nm excitation[52, 53]. Pure CdS exhibits a negative transient signal around 500–510 nm (Figure 6d), which can be tentatively associated with a ground-state bleaching related response. Upon incorporation of MoPS₃, this feature is substantially suppressed, while the dominant signal shifts to 405 nm (Figure 6g). This apparent blue shift does not

necessarily reflect a shift of the original band but rather a change in the dominant transient response. Because this region is close to the 400 nm excitation wavelength, pump-probe spectral overlap and coherent effects may also contribute to the observed signal; therefore, it is not assigned to a specific carrier species. The TA spectra extracted at representative delay times (Figure 6e and 6h) show that the transient signal decays more rapidly in the Schottky-type heterojunction, consistent with the opening of an additional charge-transfer channel. Kinetic analysis at single wavelengths (Figure 6f and 6i) further quantifies this difference: triple-exponential fitting yields shortened lifetimes across all three components for the Schottky-type heterojunction ($\tau_1 = 2.02$ ps, $\tau_2 = 35.05$ ps, $\tau_3 = 542.54$ ps vs. 4.78 ps, 192.49 ps, and 4341.54 ps for pure CdS)[54]. The pronounced reduction of the long-lived τ_3 component is consistent with efficient charge extraction, suggesting that photogenerated carriers are spatially separated before significant recombination occurs. This ultrafast charge separation process is expected to enhance the availability of photogenerated electrons for photocatalytic U(VI) reduction.

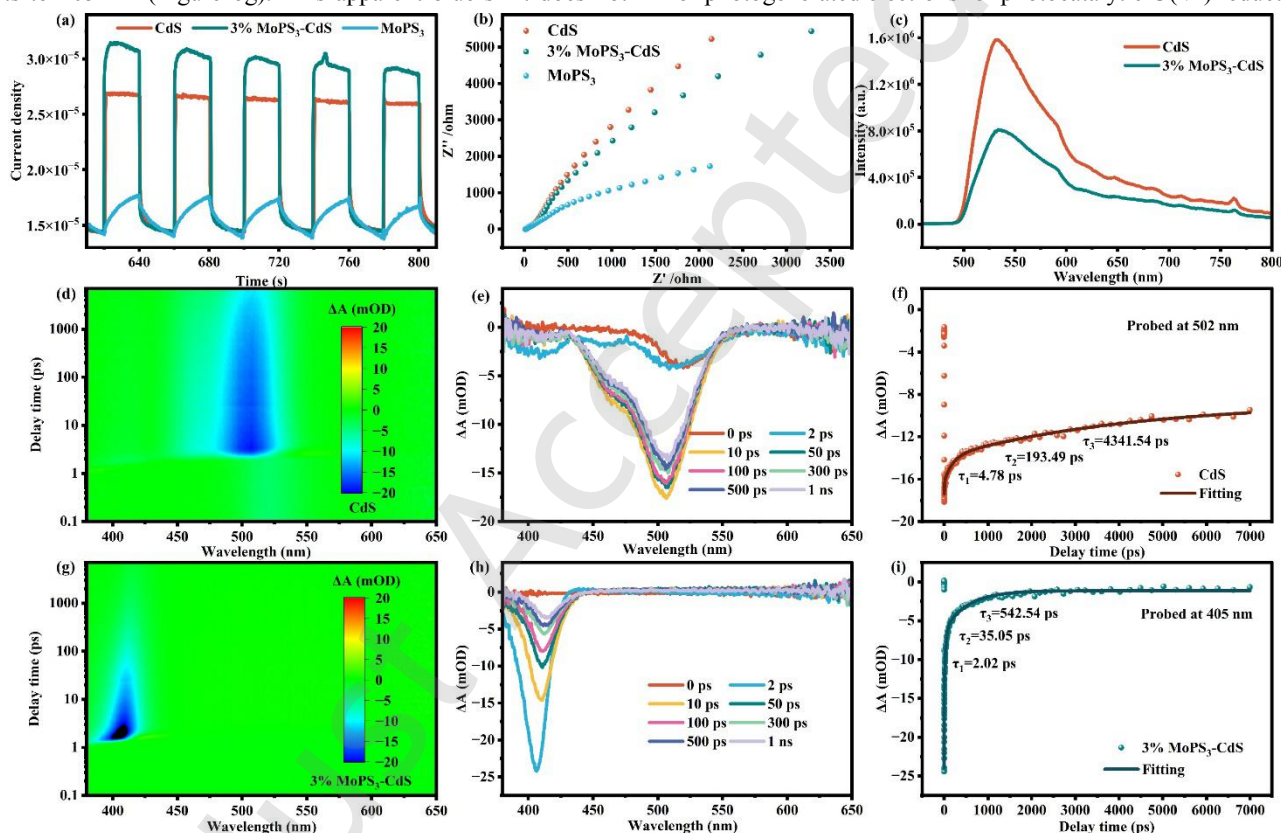


Figure 6. (a) Transient photocurrent responses, (b) Nyquist plots, and (c) steady-state PL spectra of CdS, MoPS₃, and 3%MoPS₃-CdS. Two-dimensional TA contour maps recorded for (d) CdS and (g) 3%MoPS₃-CdS. Corresponding fs-ps TA dynamic spectra are presented in (e) and (h). Normalized ground-state bleaching (GSB) decay kinetics of (f) CdS and (i) 3%MoPS₃-CdS.

To gain further insight into the interfacial electronic interaction of the MoPS₃-CdS heterostructure, DFT calculations were carried out. The calculated density-of-states (DOS) profiles of CdS and MoPS₃ are presented in Figure 7a and 7b. CdS presents a typical semiconductor band structure, with its valence band (VB) primarily attributed to S orbitals and the conduction band (CB) originating from the Cd orbital. The VB of MoPS₃ is composed of Mo and S orbitals, while the CB is primarily contributed by the Mo orbital. Furthermore, the DOS of the 3%MoPS₃-CdS heterostructure (Figure 7c) reveals strong orbital hybridization among Mo, P, Cd, and S in both the CB and VB, suggesting strong electronic interaction at the interface[55]. To clarify the interfacial electron-transfer characteristics of the MoPS₃-CdS heterostructure, the work functions (W_F) of CdS and MoPS₃ were calculated. The W_F represents the energy

required for electrons to escape from the Fermi level to the vacuum level. Therefore, a smaller W_F generally implies easier electron extraction and transfer[56]. As presented in Figure 7d and 7e, the calculated W_F of CdS and MoPS₃ are 4.23 and 5.49 eV, respectively. The corresponding Fermi levels are -2.79 and -3.48 eV, respectively. The difference in W_F and Fermi level favors electron transfer from CdS to MoPS₃ upon contact, driving Fermi-level equilibration[57]. This charge-transfer direction is further supported by the charge-density-difference calculation[58], which shows an electron transfer of approximately 0.32 e^- from CdS to MoPS₃ at the interface. The planar-averaged charge-density-difference profile of the MoPS₃-CdS heterostructure (Figure 7f) demonstrates pronounced interfacial electron redistribution, where the CdS region becomes electron-deficient while electron enrichment is

observed on the MoPS₃ side[59]. These results demonstrate pronounced interfacial charge redistribution, which can generate an associated electrostatic driving force.

Based on the above analyses, the interfacial charge-transfer process in the MoPS₃-CdS Schottky-type heterojunction is illustrated in Figure 7g. Due to the lower calculated work function of CdS (4.23 eV) compared with MoPS₃ (5.49 eV), electrons spontaneously migrate from CdS to MoPS₃ due to the difference in work functions, leading to interfacial charge redistribution[60]. Herein, “Schottky-type heterojunction” refers to the work-function-driven interfacial electronic structure and directional charge-transfer characteristics. Upon visible-light

irradiation, electrons in CdS are excited from the VB to the CB, leaving photogenerated holes in the VB. Under the influence of the interfacial electrostatic driving force, the photogenerated electrons in the CB of CdS are expected to migrate toward MoPS₃, which acts as an electron sink to participate in the reduction reaction. Meanwhile, the photogenerated holes are effectively retained in the VB of CdS for oxidation reactions. The preceding analysis suggests that the Schottky-type heterojunction formed by the introduction of MoPS₃ contributes to enhanced charge separation and improved photocatalytic performance and stability.

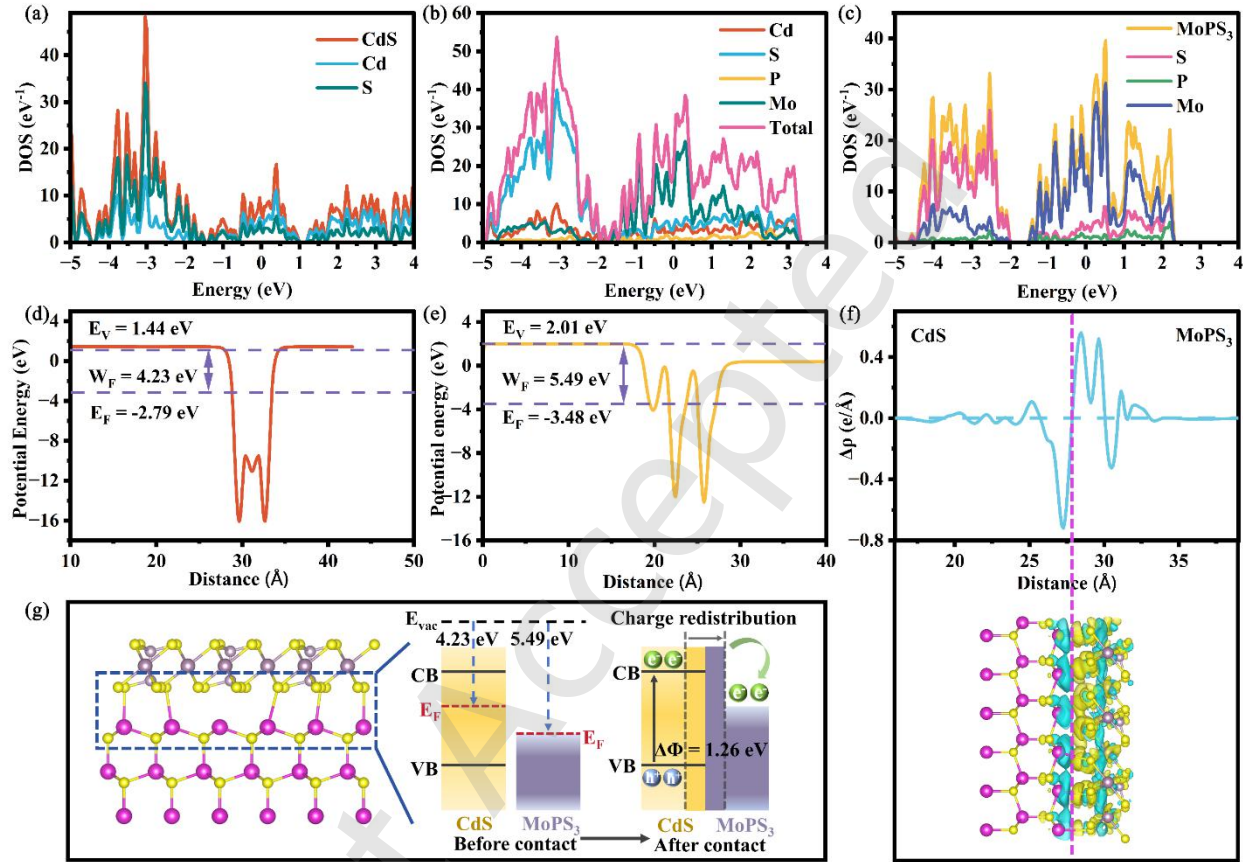


Figure 7. (a-c) Total density of states (TDOS) of CdS, MoPS₃-CdS, and MoPS₃. (d, e) Electrostatic potential distributions of CdS and MoPS₃ surfaces. (f) Planar-averaged charge density difference along the z-axis calculated from DFT. (g) Interfacial charge redistribution and electron transfer in the MoPS₃-CdS heterojunction.

Based on the above analysis and theoretical results, a possible charge-transfer mechanism associated with the Schottky-type heterojunction is proposed to explain the enhanced photocatalytic activity of the MoPS₃-CdS heterostructure. As illustrated in Fig. 8, upon light irradiation, CdS is excited to generate electron-hole pairs. The W_F difference and interfacial charge redistribution create an interfacial electrostatic driving force that drives the photogenerated electrons from the CdS conduction band (CB) to MoPS₃. The photogenerated electrons accumulated on MoPS₃ provide a favorable thermodynamic driving force for U(VI) reduction. The electrons accumulated on MoPS₃ reduce U(VI) through two parallel pathways. On one hand, electrons on the MoPS₃ surface directly transfer to the adsorbed U(VI) species, converting them into insoluble U(IV). On the other hand, a fraction of the electrons react with dissolved oxygen to generate superoxide radicals ($\cdot\text{O}_2^-$), which may act as additional reactive species and further facilitate the reduction of U(VI). Thus, the WF-driven interfacial charge

redistribution and the resulting electrostatic driving force facilitate directional charge transfer and spatial charge separation, thereby contributing to the enhanced photocatalytic U(VI) reduction and improved stability of the MoPS₃-CdS heterostructure. The main possible processes can be described as follows:



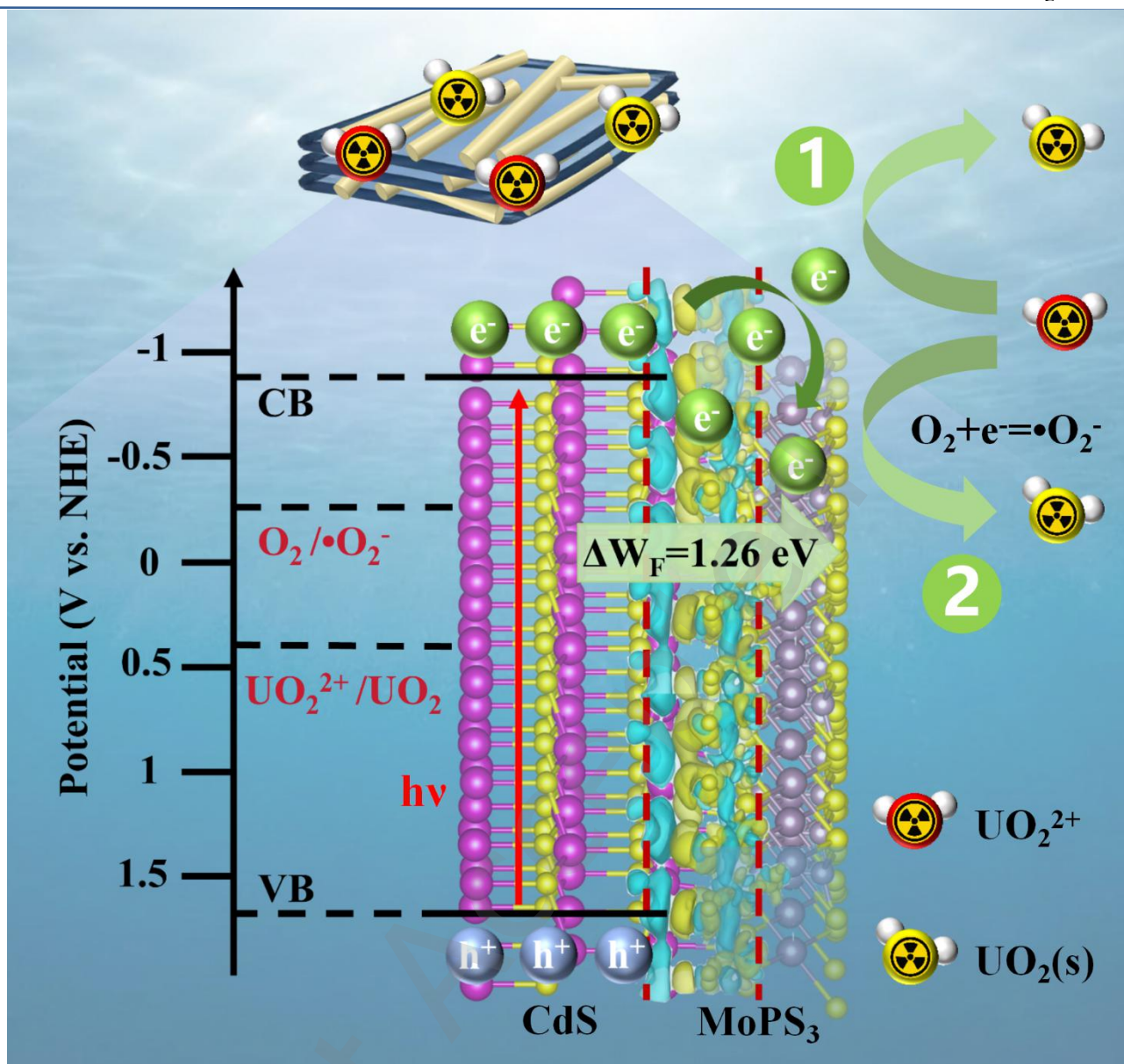


Figure 8. Proposed mechanisms for the photocatalytic reduction of U(VI) over the MoPS₃-CdS Schottky-type heterojunction.

4 Conclusion

This work demonstrates the successful construction of a MoPS₃-CdS heterostructure with a Schottky-type interfacial charge-transfer mechanism for efficient visible light driven U(VI) reduction. The integration of CdS nanorods with layered MoPS₃ nanosheets facilitates interfacial charge transfer, leading to enhanced separation of photogenerated carriers. As a result, the optimized 3%MoPS₃-CdS heterostructure achieves 99.3% U(VI) removal within 15 min, with a kinetic rate constant of 0.6493 min⁻¹, which is 12.4 and 811.6 times higher than those of pure CdS and MoPS₃, respectively. The MoPS₃-CdS heterostructure also maintains over 95% removal efficiency after five cycles, and maintains high performance across a wide U(VI) concentration range (20-200 ppm) and in the presence of coexisting ions. Mechanistic investigations and DFT calculations suggest that the favorable band alignment between CdS and MoPS₃, together with W_F-driven interfacial charge redistribution, promotes efficient electron transfer and suppresses charge recombination. Photogenerated electrons and superoxide radicals are suggested to be the primary active species responsible for U(VI) reduction. These findings highlight the great potential of MoPS₃-based heterostructures for

efficient uranium-containing wastewater remediation. This work provides a new strategy for designing efficient sulfide-based heterojunction photocatalysts for uranium recovery and environmental remediation.

Electronic Supplementary Material: Supplementary material (further details of materials, characterization of catalysts, analytical methods, and other experimental figures) is available in the online version of this article at <https://doi.org/10.26599/NR.2026.94909215>.

Data availability

All data needed to support the conclusions in the paper are presented in the manuscript and the Electronic Supplementary Material. Additional data related to this paper may be requested from the corresponding author upon request.

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Declaration of competing interest

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

Author contribution statement

Use of AI statement

None.

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Steering interfacial charge transfer via 2D-1D MoPS₃-CdS heterojunctions for highly efficient visible-light-driven uranium(VI) remediation

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Characterization of Materials

The crystal structure of the samples was characterized by X-ray diffraction (Rigaku SmartLab SE), and Fourier-transform infrared spectroscopy (Thermo Scientific iS20) was employed to analyze the functional groups of the materials. Elemental chemical states and band structures were determined using X-ray photoelectron spectroscopy (Thermo Scientific K-Alpha), while the specific surface area and porosity were evaluated by nitrogen adsorption-desorption experiments (Quantachrome EVO). Scanning electron microscopy (TESCAN MIRA LMS) and high-resolution transmission electron microscopy (JEEM-F200) were used to examine the morphology and microstructure of the samples. Ultraviolet-visible diffuse reflectance spectroscopy (PE Lambda750) and photoluminescence spectroscopy (Edinburgh FLS1000) were applied to investigate the optical absorption properties and the recombination behavior of photogenerated carriers. The photoelectrochemical performance of the materials was measured with an electrochemical workstation (CHI760E), electron spin resonance spectroscopy (Bruker EMXplus) was employed to detect radicals, and the concentrations of uranium and other ions were quantified by inductively coupled plasma atomic emission spectroscopy (ICPE-9820).

DFT Calculations

All first-principles calculations were performed using the Vienna Ab initio Simulation Package (VASP). The electron-ion interactions were treated with the projector augmented wave (PAW) method, and the exchange-correlation functional was described using PBE-GGA. The energy cutoff was set to 500 eV, and the self-consistent calculations were converged to 10^{-5} eV in energy and 0.02 eV/Å in force^[1].

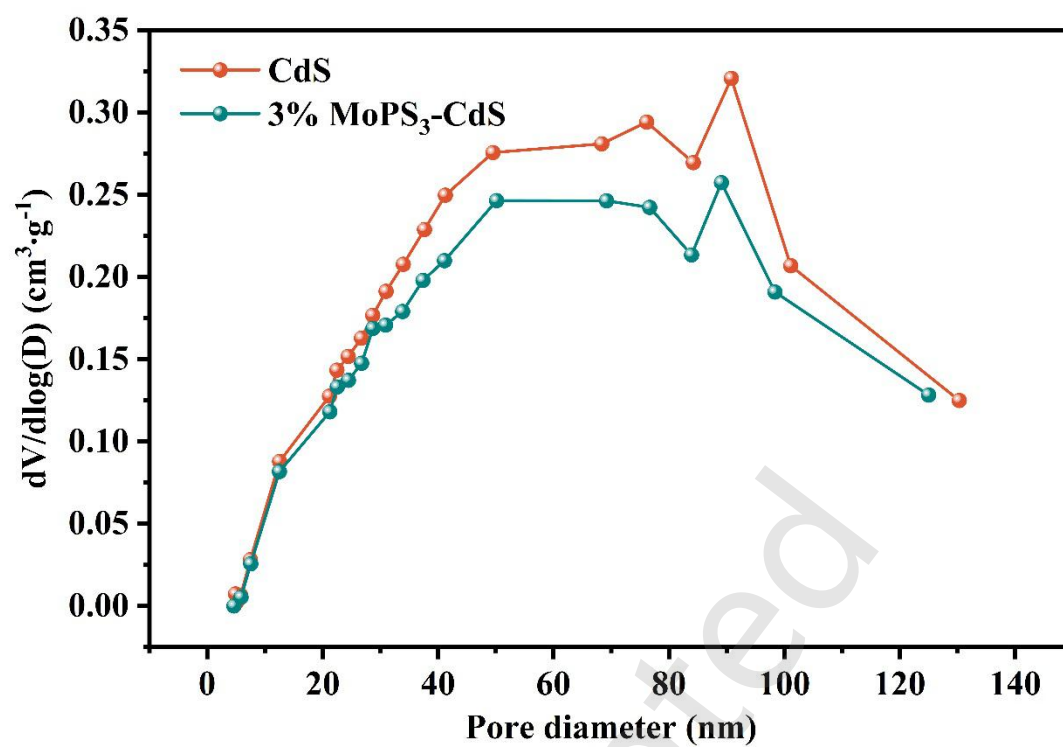


Figure S1. BJH pore size distribution of CdS and MoPS₃-CdS.

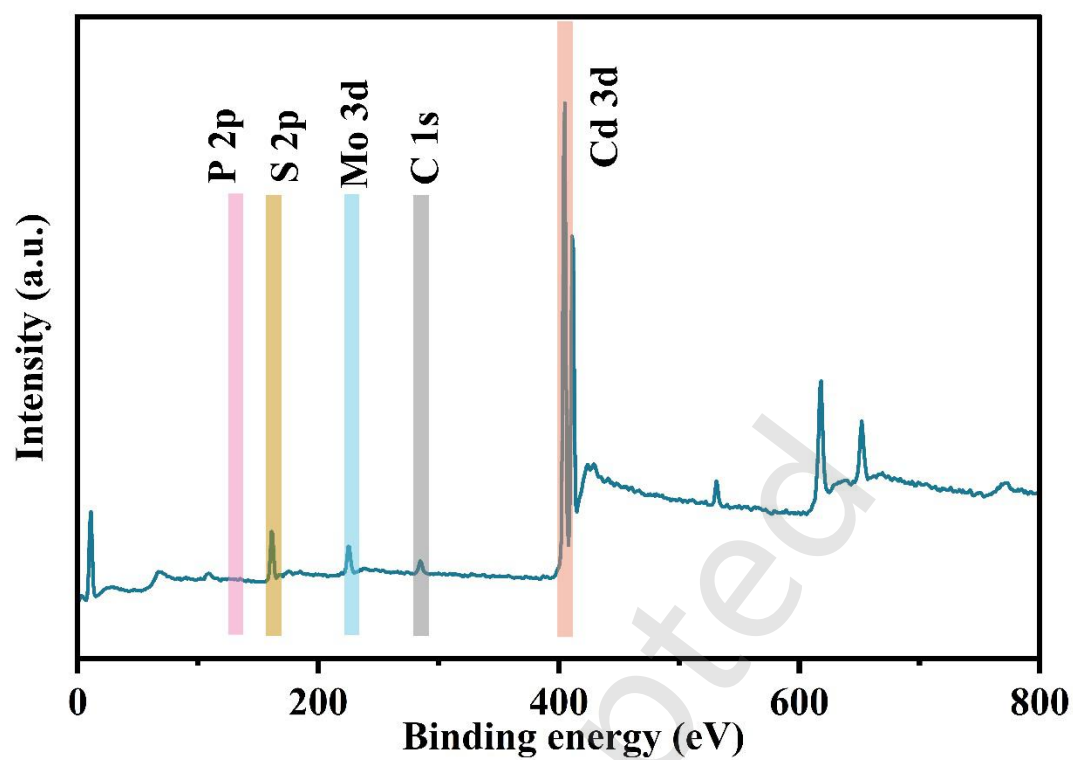


Figure S2. XPS survey spectrum of the MoPS₃-CdS composite.

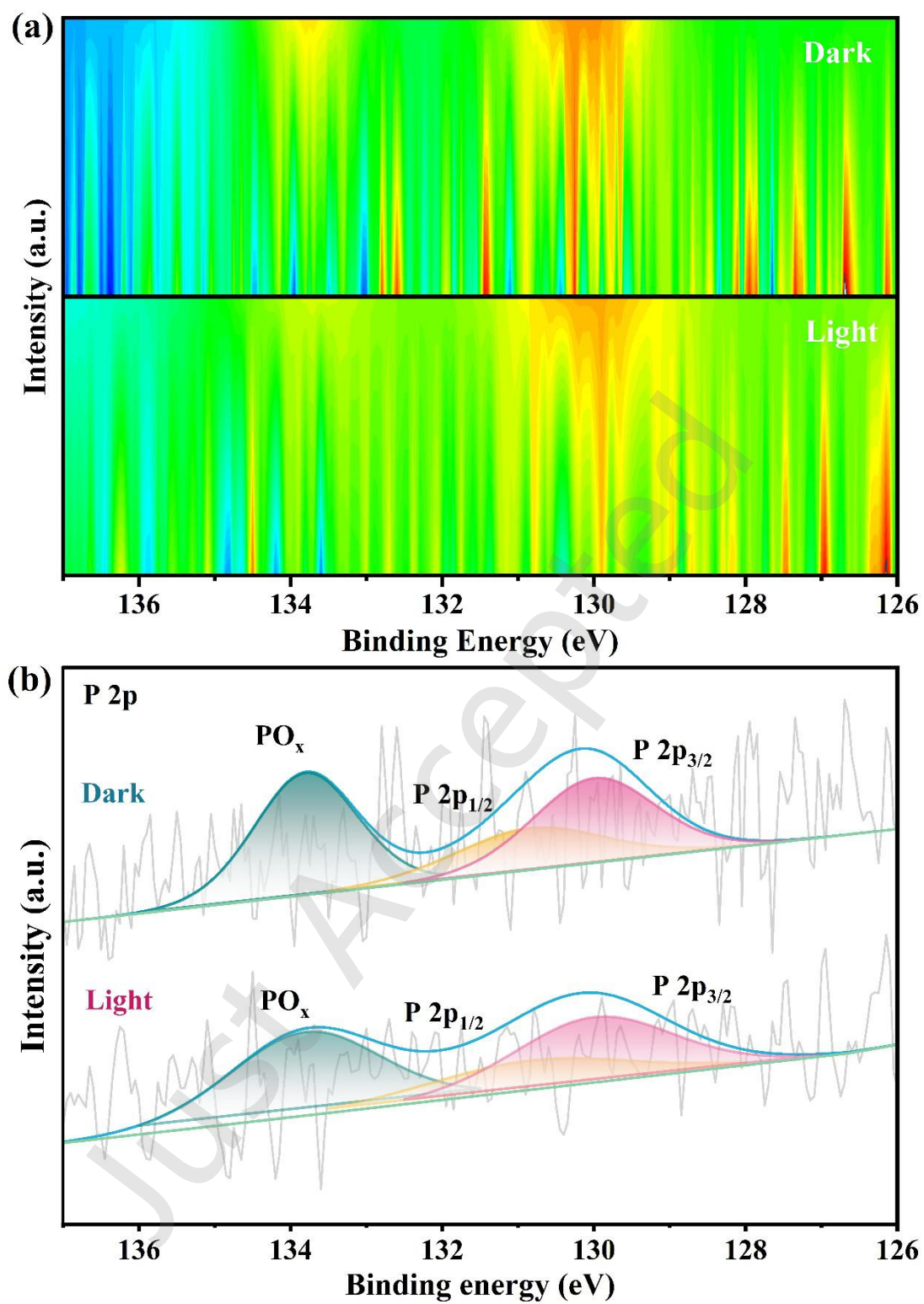


Figure S3. The in situ high-resolution XPS spectrum of (a), (b) P2p.

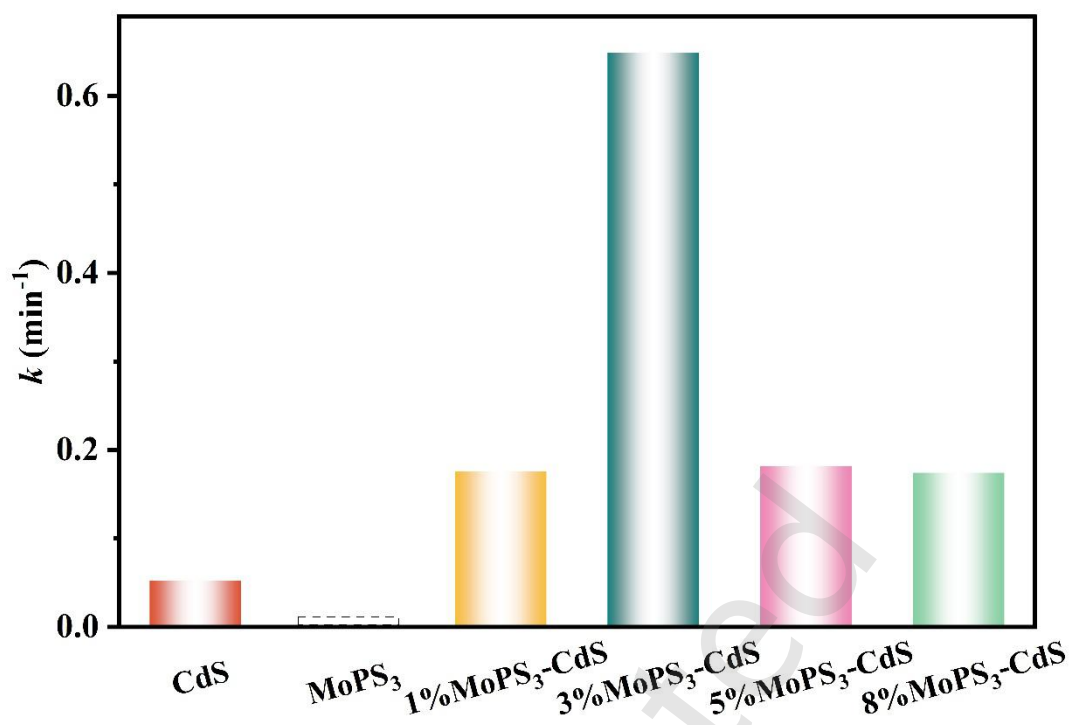


Figure S4. Comparison of the apparent rate constants for U(VI) reduction over CdS, MoPS₃, and MoPS₃-CdS

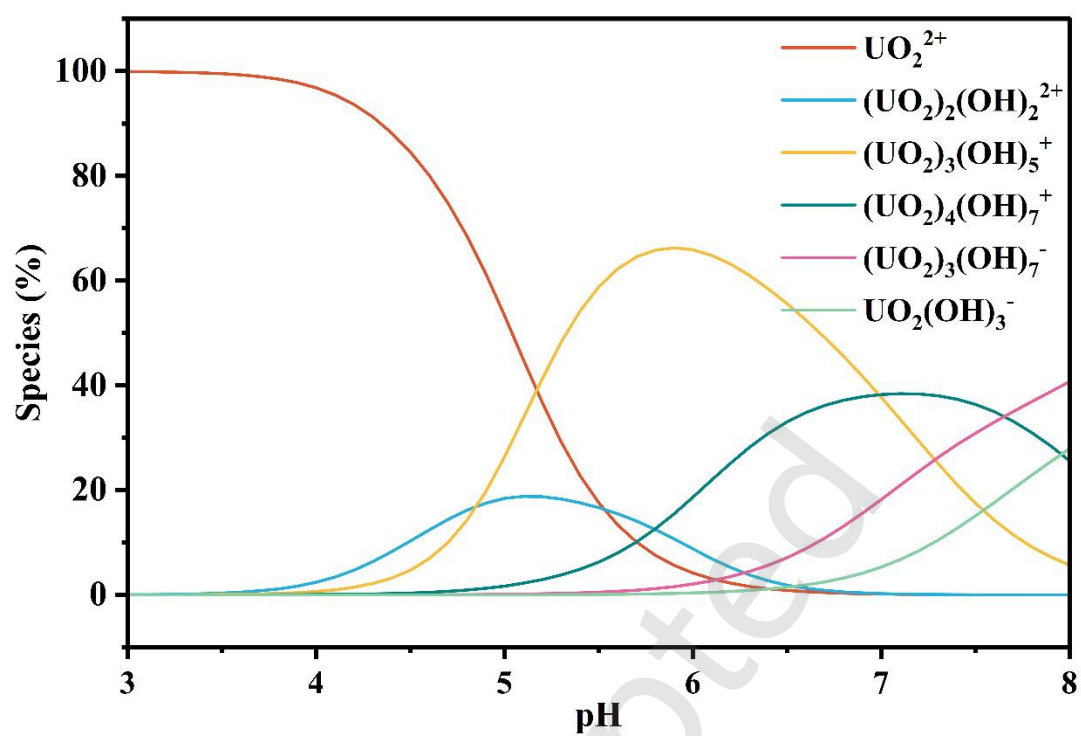


Figure S5. Calculated distribution of U(VI) species as a function of pH (3-8).

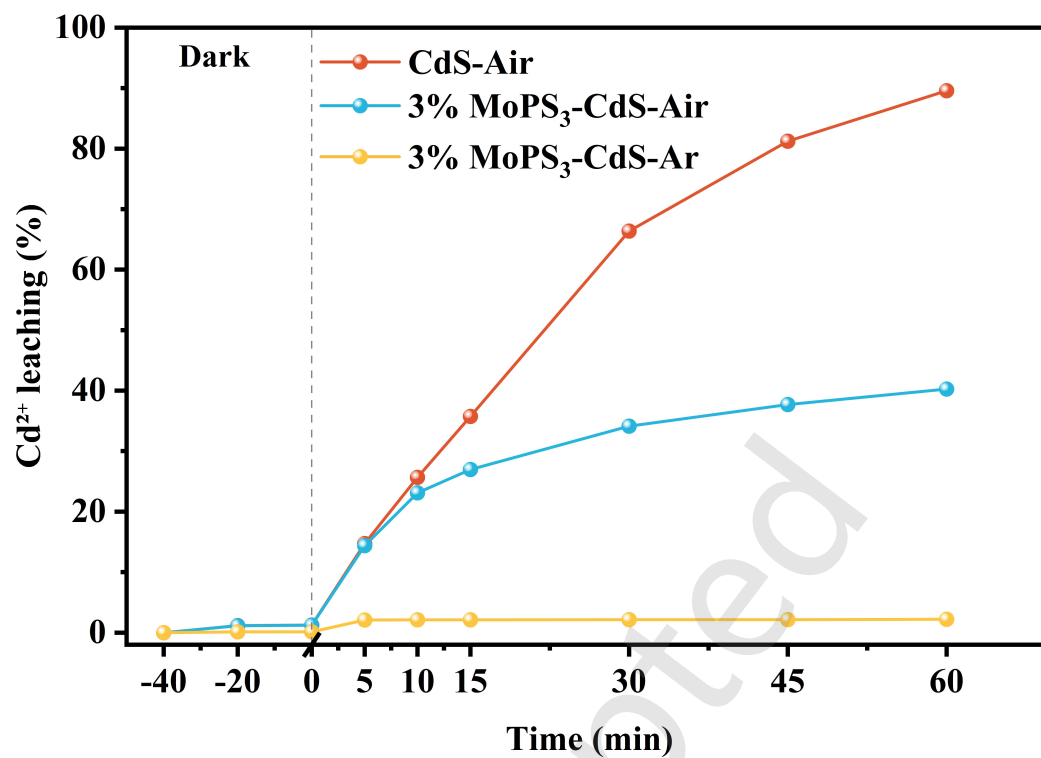


Figure S6. Cd^{2+} leaching behavior of CdS and 3% MoPS_3 -CdS under air and Ar atmospheres.

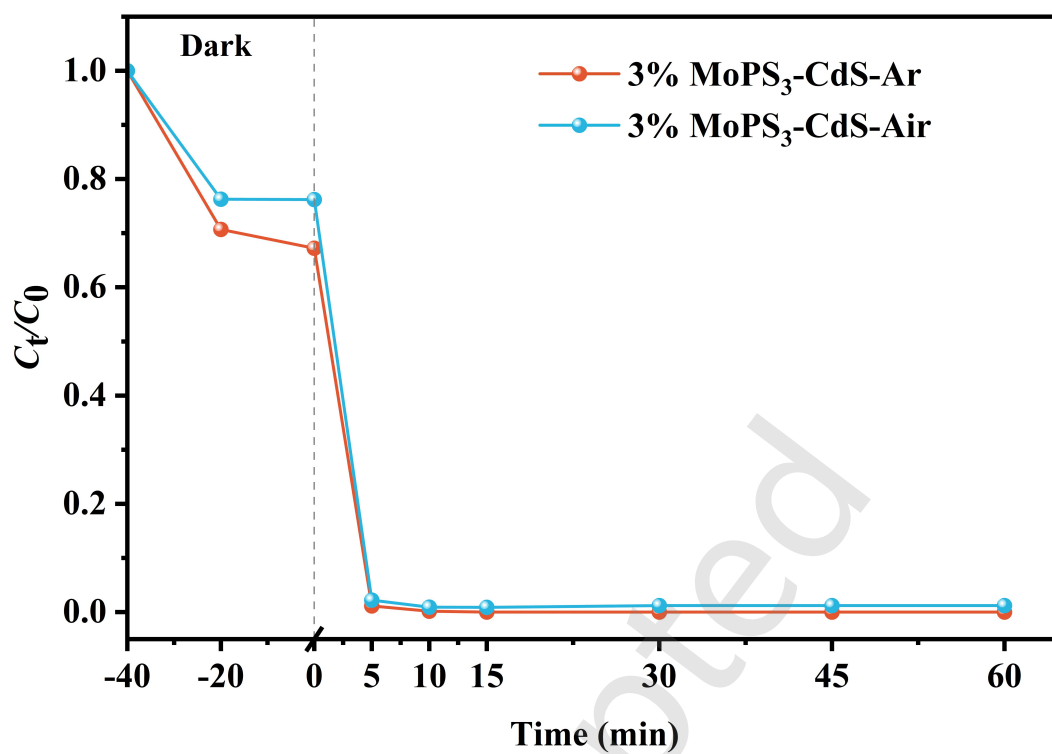


Figure S7. U(VI) removal behavior of 3% MoPS₃-CdS under air and Ar atmospheres.

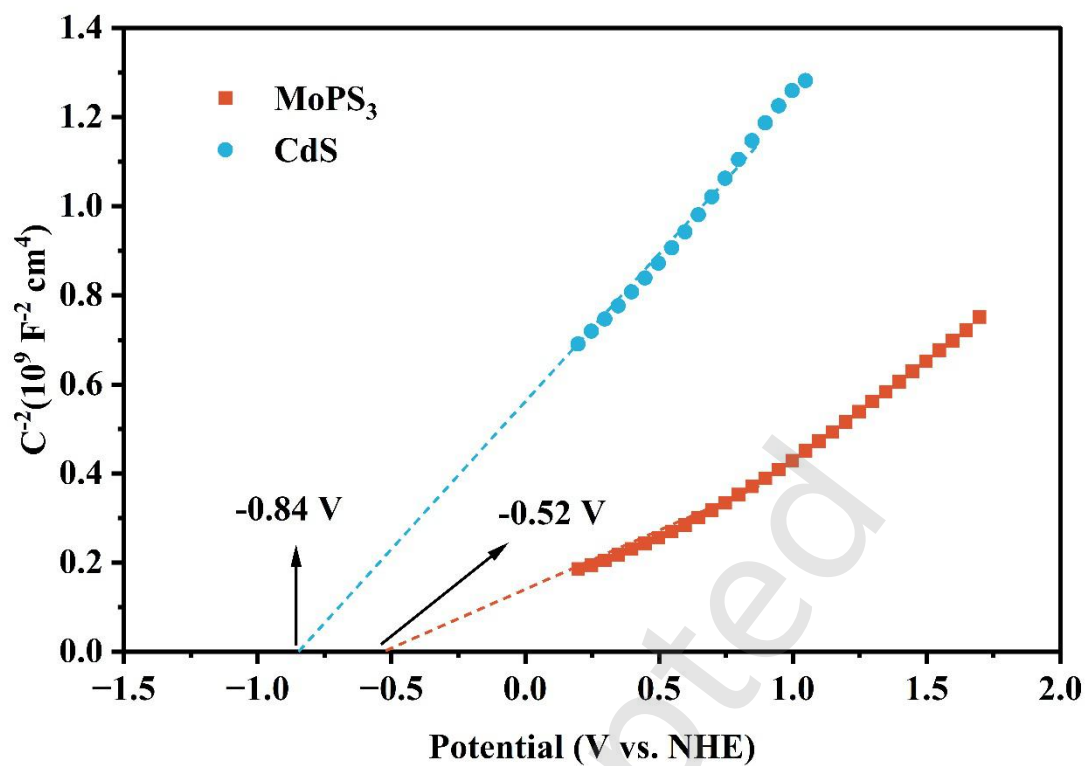


Figure S8. Mott-Schottky plots of MoPS₃ and CdS.

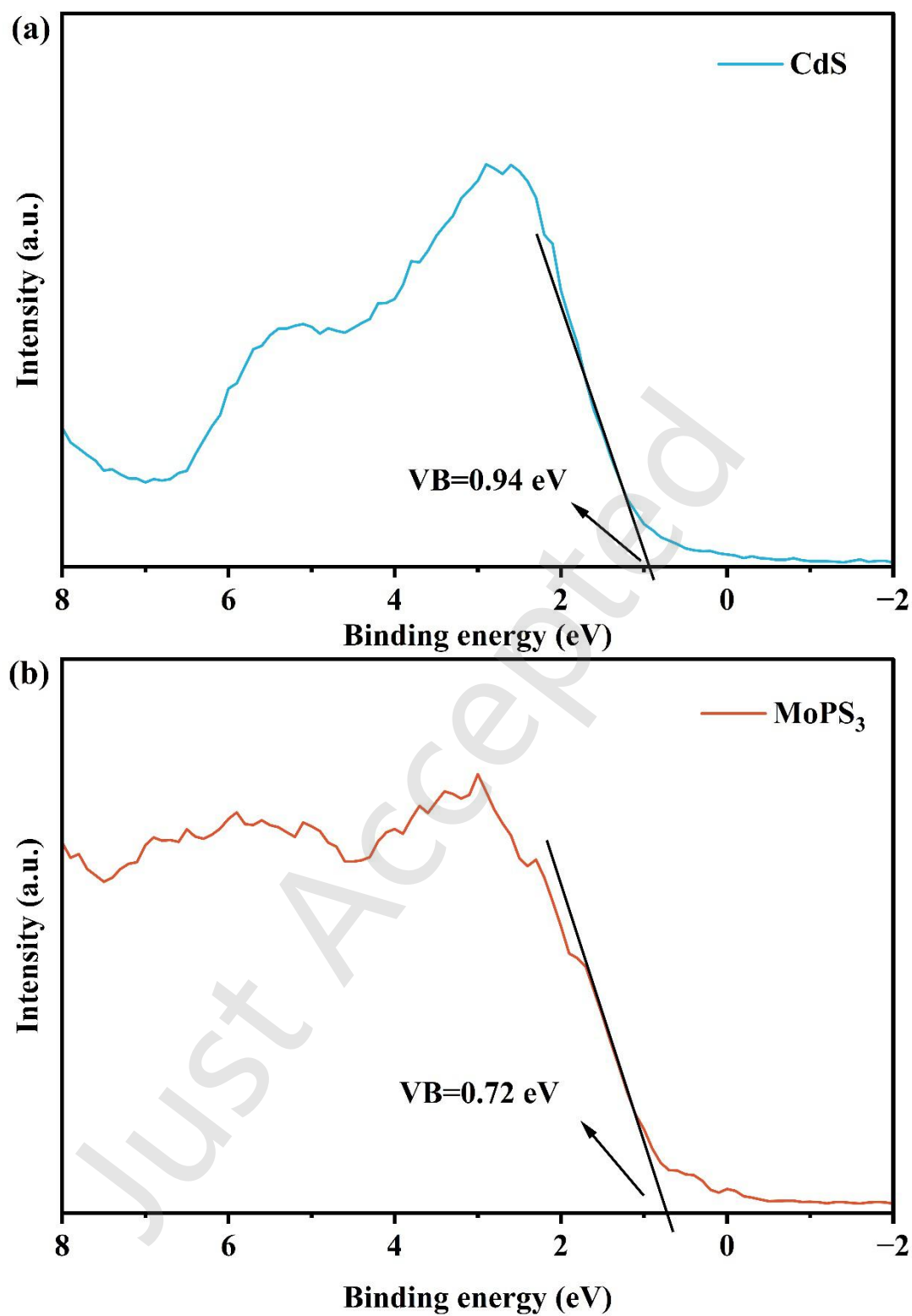


Figure S9. Valence band XPS spectrum of (a) CdS, (b) MoPS₃.

Table S1. Comparison of recently reported photocatalysts for U(VI) reduction.

Photocatalyst	Initial $C_{U(VI)}$ (ppm)	Catalyst dosage (g/L)	Time (min)	Light source	pH	Removal rate	Ref.
Gd(OH) ₃ /Cd _{0.8} Zn _{0.2} S	50	0.2	180	Visible light	6.0	95.2%	[2]
NiS@CdS-0.33	50	1	90	Solar light	5.2	98.6%	[3]
ZnS/WO ₃	50	0.3	120	Visible light	6.0	98%	[4]
CNNS@CdS	50	0.3	120	Visible light	5.0	95.7%	[5]
MoS ₂ /P-g-C ₃ N ₄	50	1	60	Visible light	5.0	99.7%	[6]
CdS H/CdS_C@PB	50	0.5	60	Visible light	8.5	98.5%	[7]
HCN-NH ₃	50	0.2	120	Visible light	4.0	95.4%	[8]
g-C ₃ N ₄ @ZnIn ₂ S ₄	50	0.1	22	Visible light	7.0	97.4%	[9]
3%MoPS₃-CdS	50	0.25	15	Visible light	6.0	99.3%	This work

Table S2. U(VI) removal performance of 3% MoPS₃- CdS in the absence and presence of mixed coexisting ions.

System	U(VI) removal at 15 min (%)
3%MoPS ₃ -CdS	99.3%
3%MoPS ₃ -CdS + mixed ions	79.1%
Mixed ions: Na ⁺ , Ca ²⁺ , Mg ²⁺ , Cl ⁻ , NO ₃ ⁻ , and SO ₄ ²⁻ .	

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