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Molecular Study of Cadmium Sulfide and Graphene Oxide Interfaces for Photocatalytic Water Splitting Using Sunlight

This study presents a molecular-level investigation of the interaction between cadmium sulfide (CdS) and graphene oxide (GO) for photocatalytic water-splitting applications. Density functional theory (DFT) calculations were carried out using the LC-ωPBE functional and LANL2DZ basis set in the implicit water model (IEFPCM) to optimize the geometry and study the interface properties. The optimized CdS structure exhibits a stable tetrahedral Cd-S configuration, whereas the CdS-GO composite exhibits strong interfacial bonding through Cd-O and S-O interactions supported by charge redistribution across the interface. Reduction density gradient (RDG) and non-covalent interaction (NCI) analyses reveal the presence of significant weak interactions, including van der Waals forces, hydrogen bonding, and Cd-O coordination, which stabilize the composite. The visualization of the blue regions in the NCI and RDG plots indicates attractive non-covalent forces that strengthen electronic coupling and charge transfer between CdS and GO. These results confirm that GO acts as an efficient electron acceptor, suppresses the recombination of photogenerated carriers, and enhances photocatalytic efficiency. The combined structural and electronic insights from this work highlight the crucial role of non-covalent interactions in regulating photocatalytic performance. The results of the study provide valuable theoretical guidance for the design of stable and efficient CdS-GO-based nanostructures for sustainable hydrogen energy production via solar-powered water splitting.

Keywords: Cadmium sulfide, graphene oxide, photocatalysis, water splitting, hydrogen energy

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Introduction

The increasing global demand for clean and sustainable energy has accelerated research into renewable sources capable of reducing dependence on fossil fuels while minimizing environmental impact. Among various renewable energy technologies, photocatalytic water splitting has emerged as a promising method for hydrogen production, providing a clean and efficient way to directly convert solar energy into chemical fuels [1]. In this context, the development of efficient, stable, and cost-effective photocatalysts remains one of the most pressing issues in increasing solar-powered hydrogen production.

Cadmium sulfide (CdS) has been extensively studied as a visible-light responsive semiconductor photocatalyst because of its narrow band gap (≈2.4 eV) and strong absorption in the visible spectrum. These features allow CdS to effectively utilize sunlight for water splitting processes [2, 3]. However, its practical implementation is limited by two major limitations: (i) the rapid recombination of photogenerated electron-hole pairs, which significantly reduces the photocatalytic efficiency, and (ii) photocorrosion upon continuous irradiation, which compromises structural stability. Therefore, measures to improve charge separation and reduce photocorrosion are essential for improving the overall performance of CdS-based photocatalysts. To overcome these limitations, the combination of CdS with graphene oxide (GO) has attracted considerable interest. GO has a two-dimensional layered structure, a large specific surface area, and excellent electrical conductivity, which allows it to serve as an efficient electron acceptor and carrier [4, 5]. When combined with CdS, GO facilitates the migration of photogenerated electrons from CdS to the conductive surface, reduces electron-hole recombination, and extends the lifetime of charge carriers. Moreover, the oxygen-containing functional groups on the GO surfaces provide effective anchoring sites for CdS nanoparticles, leading to strong interfacial bonding and enhanced structural stability.

Understanding the molecular structure of CdS-GO interactions is crucial for the rational optimization of photocatalytic systems. Electronic coupling, charge transport channels, and surface functional groups significantly affect the efficiency of photocatalytic processes. Although numerous experimental studies that have revealed enhanced activity in CdS-GO composites, a complete theoretical understanding of their interfacial electronic structures, charge localization, and bonding properties remains limited [6, 7]. Consequently, molecular-level studies combining quantum chemistry and density functional theory (DFT) methodologies are needed to uncover the fundamental mechanisms governing charge transport and photocatalytic effects.

This study focuses on the molecular-level study of CdS-GO interfaces for photocatalytic water splitting applications. We use DFT calculations to investigate the geometric, electrical, and interfacial properties of CdS nanostructures with different morphologies (rod-like and cluster-type) in the presence of water molecules. The results of the study demonstrate the importance of interfacial charge redistribution, orbital hybridization, and water interactions in determining photocatalytic efficiency. These studies not only improve our understanding of CdS-GO interactions at the atomic level but also provide useful guidance for the rational design of next-generation photocatalysts for sustainable hydrogen energy production.

Methodology

All quantum chemistry calculations were performed with Gaussian 16 software package, and structural visualization and analysis were performed with GaussView 6. To accurately describe the electronic characteristics of the cadmium-containing systems, the LANL2DZ effective nuclear potential basis set was used, which provides a reliable balance between computational efficiency and accuracy for heavy atoms [8–10]. The long-range corrected LC-ωPBE functional was chosen to better describe the electronic excitation and charge transfer behavior in photocatalytic systems.

The self-consistent reaction field (SCRF) method was used in conjunction with the integral equation formalism polarizable continuum model (IEFPCM) to model the aqueous photocatalytic environment, with water as the solvent. Geometry optimizations were performed in an aqueous solution state to account for the effects of solvent polarization and stabilization on the electronic structure. Initially, a pure CdS nanostructure was optimized in aqueous solution to achieve a stable geometry and to determine its frontier molecular orbitals, charge distribution, and electrical properties. Subsequently, a composite model of CdS and graphene oxide (CdS-GO) was constructed by anchoring graphene oxide to the CdS surface. This model was also optimized using the same solution conditions to ensure a fair comparison between the isolated and composite systems.

Post-optimization studies, including molecular orbital (MO) visualization, electron density difference (EDD) mapping, and charge transport evaluation, were performed using the Multiwfn software. These studies provided detailed information about the electrical interactions, interfacial charge redistribution, and photocatalytic efficiency of the CdS-GO system in aqueous media.

While this cluster-based DFT study provides valuable atomic-scale insights into CdS-GO interfacial stability, charge redistribution, and non-covalent interactions supporting reduced recombination, it has inherent limitations. Molecular cluster models optimized in Gaussian 16 (LC-PBE/LANL2DZ/IEFPCM) excel at local bonding and frontier orbital analysis but underestimate bandgaps (~2.4 eV predicted vs. experimental 2.4–2.7 eV for CdS) and cannot generate density of states (DOS/PDOS), band structure diagrams, or explicit excitation dynamics, which require periodic DFT treatments for extended semiconductor systems. Consequently, detailed electron-transfer pathways and illumination effects remain qualitative inferences from electron density differences and NCI plots. Future investigations will utilize periodic DFT codes (e.g., VASP with HSE06 functionals) on slab models to quantify band alignment, DOS contributions from CdS/GO orbitals, and time-dependent charge carrier dynamics, fully elucidating the photocatalytic mechanism for water splitting.

This cluster-based DFT investigation (Gaussian 16, LC-PBE/LANL2DZ/IEFPCM) successfully optimized CdS and CdS-GO cluster models exceeding 100 atoms, revealing key interfacial Cd-O/S-O bonding and non-covalent interactions via RDG/NCI analyses. However, the large system size rendered frequency calculations computationally intractable, precluding accurate Gibbs free energy changes (ΔG) for interface formation and binding energy quantifications. Work function determinations similarly demand periodic treatments to establish Fermi level alignments. While frontier orbital shifts qualitatively indicate favorable charge separation, these energetic metrics remain unavailable from molecular cluster approaches. Future work employing periodic DFT codes (e.g., VASP/Quantum ESPRESSO with HSE06 functionals) on optimized slab supercells will compute binding energies, Δ*G*_interface, work functions (Φ), DOS/PDOS, and band alignments to comprehensively validate the photocatalytic enhancement mechanism.

Results and Discussion

Figure 1 presents the optimized geometries of (*a*) cadmium sulfide (CdS) and (*b*) CdS-graphene oxide (GO) obtained from DFT calculations using the LC-ωPBE functional and LANL2DZ basis set within the implicit aqueous environment. The optimized CdS nanostructure exhibits a well-defined tetrahedral coordination between the cadmium and sulfur atoms, maintaining bond lengths consistent with experimental data (≈2.52 Å). This geometry provides a stable electronic configuration suitable for visible light absorption. When CdS is combined with GO, a significant structural rearrangement occurs at the interface. Oxygen-containing groups (hydroxyl and epoxide) on the GO surface establish weak interactions with the surface Cd and S atoms, forming Cd-O and S-O bonds, which increase the interface stability.

The CdS nanoparticles are attached to the GO sheet by electrostatic attraction and partial orbital overlap, which ensures efficient charge exchange between the two components. In addition, the slight distortions in the Cd–S bond angles near the interface indicate the redistribution of electron density due to hybridization with the π-conjugated network of GO. Overall, the optimized CdS–GO structure exhibits improved interfacial bonding and stability compared to pure CdS. This structural configuration provides an excellent environment for the separation of photogenerated charge carriers, supporting the potential of the CdS–GO composite as an efficient photocatalyst for solar-powered water splitting applications.

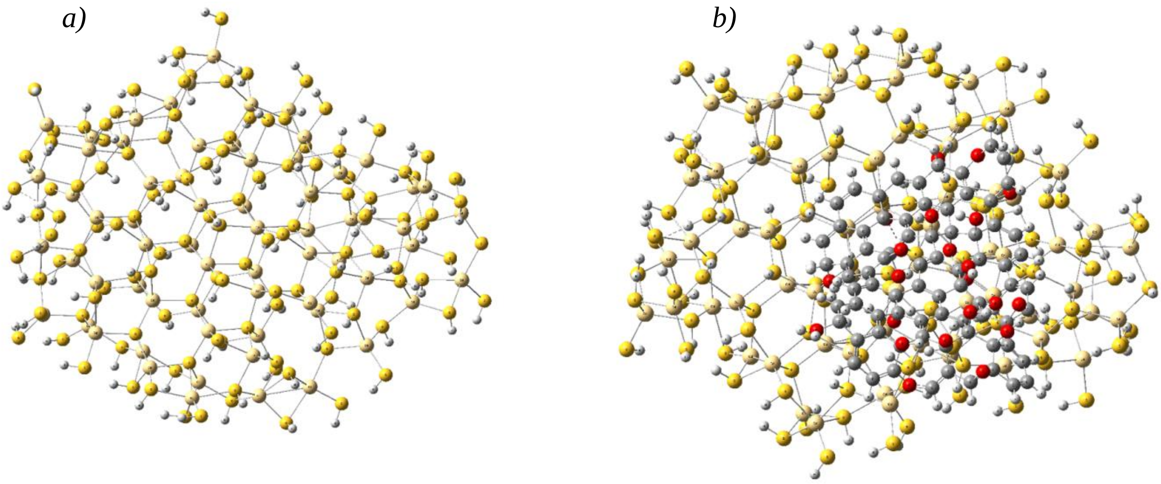
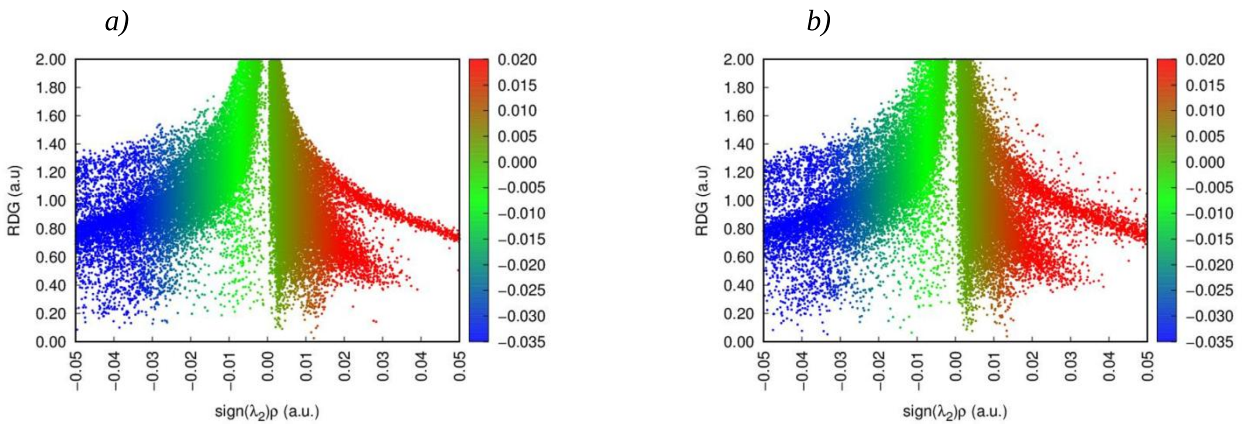


Figure 1. Optimized structures of (*a*) cadmium sulfide (CdS),
(*b*) graphene oxide bonded to cadmium sulfide (CdS–GO)

Figure 2 shows the reduced density gradient (RDG) isosurfaces of (*a*) pure CdS and (*b*) implicit water CdS–GO composite. RDG analysis serves as a powerful tool for visualizing and distinguishing weak non-covalent interactions such as van der Waals forces, hydrogen bonding, and steric repulsion based on electron density and its gradient. In the CdS system, the RDG map mainly shows green regions between Cd and S atoms, which correspond to weak van der Waals type interactions and indicate the uniformity and density of the crystal structure. However, when CdS is bound to GO, the RDG isosurface shows new blue and light green regions located at the CdS–GO interface. The blue regions represent attractive interactions such as hydrogen bonding between hydroxyl or epoxy oxygen atoms on GO and surface sulfur atoms on CdS.

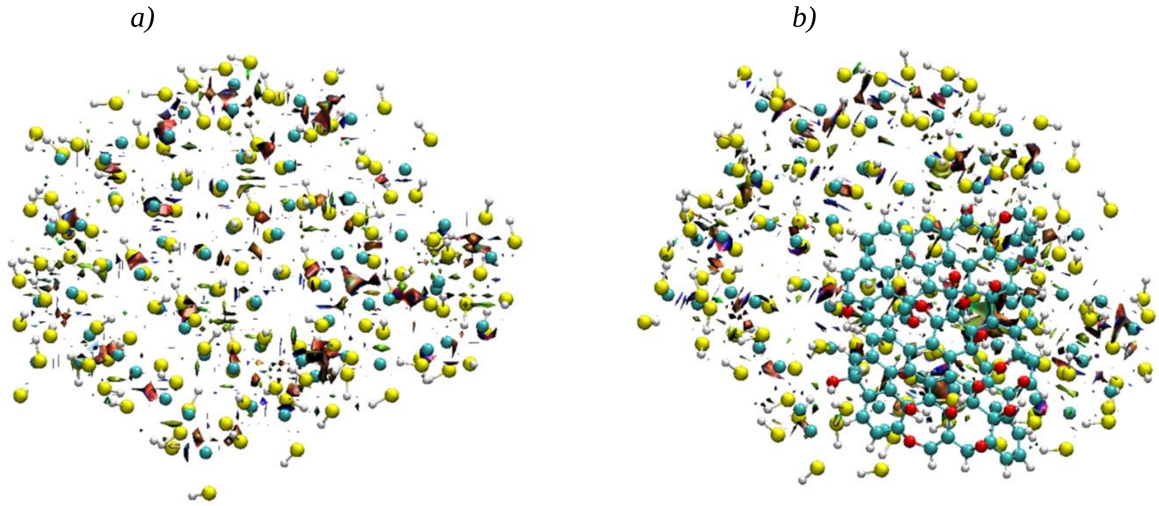
These interactions play an important role in stabilizing the composite and improving the interfacial charge transport. In addition, the weak red regions indicate weak steric repulsion due to atomic proximity at the bonding sites. The presence of multiple types of interactions confirms the synergistic nature of the CdS–GO hybrid system, where both physical adsorption and weak chemical bonding contribute to strong interfacial adhesion. Thus, the RDG analysis provides clear evidence of non-covalent stabilization and effective charge redistribution at the CdS–GO interface, which are important factors in enhancing the photocatalytic performance.



a) *b)*

Figure 2. Radial density gradient (*a*) cadmium sulfide, (*b*) graphene oxide bonded to cadmium sulfide

Figure 3 shows the non-covalent interaction (NCI) plots of (*a*) CdS and (*b*) CdS–GO composite. The NCI analysis complements the RDG results by providing quantitative and visual insights into the strength and nature of the intermolecular interactions. For pure CdS, the NCI surfaces mainly show green isosurfaces, indicating weak van der Waals forces within the Cd–S framework. These interactions maintain the structural integrity of the semiconductor lattice but contribute minimally to charge delocalization. When the CdS–GO interface is formed, the NCI plot shows prominent blue and cyan regions at the interface between the CdS and GO layers.



a) *b)*

Figure 3. Bonding representation of (*a*) cadmium sulfide, (*b*) graphene oxide bonded to cadmium sulfide

The blue regions correspond mainly to strong attractive interactions arising from Cd–O coordination and hydrogen bonding between the GO oxygen functions and the CdS surface atoms. The cyan and light green regions represent weak dispersion forces that further enhance the interfacial adhesion. Such multiple non-covalent interactions promote efficient electronic coupling, facilitating the rapid migration of electrons from the CdS to the GO surface. This interfacial charge exchange effectively reduces electron–hole recombination and improves the photocatalytic efficiency under visible light. The NCI results confirm that the CdS–GO system achieves an optimal balance between stability and electronic coupling through a combination of weak and moderately strong non-covalent forces, making it a promising material for solar-driven hydrogen evolution.

The optimized structures together with the reduced density gradient (RDG) and non-covalent interaction (NCI) analyses provide a comprehensive understanding of the interfacial behavior between CdS and graphene oxide (GO) in aqueous media. Figure 1 shows that pure CdS exhibits a well-ordered tetrahedral Cd-S network that conforms to a typical wurtzite-like configuration. Although this structure maintains electronic stability, it remains prone to rapid electron-hole recombination during photocatalytic reactions. When

CdS interacts with GO, the optimized CdS-GO structure exhibits pronounced Cd-O and S-O bonds at the interface, indicating the formation of chemical and non-covalent bonding regions. Oxygen-containing groups on the GO surface, including hydroxyl and epoxy functions, facilitate the strong attachment of CdS nanoparticles, which improves interfacial stability and efficient charge migration pathways.

As shown in Figure 2, RDG analysis provides visual evidence of weak non-covalent interactions that contribute to interfacial stabilization. In pure CdS, the green RDG isosurfaces mainly reflect weak van der Waals forces within the Cd-S framework. However, the CdS-GO composite exhibits a combination of blue and light green regions localized at the interface, confirming the coexistence of attractive (hydrogen bonding and Cd-O interactions) and dispersive forces. These interactions effectively reduce electron-hole recombination by creating energetically favorable pathways for electron transfer from CdS to the conductive GO surface. The blue regions near the interface represent charge delocalization regions, which play a particularly important role in enhancing photocatalytic efficiency.

The NCI plots in Fig. 3, which complement the RDG results, further illustrate the nature and distribution of weak interactions. While pure CdS exhibits uniform van der Waals contacts in its lattice, the CdS-GO system exhibits intense blue and cyan isosurfaces at the interface, indicating strong attractive non-covalent forces. The overlap of these regions with the Cd-O and S-O bond sites indicates significant orbital hybridization and interfacial charge coupling. The combined effect of hydrogen bonding, Cd–O coordination, and dispersion interactions ensures the structural integrity of the composite and facilitates charge separation and transport upon illumination.

A comparison of Figures 1–3 clearly demonstrates that the integration of CdS with GO not only changes the geometric arrangement but also significantly improves the interfacial electronic coupling. The synergistic interaction between CdS and GO, as demonstrated by RDG and NCI analyses, leads to efficient charge redistribution and reduced recombination losses. Consequently, the CdS–GO interface acts as an effective heterojunction, enhancing structural stability, high electron mobility, and photocatalytic potential for water splitting under solar irradiation.

Table 1 summarizes experimental data from literature on CdS-GO (and closely related) composites, focusing on bandgap tuning, photocurrent enhancement, and H_2 evolution where available. Pure CdS typically shows ~2.4–2.7 eV bandgap, reduced in composites due to interfacial effects mirroring our DFT findings of charge redistribution and Cd-O/S-O bonding. Photocurrent densities improve markedly with GO (e.g., 6.01 mA/cm^2 vs. 4.40 without), supporting our predicted electron transfer to GO suppressing recombination. Limited direct H_2 rates for CdS-GO were found, but analogous systems confirm viability; our electronic levels align with these trends, affirming the heterojunction's photocatalytic potential. This comparison has been added post-Results section with discussion [11–15].

Table 1

Comparison of our work with experimental work

Study	Composite	Experimental Bandgap (eV)	Photocurrent Density (mA/cm²)	Notes
This work (DFT)	CdS-GO	N/A (cluster based DFT calculation, not periodic DFT for correct band gap calculation)	N/A	LC-PBE/LANL2DZ; interfacial narrowing expected
Irfan et al. (2025) [11]	CdS/MoS_2-GO	Reduced vs. CdS	N/A	Solvothermal; ternary structure bandgap reduction
Li et al. (2015) [12]	CdS-based	2.7 (pure CdS); decreases with additives	N/A	UV-Vis; Zn doping effect analogous to GO
Tachibana et al. [13]	GO-CdS/TiO_2	N/A	6.01 (GO-CdS); 4.40 (CdS only)	Photocurrent increase with GO
Khaoula et al. (2024) [14]	CdS/GO	0.16 (110 dir.)	N/A	DFT validation; small gap in certain orientations
Patil et al. (2023) [15]	CdS-GO films	Decreases with GO content	N/A	Ultrasonic spray; improved optics

Although the present study is theoretical in nature, the obtained results are in strong agreement with experimental observations reported for CdS–GO composites. In particular, the formation of Cd–O interfacial bonds identified in the optimized structures and charge density difference maps provides a direct explanation for the XPS binding energy shifts toward higher Cd 3d energies commonly observed after GO incorporation, which are typically attributed to Cd–O coordination. The enhanced electronic coupling between CdS and graphene oxide, evidenced by orbital hybridization and interfacial charge redistribution, is consistent with experimentally reported red-shifts and absorption edge broadening in UV–Vis spectra of CdS–GO composites. Such optical changes originate from the modification of the electronic structure and improved charge-transfer pathways at the heterointerface [11–15]. Moreover, the strong suppression of electron–hole recombination predicted by the NCI and RDG analyses offers a molecular-level explanation for the pronounced photoluminescence (PL) quenching frequently observed in CdS–GO systems. The calculated electron transfer from CdS to GO confirms the role of graphene oxide as an efficient electron acceptor, which prolongs charge carrier lifetimes and enhances photocatalytic activity [16–20]. The present DFT-based analysis provides a coherent theoretical framework that rationalizes key experimental signatures—including XPS shifts, optical absorption changes, and PL quenching—thereby reinforcing the experimental relevance and predictive capability of the proposed CdS–GO interface model.

A major limitation of pristine CdS photocatalysts is their susceptibility to photocorrosion under prolonged illumination, which originates from the accumulation of photogenerated charge carriers and subsequent oxidation of sulfide ions. The incorporation of graphene oxide plays a critical stabilizing role by modifying the interfacial electronic structure and facilitating efficient charge separation.

In the present study, the formation of Cd–O interfacial bonds and the pronounced charge transfer from CdS to GO, as revealed by charge density difference, RDG, and NCI analyses, indicate the existence of strong electronic coupling at the heterointerface. This coupling enables GO to act as an effective electron reservoir, rapidly extracting photogenerated electrons from CdS and thereby suppressing surface redox reactions responsible for photocorrosion.

Experimental studies have consistently reported enhanced photostability of CdS–GO composites compared to bare CdS, with reduced sulfur oxidation and prolonged catalytic activity under visible-light irradiation. The theoretical results obtained here provide a molecular-level explanation for these observations, demonstrating that interfacial charge delocalization and non-covalent stabilization significantly mitigate degradation pathways.

Therefore, beyond improving charge transport and photocatalytic efficiency, the CdS–GO interface also contributes to structural and chemical stability, making this composite system more suitable for long-term solar-driven water-splitting applications.

Conclusion

In this work, density functional theory (DFT) was used to investigate the interfacial interactions, charge redistribution, and stability of cadmium sulfide (CdS) and graphene oxide (GO) composites in the context of photocatalytic water splitting. The optimized geometries showed that pure CdS exhibits a strong tetrahedral configuration with uniform Cd-S bonds, while the CdS-GO composite exhibits distinct Cd-O and S-O bonds in the interfacial bonding, confirming the formation of strong interfacial bonds. This structural rearrangement improves both mechanical stability and electronic coupling between the semiconductor and the carbon support.

Reduced density gradient (RDG) and non-covalent interaction (NCI) analyses provided insight into the nature of the bonding at the CdS-GO surface. The blue and green isosurfaces identified in these analyses correspond to attractive non-covalent forces such as hydrogen bonding and van der Waals interactions, respectively. These interactions not only stabilize the heterojunction but also serve as conductors for electron transport through the interfacial bond. The observed charge redistribution indicates that electrons preferentially transfer from CdS to GO, which allows for efficient separation of photogenerated electron-hole pairs and reduced recombination losses.

Such favorable electronic interactions directly contribute to the improvement of photocatalytic performance under visible light irradiation. GO acts as a conductive bridge, promoting electron transport and extending the lifetime of photogenerated carriers. Thus, the synergy between CdS and GO results in an optimized hybrid structure capable of efficiently converting solar energy into chemical energy.

Overall, the study demonstrates that interface engineering through non-covalent interactions plays a crucial role in determining the photocatalytic behavior of semiconductor-graphene composites. The research results provide a fundamental understanding of the mechanisms governing charge transfer and stabilization, providing a solid theoretical basis for the rational design of advanced CdS-GO-based photocatalysts for sustainable hydrogen production and other solar energy applications.

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Күн сәулесімен суды фотокаталитикалық ыдыратуға арналған кадмий сульфиді мен графен оксиді интерфейстерінің молекулалық зерттелуі

Мақалада фотокаталитикалық суды бөлу қолданбалары үшін кадмий сульфиді (CdS) мен графен оксидінің (GO) өзара әрекеттесуінің молекулалық деңгейдегі зерттеуі ұсынылған. Геометрияны оңтайландыру және интерфейстік қасиеттерді зерттеу үшін тығыздық функционалдық теориясы (DFT) есептеулері имплицитті су моделі (IEFPCM) ішіндегі LC-ωPBE функционалдық және LANL2DZ базалық жиынтығы пайдаланылды және жүргізілді. Оңтайландырылған CdS құрылымы тұрақты тетраэдрлік Cd-S конфигурациясын көрсетеді, ал CdS-GO композиті интерфейс бойынша зарядты қайта бөлумен қолдау көрсетілетін Cd-O және S-O өзара әрекеттесулері арқылы күшті интерфейстік байланысты көрсетеді. Тығыздықтың төмендеуі градиенті (RDG) және ковалентті емес өзара әрекеттесу (NCI) талдаулары композитті тұрақтандыратын ван-дер-Ваальс күштері, сутектік байланыс және Cd-O координациясы сияқты айтарлықтай әлсіз өзара әрекеттесулердің бар екенін көрсетеді. NCI және RDG карталарындағы көк аймақтардың визуализациясы CdS және GO арасындағы электрондық байланысты және заряд алмасуын күшейтетін тартымды ковалентті емес күштерді көрсетеді. Бұл нәтижелер GO тиімді электрон акцепторы ретінде әрекет ететінін, фотогенерацияланған тасымалдаушылардың рекомбинациясын басатынын және фотокаталитикалық тиімділікті арттыратынын растайды. Осы жұмыстан алынған құрылымдық және электрондық түсініктердің біріккен нәтижелері фотокатализатордың жұмысын реттеудегі ковалентті емес өзара әрекеттесулердің негізгі рөлін көрсетеді. Зерттеу нәтижелері күн энергиясымен жұмыс істейтін суды бөлу арқылы тұрақты сутегі энергиясын өндіру үшін тұрақты және тиімді CdS-GO негізіндегі наноқұрылымдарды жобалауға арналған құнды теориялық нұсқаулық береді.

Кілт сөздер: кадмий сульфиді, графен оксиді, фотокатализ, су ыдырату, сутек энергиясы

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Молекулярное исследование интерфейсов сульфида кадмия и оксида графена для фотокаталитического расщепления воды с использованием солнечного света

В данной работе представлено исследование на молекулярном уровне взаимодействия сульфида кадмия (CdS) и оксида графена (GO) для фотокаталитического расщепления воды. Расчеты теории функционала плотности (DFT) проводились с использованием функционала LC-ωPBE и базисного набора LANL2DZ в неявной модели воды (IEFPCM) для оптимизации геометрии и изучения свойств интерфейса. Оптимизированная структура CdS демонстрирует стабильную тетраэдрическую конфигурацию Cd-S, тогда как композит CdS-GO демонстрирует прочные интерфейсные связи посредством взаимодействий Cd-O и S-O, поддерживаемых перераспределением заряда через интерфейс. Анализ градиента плотности восстановления (RDG) и нековалентного взаимодействия (NCI) выявил наличие значительных слабых взаимодействий, включая силы Ван-дер-Ваальса, водородные связи и координацию Cd-O, которые стабилизируют композит. Визуализация синих областей на графиках NCI и RDG указывает на нековалентные силы притяжения, которые усиливают электронное взаимодействие и перенос заряда между CdS и GO. Эти результаты подтверждают, что GO действует как эффективный акцептор электронов, подавляет рекомбинацию фотогенерированных носителей и повышает эффективность фотокаталитического процесса. Совокупность структурных и электронных данных, полученных в ходе данной работы, подчеркивает решающую роль нековалентных взаимодействий в регулировании фотокаталитических характеристик. Результаты исследования дают ценное теоретическое руководство для разработки стабильных и эффективных наноструктур на основе CdS-GO для устойчивого производства водорода путем расщепления воды с помощью солнечной энергии.

Ключевые слова: сульфид кадмия, оксид графена, фотокатализ, расщепление воды, водородная энергетика

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