

Selenium Alloying in CdSeTe Colloidal Quantum Wells as an Effective Strategy for High Efficiency and Enhanced Stability

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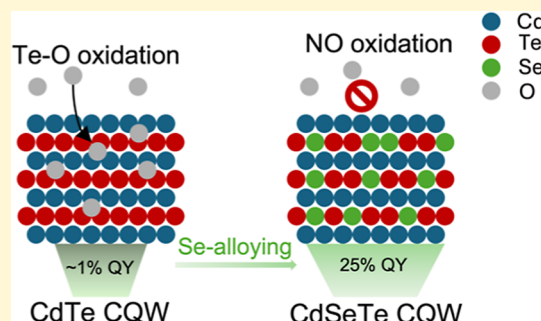


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Supporting Information

ABSTRACT: CdTe colloidal quantum wells (CQWs) exhibit very low quantum yields (QYs) (<1%) and suffer significant stability challenges unlike their CdSe counterparts, which feature near unity QY and high stability under ambient conditions. Here, we synthesized highly stable CdSeTe CQWs with photoluminescence quantum efficiency (PLQY) reaching 25%, which far exceeds the previously best-reported PLQYs from CdTe CQWs while preserving the PL spectral characteristics (PL peak position and full-width-at-half-maximum (fwhm) of PL emission) similar to those of CdTe CQWs. In these as-synthesized CdSeTe nanoplatelets, a progressive increase in the Se/Te ratio leads to a notable enhancement in their quantum yield, accompanied by extended photoluminescence lifetimes, strongly indicating that higher Se incorporation effectively mitigates nonradiative recombination channels. In addition, we demonstrate that these CdSeTe CQWs are stable under ambient conditions unlike pristine CdTe CQWs through systematic studies with X-ray photoelectron spectroscopy (XPS). Using density functional theory (DFT) calculations we demonstrate that, under oxygen-rich conditions, O atoms weaken Cd–Te bonds and destabilize CdTe nanoplatelets, whereas in Se-alloyed CdSeTe CQWs, oxygen atoms preferentially adsorb onto the surface without penetrating the structure, effectively suppressing bond destabilization, which is consistent with our XPS observations. The enhanced optical properties, stability, and robustness of these CdSeTe-alloyed nanoplatelets offer a practical solution to overcoming the inherent limitations of CdTe CQWs and position them as highly attractive materials for practical use in advanced optoelectronic applications.



INTRODUCTION

Colloidal quantum wells (CQWs), commonly known as nanoplatelets, have emerged as a promising class of nanomaterials, thanks to their remarkable optoelectronic properties.^{1–4} These include narrow photoluminescence emission,^{3,4} near-unity photoluminescence quantum yield (PLQY),⁵ directed emission because of anisotropic transition dipole moments,⁶ giant oscillator strength,⁷ and suppressed Auger recombination,⁸ which make them superior in various applications. Especially, the narrow photoluminescence emission leading saturated colors and directed emission resulting in high outcoupling efficiencies are advantageous for display and imaging applications.^{9,10} For example, core CQWs with ~10 nm of full-width-at-half-maximum (fwhm) of PL can be easily obtained without alloying¹ while fwhm of CQDs is usually around 30 nm¹¹ which make them superior in light-emitting diodes (LED) applications together with their directed emission.¹² In addition, CQWs provide unprecedented opportunities for the design of advanced heterostructures owing to the possibility of growing laterally a crown selectively and isotropically a shell unlike the QDs, which are limited by only shell growth.¹³ Such flexibility of obtaining advanced

heterostructures of CQWs is allowed for LEDs with EQE of ~26%.¹²

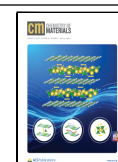
CQWs have been successfully obtained with monolayer-level thickness control in different compositions including CdSe and CdS using synthetic wet chemistry techniques.^{1,14} Among various semiconductor materials explored, significant attention has been directed toward CdSe and CdS CQWs for applications in devices such as LEDs,^{15,16} photodetectors,¹⁷ and energy harvesting.^{18,19} In contrast, the synthesis of CdTe CQWs has been investigated in only few studies and CdTe CQWs have been shown to inherently possess relatively poor optical performance primarily due to lattice defects.¹ This limitation restricts the potential integration of CdTe with other Cd-chalcogenides, such as CdSe and CdS, particularly in the development of sophisticated core–shell^{20,21} and core–crown–shell²² heterostructures. However, CdTe exhibits a relatively

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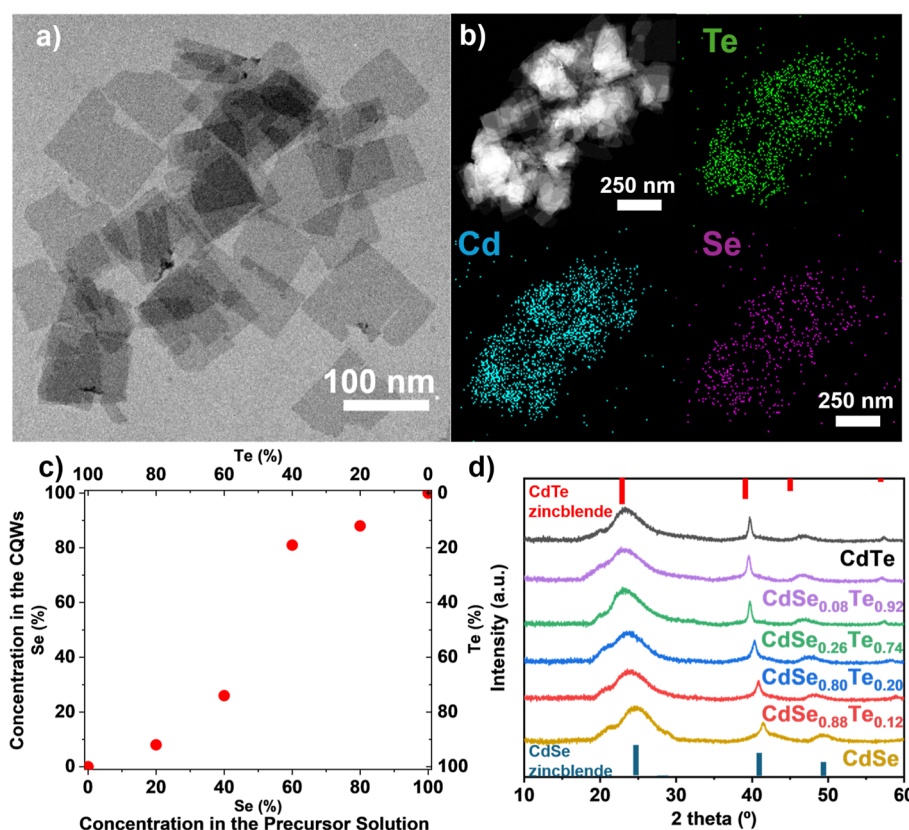


Figure 1. Structural characterization of CdSeTe-alloyed cores. (a) Representative TEM image of CdSe_{0.80}Te_{0.20} CQWs. (b) TEM–EDX mapping of CdSe_{0.26}Te_{0.74} CQWs. (c) Comparison of the Se/(Se + Te) ratio in the precursor and EDX-measured alloy composition of CdSeTe CQWs. (d) X-ray diffraction (XRD) patterns of CdSe_xTe_{1−x} ($0 < x < 1$) nanoplalets along with pure CdTe ($x = 0$) and pure CdSe ($x = 1$) nanoplalets, compared with bulk CdTe and CdSe zinc-blende structures, demonstrating peak shifts indicative of alloy formation.

low band gap of approximately 1.44 eV, distinctly lower than CdSe (around 1.74 eV) and CdS (approximately 2.24 eV) which makes CdTe especially promising for photovoltaic and photodetection applications.²³

To date, the reported set of two-dimensional (2D) CdTe nanostructures primarily includes CQWs with a zincblende crystal structure¹ and nanoribbons in the wurtzite structure.²⁴ Among them, these CdTe CQWs suffer from poor control over thickness during synthesis unlike CdSe CQWs whose thickness can be precisely controlled at an atomic level.²³ In addition, a recent study by Ahmed et al. shows islands of different monolayers (MLs) on the same CQW which exhibit two spectrally separated co-localized emission peaks.²⁵ This inadequate thickness control negatively impacts their optoelectronic properties by introducing inhomogeneity in the PL emission, thereby restricting their potential in light-emitting applications such as LEDs and lasers. Additionally, the PLQY of the reported CdTe CQWs is around 1%, which is significantly lower than the PLQY of CdSe CQWs and their heterostructures reaching near-unity PLQY, significantly limiting their usage. Recently, the Moreels group successfully reported a PLQY of 9% for CdTe CQWs by varying different Te-precursors, subsequently improving it to 12% in a follow-up study.^{26,27} Moreover, beyond a low PLQY, practical implementation of CdTe CQWs has been severely constrained by persistent stability issues. When exposed to ambient environmental conditions, CdTe nanostructures undergo degradation processes²⁸ that markedly compromise their optoelectronic properties over prolonged periods.²⁹ Such

instability presents a critical obstacle, effectively limiting their viability for real-world technological applications.

In this study, we present synthesis and systematic optical characterization of efficient and stable CdSeTe CQWs exhibiting QYs as high as 25%, surpassing the previously reported highest efficiencies from CdTe-based systems (the maximum previous value reaching 12%)²⁷ while keeping the PL spectral characteristics including PL peak position and full-width-at-half-maximum (fwhm) of PL emission similar to those of CdTe CQWs. In addition, we studied the emission kinetics of CdSeTe CQWs having different amounts of Se/Te using time-resolved fluorescence (TRF). In these CQWs, QY increases as the Se/Te ratio raised, which is accompanied by an increase in PL lifetime. This indicates the successful suppression of nonradiative recombination pathways. Moreover, we demonstrated that those alloyed CdSeTe CQWs show significantly enhanced stability to oxidation compared to pure CdTe CQWs by investigating experimentally the level of their degradation of our CdSeTe CQWs in an ambient environment experimentally using X-ray photoelectron spectroscopy (XPS) and theoretically by density functional theory (DFT) calculations. These findings underscore the effectiveness of selenium alloying in substantially enhancing the chemical robustness and optical efficiency of the CdTe quantum wells.

RESULTS AND DISCUSSION

We synthesized 3-monolayer CdSeTe-alloyed CQWs using a cadmium precursor solution containing Cd-acetate dihydrate

for anisotropic 2D growth and octadecene-triethylphosphine (ODE-TOP) solution with varying ratios of Se and Te with a constant injection rate at 200 °C. In this work, we varied this Se/Te ratio in the precursor solution to synthesize CdSeTe CQWs with different incorporation amounts of Se/Te. The detailed synthesis procedure is given in the Experimental Section. The transmission electron microscopy (TEM) image depicted in Figure 1a clearly demonstrates the successful synthesis of CdSeTe nanoplatelets exhibiting distinct 2D characteristics.¹ These CQWs show a clear rectangular shape within the size range of $102 \pm 6 \times 98 \pm 5$ nm². Figure 1b presents the TEM-electron dispersive spectroscopy (EDX) mapping results for Cd, Se, and Te elements in 3 ML of thick CdSe_{0.26}Te_{0.74} CQWs. The EDX mapping distinctly reveals a uniform spatial distribution of Cd, Se, and Te across the CQWs, confirming the homogeneous elemental composition and absence of significant phase segregation or observable clustering. Notably, the overlap between Se and Te maps demonstrates effective alloy formation at the atomic scale, indicative of successful incorporation of Se into the Te-rich lattice structure or vice versa. Additional TEM–EDX results from CdSeTe CQWs with various concentrations of Se and Te are also added into Supporting Information as Figure S1, showing homogeneous elemental composition in all cases.

We obtained the Se/(Se + Te) composition in CdSeTe CQWs using EDX analyses for CQWs synthesized by using different Se/(Se + Te) ratios as presented in Figure 1c. This figure shows how the precursor composition translates into the final alloy composition within the synthesized CdSeTe nanoplatelets with EDX analysis. The measured elemental compositions reveal a distinct one-to-one correlation between the precursor ratios and the final nanoplatelet compositions. Specifically, it is observed that the element initially present in a greater proportion within the precursor solution is preferentially incorporated at an even higher ratio in the resultant nanoplatelets, as clearly detailed in Table 1. For instance, a

Table 1. Comparison of Te Concentrations in the Precursor and Inside the CdSeTe Alloys Obtained Using EDX

	Se concentration in the precursor (%)	Se concentration in CQWs (%)
CdSe _{0.08} Te _{0.92}	20	8
CdSe _{0.26} Te _{0.74}	40	26
CdSe _{0.80} Te _{0.20}	60	80
CdSe _{0.88} Te _{0.12}	80	88

precursor mixture richer in Te results in nanoplatelets with a disproportionately higher Te content compared to that of Se. Similar trends of preferential elemental incorporation and compositional deviations from precursor stoichiometry have been widely reported in colloidal semiconductor alloy syntheses, emphasizing the complexity of accurately predicting alloy composition solely based on the initial precursor ratios.^{30,31}

The XRD patterns presented in Figure 1d provide complementary structural insights, distinctly presenting the zincblende crystalline nature of the synthesized CdSeTe alloys with varying Se/Te ratios (8:92, 26:74, 80:20, and 88:12). The patterns reveal that all nanoplatelets consistently retain the zincblende crystal structure inherent to both pure CdSe and CdTe materials. Notably, the observed shift of diffraction peaks to smaller angles as Se concentration is decreased can be

attributed to the larger lattice parameter of CdTe compared to that of CdSe. Furthermore, diffraction peaks display noticeable broadening compared to the bulk, which is primarily associated with reduced dimensionality and finite crystallite size inherent to ultrathin two-dimensional quantum wells. Crucially, no additional phases were observed in the diffraction patterns, confirming the phase purity. Collectively, these findings unequivocally indicate the successful formation of uniform CdSeTe alloy compositions across all examined Se/Te ratios, where the extent of lattice variation directly correlates with the Se/Te ratio.

A comprehensive evaluation of the optical properties exhibited by 3 ML CdSeTe nanoplatelets synthesized with varying Se contents is presented in Figure 2a–c. The absorption spectra normalized by their first excitonic peak (Figure 2a) exhibit a clear and systematic band bowing as the Se fraction increases, highlighting a direct correlation between the alloy composition and the band gap modulation.^{32,33} This band bowing indicates that Se incorporation modifies the energy band gap while keeping the overall behavior the same.

PL emission profiles of CdSeTe CQWs are given in Figure 2b,c. A detailed analysis shown in Figure 2c reveals a systematic band bowing that varies from 507 to 525 nm as the Se fraction increases compared to pure 3 ML CdTe nanoplatelets emitting around 500 nm. This observation confirms that the alloying process influences electronic transitions and effectively tunes the band gap while preserving the characteristic optical emission profile typical of CdTe-based nanoplatelets. These results are consistent with previous alloying studies,^{32,33} which also report similar controlled band gap engineering through compositional variations in colloidal quantum wells.

A crucial aspect of this study involves evaluating the impact of Se alloying on structural quality, assessed by measuring the fwhm values of the emission peaks, as summarized in Table 2. The obtained fwhm values, namely, 12, 15, 20, and 15 nm, for varying Se fractions indicate that the alloying process introduces minimal inhomogeneous broadening. In contrast, the previous study by Ithurria et al. reports significantly broader emission line widths, reaching up to 80 nm, primarily due to the pronounced inhomogeneous distribution of the alloy components within their nanoplatelets.³² The observation of limited broadening in our 3 ML CdSeTe CQWs emphasizes excellent compositional uniformity and structural homogeneity, which are essential for optoelectronic device applications where narrow emission line widths are highly desirable for high color purity and enhanced device efficiency. In addition, the synthesis procedure was repeated for multiple batches under identical reaction conditions, and the obtained CdSeTe CQWs consistently exhibited highly similar optical properties. The emission peak position varied within ± 4 nm, and fwhm remained consistent within ± 3 nm.

Notably, a significant advancement reported in this study is the remarkable enhancement of the QY, increasing substantially from approximately 1% for pure CdTe nanoplatelets to up to 25% with increased Se content. The PLQY values reported were obtained using an integrating-sphere measurement based on the technique developed by De Mello et al.³⁴ at an excitation wavelength of 430 nm. The PLQY values of the CdSeTe CQWs were measured for multiple batches for consistency and reproducibility. The PLQY values differ by no more than 3% for multiple batches. This QY is higher than twice the best-reported QY values from 3 ML CdTe CQWs

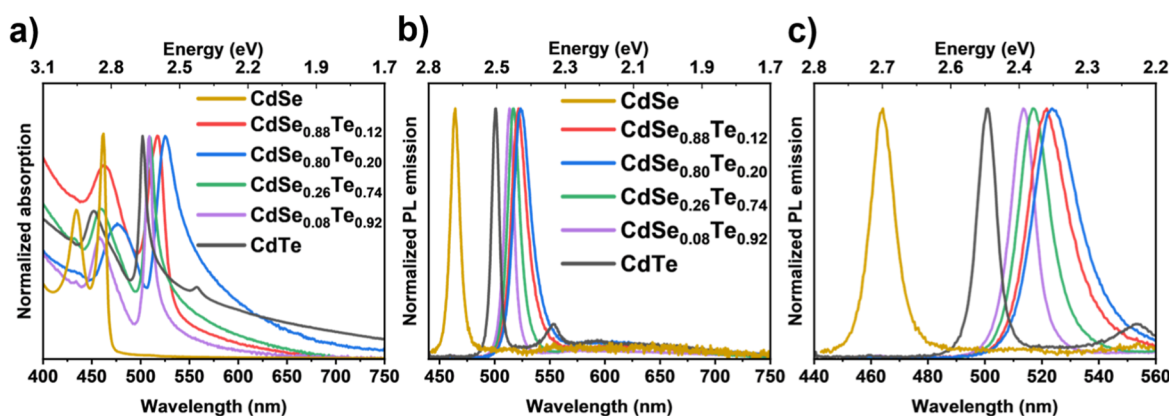


Figure 2. Optical characterization of CQWs of varied CdSeTe alloys. (a) Normalized absorption spectra, (b) normalized photoluminescence emission spectra, and (c) zoomed-in normalized photoluminescence emission spectra in the closed range of alloyed samples in comparison with CdSe and CdTe.

Table 2. FWHM and QY of CdSe_xTe_{1-x} Alloys with Varying Compositions

	fwhm (nm)	QY (%)
CdTe	11	1
CdSe _{0.08} Te _{0.92}	12	4
CdSe _{0.26} Te _{0.74}	15	12
CdSe _{0.80} Te _{0.20}	20	20
CdSe _{0.88} Te _{0.12}	15	25

achieved via post synthesis treatment. This result marks a substantial improvement over values previously reported in the literature for CdTe-based nanoplatelets, which typically exhibit quantum yields from less than 1% due to elevated densities of surface defects and nonradiative recombination pathways along with inherent instability issues. The increased quantum yield observed in the present CdSeTe alloys suggests that Se incorporation effectively passivates defect states or reduces their density, thereby suppressing nonradiative recombination losses and promoting more efficient radiative recombination processes. The observed enhancements in optical performance can be directly attributed to compositional adjustments rather than thickness-dependent variations typically associated with quantum confinement effects. This controlled comparison reinforces the conclusion that selenium incorporation directly enhances the optical efficiency and material stability.

As clearly demonstrated in Figure 2a–c, alloyed samples exhibit narrow, single-peak emission profiles consistent with uniform thickness across the nanoplatelet architecture. In contrast, CdTe samples suffer from inadequate thickness control, reflected in multiple emission peaks that arise during synthesis.^{1,23} Additionally, recent findings by Ahmed et al. reveal simultaneous coexistence of 3 and 4 ML nanoplatelets, characterized by heterogeneous emission profiles that highlight thickness inconsistencies within CdTe nanoplatelets.²⁵ Consequently, the alloyed CdSeTe CQWs in this work demonstrate improved thickness uniformity and compositional homogeneity relative to their CdTe counterparts, further underscoring their potential advantages for optoelectronic applications.

Figure 3 presents a detailed analysis of TRF decay characteristics for alloyed 3 ML CdSeTe nanoplatelets with varying Se concentrations. The decay curves depicted in Figure 3a demonstrate fluorescence dynamics across different alloy compositions. These decay curves were fitted using a triexponential decay model, and the resulting intensity-averaged lifetimes calculated from the fitting parameters are provided in Table S1. The calculated intensity-averaged lifetimes for each alloy composition are plotted in Figure 3b, clearly showing a systematic increase in lifetime with rising Se content. This observation highlights the beneficial role of Se incorporation in mitigating nonradiative recombination path-

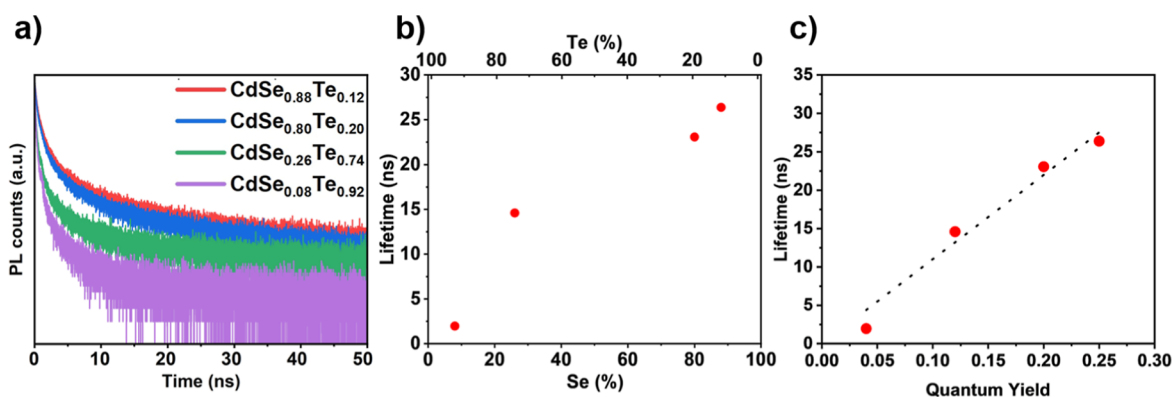


Figure 3. TRF analysis of alloyed 3 ML CdSe_xTe_{1-x} samples. (a) TRF decay curves of the alloyed samples. (b) Comparison of fluorescence intensity-averaged lifetimes for each alloy composition, including CdTe and CdSe, and (c) linear relationship between intensity-averaged lifetime with quantum yield.

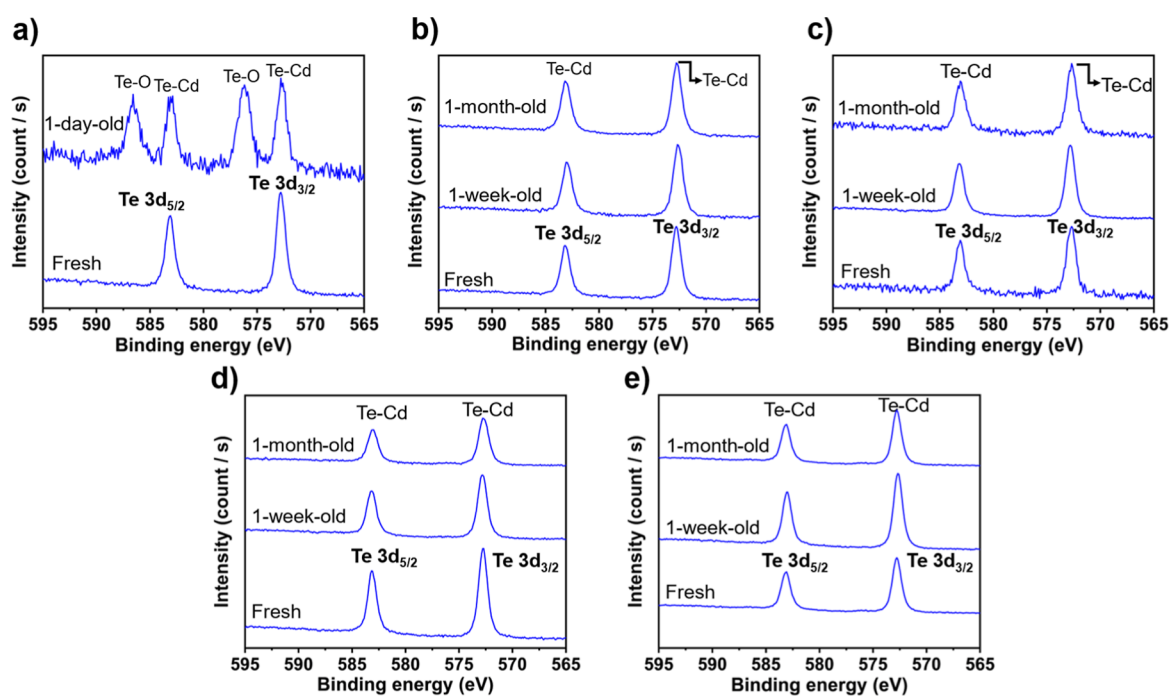


Figure 4. XPS measurements focusing on Te range for (a) CdTe, (b) CdSe_{0.80}Te_{0.20}, (c) CdSe_{0.26}Te_{0.74}, (d) CdSe_{0.88}Te_{0.12}, and (e) CdSe_{0.08}Te_{0.92}, measured after different durations of exposure under ambient conditions.

ways and facilitating more efficient radiative processes. To further elucidate the correlation between enhanced lifetimes and photoluminescence efficiency, Figure 3c presents a plot of intensity-averaged lifetime versus QY for alloyed CdSeTe nanoplatelets. This graph reveals a strong linear relationship within the alloyed samples, characterized by a coefficient of determination (R^2) of >0.99 . The slope obtained from this linear fit is approximately 110 ns, corresponding directly to the intrinsic radiative lifetime of the alloyed nanoplatelets. This linear correlation confirms that improvements in QY primarily arise from the suppression of nonradiative recombination channels rather than from changes in intrinsic radiative decay rates. Notably, the alloyed CdSeTe structures consistently exhibit longer fluorescence lifetimes compared to their binary counterparts, with the composition of 88:12 Se/Te achieving the longest measured lifetime of 26.4 ns, significantly surpassing the lifetimes of 7.9 and 9.1 ns observed for pure CdTe and pure CdSe, respectively. This comprehensive analysis demonstrates that compositional tuning via Se alloying effectively passivates nonradiative recombination channels, resulting in substantial enhancements in both fluorescence lifetime and quantum efficiency.

Figure 4a–e presents XPS spectra obtained for CdTe and CdSeTe-alloyed nanoplatelets with varying compositions (CdSe_{0.88}Te_{0.12}, CdSe_{0.80}Te_{0.20}, CdSe_{0.26}Te_{0.74}, and CdSe_{0.08}Te_{0.92}) under an ambient environment. Initially, the freshly prepared CdTe sample exhibits only peaks corresponding to Te–Cd interactions at the binding energies of 573 eV (Te 3d_{5/2}) and 583.5 eV (Te 3d_{3/2}), without any detectable presence of Te–O binding energy peaks at 576.5 eV (Te 3d_{5/2}) or 587 eV (Te 3d_{3/2}).²⁹ However, a marked difference emerges after only 1 day of exposure to air, with prominent new peaks corresponding to Te–O interactions appearing alongside the original Te–Cd peaks. The intensity of these Te–O peaks becomes comparable to that of the Te–Cd signals, indicative of extensive oxidation occurring in pure

CdTe samples. This rapid and significant oxidation highlights the intrinsic instability of pure CdTe nanoplatelets and their pronounced susceptibility to environmental oxidation processes.

In contrast, for all CdSeTe CQWs, the recorded spectra consistently exhibit only peaks corresponding to the Te–Cd interactions without any detectable presence of Te–O peaks after one month exposure to an ambient environment. The consistent absence of oxidation peaks conclusively demonstrates CdSeTe CQWs maintain exceptional chemical stability when exposed to air over extended periods. The absence of oxidation-related features in CdSeTe CQWs strongly suggests that the incorporation of Se into the CdTe lattice significantly alters the local electronic and structural environments around tellurium atoms, reducing their susceptibility to oxidation.

The bond energy associated with the CdTe CQWs is smaller than that of CdSe CQWs which makes CdTe CQWs thermodynamically less stable²⁵ and therefore vulnerable to oxidation, as demonstrated in our work (Figure 4). Such oxidized sites can act as nonradiative recombination centers in CdTe CQWs. The alloyed structure of CdSeTe as also shown in our work is much more stable than the pristine CdTe structure which makes CdSeTe alloys resistant to formation of defect sites acting as nonradiative recombination centers compared to pristine CdTe structures. Therefore, we attribute the superior optical performance of our CdSeTe CQWs to their thermodynamically stable lattice compared with CdTe CQWs.

Ultimately, the results demonstrated in Figure 4 provide compelling evidence of the critical advantage offered by Se incorporation into enhancing the long-term stability against oxidation for CdTe-based nanoplatelets. The substantial resistance to oxidation exhibited by CdSeTe alloys signifies a major advancement, directly addressing one of the primary obstacles hindering practical applications of CdTe-based materials. Consequently, this improved stability represents a

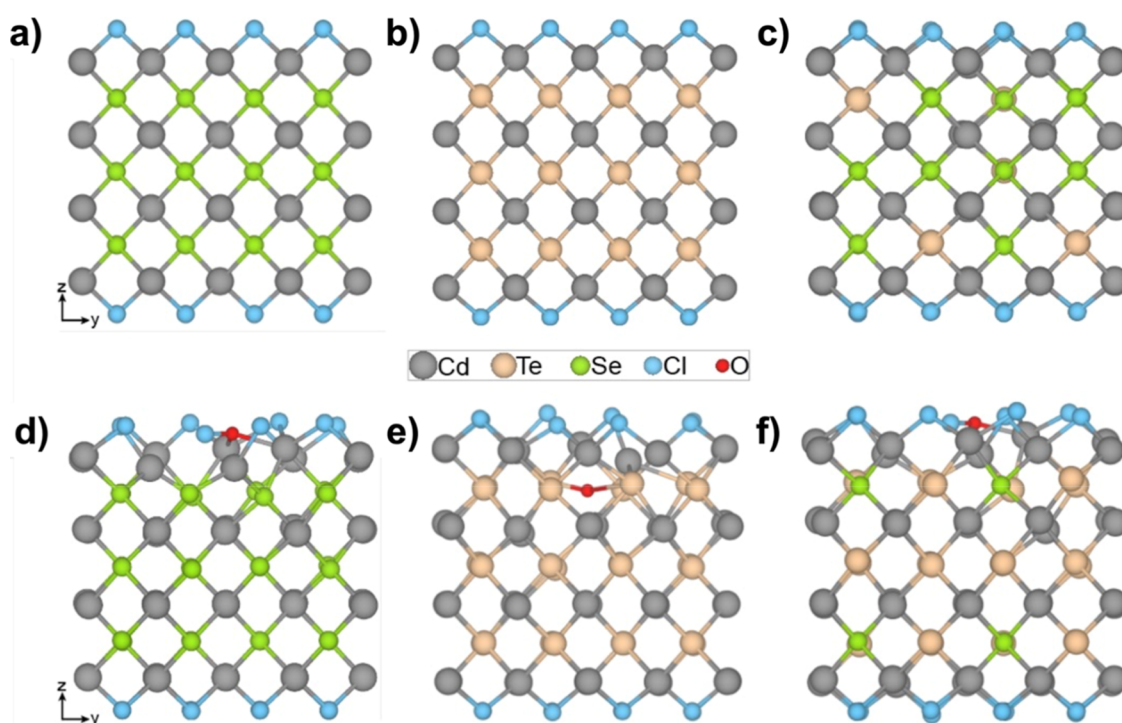


Figure 5. Side view of the seven-layer slab models of (a) pure CdSe, (b) pure CdTe, and (c) CdTe_{0.4}Se_{0.6}. The side-view representation of optimized nanoplatelets with O-adatom (d) CdSe, (e) CdTe, and (f) CdTe_{0.8}Se_{0.2}.

significant breakthrough for realizing high-performance, durable semiconductor devices in photovoltaics, photo-detectors, and advanced optoelectronics, emphasizing the broader technological relevance and potential of CdSeTe alloys.

As discussed in the previous sections, we now turn our attention to the physical understanding of the stability of CdTe nanoplatelets upon Se alloying under oxygen-rich conditions. The first-principles calculations were performed within the framework of DFT to explore the stability of 3 ML CdSeTe CQWs in various compositions, along with pure CdSe and pure CdTe CQWs under O-rich conditions. Initially, ideal CdSe and CdTe nanoplatelets are modeled as 3 ML slab structures terminated with Cd on the top and bottom to represent experimental nanoplatelets. These slab models are derived from the [100] plane of bulk CdSe or CdTe structures, belonging to the $F\bar{4}3m$ space group. The fully optimized bulk lattice parameters are found to be $a = b = c = 0.62$ nm for CdSe, and 0.66 nm for CdTe, showing good agreement with previously reported experimental values.³⁵

To investigate the influence of Se alloying, CdTe_{*x*}Se_{1-*x*} slab models were randomly generated by varying the Se concentration to match approximately 20%, 40%, 60%, and 80%. The structural optimizations reveal surface deformation and Cd atom dissociation in all alloy compositions, particularly pronounced at Se concentrations of 20% and 80%, as illustrated in Figure S2 of the Supporting Information. Additionally, oxygen adsorption calculations performed on experimentally stable, bare CdSe slab surfaces indicate similar deformation and dissociation phenomena. However, experimental observations do not detect any surface deformation or Cd dissociation for CdTe_{*x*}Se_{1-*x*} nanoplatelets across the studied Se concentration range nor for bare CdSe nanoplatelets. This discrepancy underscores the limitations of using bare CdSe, CdTe, and CdTe_{*x*}Se_{1-*x*} slab models to accurately

simulate real nanoplatelets, which are typically passivated with organic ligands, such as oleate.

Therefore, we improved our modeling approach by fully passivating both surfaces of CdSe, CdTe, and CdTe_{*x*}Se_{1-*x*} nanoplatelets with chlorine atoms to better mimic experimentally synthesized oleate-passivated nanoplatelets. Average cohesive energy calculations demonstrate full passivation on the Se or Te hollow sides (illustrated in Figure S3 of Supporting Information) provided the most energetically favorable configuration, as shown in Figure 5. Subsequent DFT optimizations confirmed that fully Cl-passivated CdTe_{*x*}Se_{1-*x*} nanoplatelets exhibit no significant surface deformation or dissociation. Minor atomic displacements occurred due to the shorter Se–Te bond compared to Te–Te bonds.

Next, comparative oxygen adsorption calculations were carried out on Cl-passivated CdSe and CdTe nanoplatelets to elucidate the origin of the instability observed in CdTe under O-rich conditions. Oxygen adsorption was analyzed on four distinct adsorption sites, shown in Figure S3b of Supporting Information. For the CdSe nanoplatelet, O atoms are adsorbed onto the surface except at the Cd hollow site, where they directly bond with surface Cd atoms. Conversely, for the CdTe nanoplatelet, oxygen adsorption occurs at three surface sites, but at the Cd hollow site, the O atom penetrates deeper into the nanoplatelet surface, forming bonds with underlying Te atoms (Figure 5e). The pronounced susceptibility of CdTe nanoplatelets to oxidation primarily arises from the high chemical reactivity of surface Te atoms, whose stereochemically active lone pairs readily interact with ambient oxygen. This interaction promotes the formation of detrimental tellurium oxides.^{36,37} Under O-rich conditions, oxygen atoms penetrate the surface and bind to Te sites, weakening Cd–Te bonds and leading to the structural destabilization of the nanoplatelets.

To further clarify the stabilizing effect of Se alloying, we conducted additional oxygen adsorption simulations using the $\text{CdTe}_{0.4}\text{Se}_{0.6}$ alloy models. Adsorption at the critical Cd hollow site, where oxygen penetration is observed in pure CdTe, was specifically investigated for models exhibiting both symmetric and asymmetric Se distributions. Regardless of Se arrangement, oxygen atoms consistently are adsorbed onto the surface without penetration. Additionally, even in alloy models with a lower Se content ($\text{CdTe}_{0.8}\text{Se}_{0.2}$), oxygen atoms are adsorbed onto the surface, demonstrating the effective suppression of oxygen penetration (Figure 5f). This significant enhancement in chemical stability can be attributed to Se incorporation altering the electronic structure of the nanoplatelets, which reduces electron density localization on Te sites and mitigates their reactivity toward oxygen.³⁸ Additionally, Se alloying suppresses oxygen penetration into the nanoplatelet matrix by electronically passivating reactive Te sites and disrupting diffusion pathways.

Our DFT results align closely with experimental observations, clearly indicating that pure CdTe nanoplatelets become unstable under O-rich conditions due to oxidation. However, alloying with Se at various concentrations effectively mitigates this instability, enhancing the structural integrity of CdTe-based nanoplatelets against oxidation.

CONCLUSION

In conclusion, this study successfully demonstrated the synthesis and comprehensive characterization of CdSeTe-alloyed CQWs that possess significantly higher PLQY and stability compared with pristine CdTe nanoplatelets. Here, the controlled incorporation of Se resulted in nanoplatelets exhibiting a precise 2D morphology, superior crystallinity, and exact compositional control, verified through TEM, EDX, and XRD analyses. The quantum yields of these CdSeTe CQWs reach 25%, surpassing the previously best-reported efficiency level for pristine CdTe CQWs by more than two times. TRF studies confirm extended fluorescence lifetimes with increasing Se content accompanied by a continuous increase in QY, highlighting effective defect passivation and improved carrier recombination dynamics in these alloyed CdSeTe CQWs compared to pristine CdTe CQWs. In addition, we show that the cosynthesized CdSeTe alloys showed exceptional resistance to oxidation during prolonged ambient exposure, in stark contrast to the rapid oxidation observed in pure CdTe samples using XPS. DFT calculations indicate that oxygen atoms compromise the stability of CdTe nanoplatelets under oxygen-rich conditions by weakening the Cd–Te bonds. In contrast, for alloyed CdSeTe CQWs, oxygen atoms predominantly adsorb onto the surface, significantly hindering further oxygen penetration and aligning closely with our XPS experimental observations. These findings establish selenium alloying as a powerful and scalable strategy for addressing stability challenges and enhancing the efficiency of CdTe based colloidal quantum wells with potential applications spanning advanced photovoltaics, high-efficiency photodetectors, and next-generation LEDs. The superior stability, efficiency, and robustness of CdSeTe CQWs, overcoming the intrinsic limitations associated with CdTe nanoplatelets, position these materials as highly promising candidates for practical implementation in sustainable energy technologies, optical sensing platforms, and high-resolution displays, addressing essential demands within contemporary optoelectronics.

EXPERIMENTAL SECTION

Synthesis of 3 ML CdSe CQWs

530 mg of cadmium acetate dihydrate, 40 mL of octadecene (ODE), 0.6 mL of oleic acid (OA), and 7 mL of a 0.19 M selenium-ODE stock solution were combined in a three-neck flask and degassed at 60 °C under constant stirring for 1 h. After degassing, the temperature was raised rapidly to 245 °C under inert atmosphere; immediately upon reaching this target temperature, the reaction was quenched by removing the heat source. Once the solution cooled to room temperature, it was transferred into a centrifuge tube. Subsequently, 10 mL of hexane (as the solvent) and 10 mL of ethanol (as the antisolvent) were added. The resulting mixture was centrifuged at 6000 rpm for 6 min to isolate the colloidal quantum wells from residual reaction byproducts.

Synthesis of 3 ML CdTe and 3 ML $\text{CdSe}_x\text{Te}_{1-x}$ CQWs

A mixture consisting of 25 mL of the ODE and 2 mL of the anisotropic growth mixture was introduced into a three-neck flask and degassed under continuous stirring at 60 °C for 30 min. Subsequently, the reaction temperature was elevated to 210 °C under an inert atmosphere. At this temperature, a 4 mL solution of 0.03 M Se- and Te-containing TOP precursors dissolved in ODE (0.03 M ODE-TOP- $\text{Se}_y\text{Te}_{1-y}$), which had been previously prepared under the nitrogen atmosphere inside a glovebox, was injected at a controlled rate of 20 mL/h. The selenium-to-tellurium ratio (y) in the precursor solution was tuned by adjusting the relative proportions of the ions of the ions of the ODE-TOP-Se and ODE-TOP-Te, allowing precise control over the composition of the synthesized $\text{CdSe}_x\text{Te}_{1-x}$ CQWs and $y = 0$ for CdTe CQWs. Immediately after the full injection of the precursor solution, the reaction was rapidly quenched. Upon cooling, the mixture was combined with 10 mL of hexane as the solvent and 10 mL of ethanol as the antisolvent, followed by centrifugation at 6000 rpm for 6 min to separate the CQWs from reaction byproducts.

Computational Details

The first-principles calculations were performed within the framework of DFT using the Vienna Ab initio Simulation Package (VASP).³⁹ The exchange–correlation interactions were described by the generalized gradient approximation employing the Perdew–Burke–Ernzerhof (PBE) functional,⁴⁰ together with projector augmented wave pseudopotentials.⁴¹ A plane-wave basis set with a kinetic energy cutoff of 400 eV was used throughout the simulations.

Using three-layer alloy slab models, subsequent oxygen adsorption calculations were conducted within $2 \times 2 \times 1$ supercells. Brillouin zone integrations were performed by using a $6 \times 6 \times 1$ Monkhorst–Pack k-point mesh. Electronic occupancies were treated using Gaussian smearing with a smearing width of 0.05 eV. Additionally, van der Waals interactions were accounted for using Grimme's DFT-D2 dispersion correction method.⁴²

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.chemmater.5c02327>.

Detailed synthesis procedure of CdTe, CdSe, and alloyed CdSeTe core CQWs; TEM images and EDX mapping of CdSeTe-alloyed CQWs with various compositions; tabulated TRF fitting parameters; alloy slab models of CdSeTe-alloyed CQWs with various compositions; pristine and Cl-passivated versions; and PL intensity measurements over time (PDF)

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Author Contributions

[§]A.A.G. and S.D. contributed equally to this work. H.V.D., A.A.G., and S.D. conceived the idea and H.V.D. supervised the research at all stages. A.A.G. prepared the samples, performed the absorption and PL measurements, conducted XRD measurements, analyzed the data, and performed the TRF measurements. A.A.G. and S.D. analyzed the data. A.A.G. performed XPS measurements and analyzed the data. E.G.D. took the TEM images and EDX mapping. T.G., E.D., and F.I. designed the simulation. E.D. supervised the simulation part. T.G. and E.G. performed and analyzed the DFT calculations.

A.A.G. wrote the draft manuscript with inputs from S.D., H.V.D., T.G., and E.D. The manuscript was written through contributions of all authors. All authors have given approval to the final version of the manuscript.

Notes

The authors declare no competing financial interest.

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REFERENCES

- (1) Ithurria, S.; Tessier, M. D.; Mahler, B.; Lobo, R. P. S. M.; Dubertret, B.; Efros, A. L. Colloidal Nanoplatelets with Two-Dimensional Electronic Structure. *Nat. Mater.* **2011**, *10* (12), 936–941.
- (2) Diroll, B. T.; Guzelturk, B.; Po, H.; Dabard, C.; Fu, N.; Makke, L.; Lhuillier, E.; Ithurria, S. 2D II–VI Semiconductor Nanoplatelets: From Material Synthesis to Optoelectronic Integration. *Chem. Rev.* **2023**, *123* (7), 3543–3624.
- (3) Ithurria, S.; Dubertret, B. Quasi 2D Colloidal CdSe Platelets with Thicknesses Controlled at the Atomic Level. *J. Am. Chem. Soc.* **2008**, *130* (49), 16504–16505.
- (4) Guzelturk, B.; Erdem, O.; Olutas, M.; Kelestemur, Y.; Demir, H. V. Stacking in Colloidal Nanoplatelets: Tuning Excitonic Properties. *ACS Nano* **2014**, *8* (12), 12524–12533.
- (5) Liu, B.; Altintas, Y.; Wang, L.; Shendre, S.; Sharma, M.; Sun, H.; Mutlugun, E.; Demir, H. V. Record High External Quantum Efficiency of 19.2% Achieved in Light-Emitting Diodes of Colloidal Quantum Wells Enabled by Hot-Injection Shell Growth. *Adv. Mater.* **2020**, *32* (8), 1905824.
- (6) Scott, R.; Heckmann, J.; Prudnikau, A. V.; Antanovich, A.; Mikhailov, A.; Owschimikow, N.; Artemyev, M.; Climente, J. I.; Woggon, U.; Grosse, N. B.; Achtstein, A. W. Directed Emission of CdSe Nanoplatelets Originating from Strongly Anisotropic 2D Electronic Structure. *Nat. Nanotechnol.* **2017**, *12* (12), 1155–1160.
- (7) Naeem, A.; Masia, F.; Christodoulou, S.; Moreels, I.; Borri, P.; Langbein, W. Giant Exciton Oscillator Strength and Radiatively Limited Dephasing in Two-Dimensional Platelets. *Phys. Rev. B* **2015**, *91* (12), 121302.
- (8) Taghipour, N.; Delikanli, S.; Shendre, S.; Sak, M.; Li, M.; Isik, F.; Tanriover, I.; Guzelturk, B.; Sum, T. C.; Demir, H. V. Sub-Single Exciton Optical Gain Threshold in Colloidal Semiconductor Quantum Wells with Gradient Alloy Shelling. *Nat. Commun.* **2020**, *11* (1), 3305.
- (9) Baruj, H. D.; Bozkaya, I.; Canimkurbey, B.; Isik, A. T.; Shabani, F.; Delikanli, S.; Shendre, S.; Erdem, O.; Isik, F.; Demir, H. V. Highly-Directional, Highly-Efficient Solution-Processed Light-Emitting Diodes of All-Face-Down Oriented Colloidal Quantum Well Self-Assembly. *Small* **2023**, *19* (29), 2206582.
- (10) Canimkurbey, B.; Isik, F.; Delikanli, S.; Bozkaya, I.; Unal, E.; Isik, A. T.; Dikmen, Z.; Shabani, F.; Ozkan, I.; Piravadi, S.; Demir, H. V. Flexible Colloidal Light-Emitting Diodes of Self-Assembled Quantum Well Monolayers. *Small* **2025**, *21* (32), 2502314.
- (11) Guzelturk, B.; Kelestemur, Y.; Gungor, K.; Yeltik, A.; Akgul, M. Z.; Wang, Y.; Chen, R.; Dang, C.; Sun, H.; Demir, H. V. Stable and Low-Threshold Optical Gain in CdSe/CdS Quantum Dots: An All-Colloidal Frequency Up-Converted Laser. *Adv. Mater.* **2015**, *27* (17), 2741–2746.

- (12) Zhu, Y.; Deng, Y.; Bai, P.; Wu, X.; Yao, Y.; Liu, Q.; Qiu, J.; Hu, A.; Tang, Z.; Yu, W.; Li, Y.; Jiang, P.; Liu, Z.; Gao, P.; Hao, Y.; Jin, W.; Chen, D.; Zhu, X.; Jin, Y.; Gao, Y. Highly Efficient Light-Emitting Diodes Based on Self-Assembled Colloidal Quantum Wells. *Adv. Mater.* **2023**, *35* (49), 2305382.
- (13) Sharma, M.; Delikanli, S.; Demir, H. V. Two-Dimensional CdSe-Based Nanoplatelets: Their Heterostructures, Doping, Photo-physical Properties, and Applications. *Proc. IEEE* **2020**, *108* (5), 655–675.
- (14) Li, Z.; Qin, H.; Guzun, D.; Benamara, M.; Salamo, G.; Peng, X. Uniform Thickness and Colloidal-Stable CdS Quantum Disks with Tunable Thickness: Synthesis and Properties. *Nano Res.* **2012**, *5* (5), 337–351.
- (15) Chen, Z.; Nadal, B.; Mahler, B.; Aubin, H.; Dubertret, B. Quasi-2D Colloidal Semiconductor Nanoplatelets for Narrow Electroluminescence. *Adv. Funct. Mater.* **2014**, *24* (3), 295–302.
- (16) Qu, J.; Rastogi, P.; Gréboval, C.; Livache, C.; Dufour, M.; Chu, A.; Chee, S.-S.; Ramade, J.; Xu, X. Z.; Ithurria, S.; Lhuillier, E. Nanoplatelet-Based Light-Emitting Diode and Its Use in All-Nanocrystal LiFi-like Communication. *ACS Appl. Mater. Interfaces* **2020**, *12* (19), 22058–22065.
- (17) Dutta, A.; Medda, A.; Bera, R.; Sarkar, K.; Sain, S.; Kumar, P.; Patra, A. Hybrid Nanostructures of 2D CdSe Nanoplatelets for High-Performance Photodetector Using Charge Transfer Process. *ACS Appl. Nano Mater.* **2020**, *3* (5), 4717–4727.
- (18) Naskar, S.; Lübke, F.; Hamid, S.; Freytag, A.; Wolf, A.; Koch, J.; Ivanova, I.; Pfnür, H.; Dorfs, D.; Bahnemann, D. W.; Bigall, N. C. Synthesis of Ternary and Quaternary Au and Pt Decorated CdSe/CdS Heteronanostructures with Controllable Morphology. *Adv. Funct. Mater.* **2017**, *27* (8), 1604685.
- (19) Li, Q.; Zhao, F.; Qu, C.; Shang, Q.; Xu, Z.; Yu, L.; McBride, J. R.; Lian, T. Two-Dimensional Morphology Enhances Light-Driven H₂ Generation Efficiency in CdS Nanoplatelet-Pt Heterostructures. *J. Am. Chem. Soc.* **2018**, *140* (37), 11726–11734.
- (20) Mahler, B.; Nadal, B.; Bouet, C.; Patriarche, G.; Dubertret, B. Core/Shell Colloidal Semiconductor Nanoplatelets. *J. Am. Chem. Soc.* **2012**, *134* (45), 18591–18598.
- (21) Tessier, M. D.; Mahler, B.; Nadal, B.; Heuclin, H.; Pedetti, S.; Dubertret, B. Spectroscopy of Colloidal Semiconductor Core/Shell Nanoplatelets with High Quantum Yield. *Nano Lett.* **2013**, *13* (7), 3321–3328.
- (22) Kelestemur, Y.; Guzel, B.; Erdem, O.; Olutas, M.; Gungor, K.; Demir, H. V. Platelet-in-Box Colloidal Quantum Wells: CdSe/CdS@CdS Core/Crown@Shell Heteronanostructures. *Adv. Funct. Mater.* **2016**, *26* (21), 3570–3579.
- (23) Pedetti, S.; Nadal, B.; Lhuillier, E.; Mahler, B.; Bouet, C.; Abécassis, B.; Xu, X.; Dubertret, B. Optimized Synthesis of CdTe Nanoplatelets and Photoresponse of CdTe Nanoplatelets Films. *Chem. Mater.* **2013**, *25* (12), 2455–2462.
- (24) Son, J. S.; Wen, X.-D.; Joo, J.; Chae, J.; Baek, S.; Park, K.; Kim, J. H.; An, K.; Yu, J. H.; Kwon, S. G.; Choi, S.-H.; Wang, Z.; Kim, Y.-W.; Kuk, Y.; Hoffmann, R.; Hyeon, T. Large-Scale Soft Colloidal Template Synthesis of 1.4 Nm Thick CdSe Nanosheets. *Angew. Chem.* **2009**, *121*, 6993–6996.
- (25) Ahmed, T.; Tan, X.; Li, B. Y.; Cook, E.; Williams, J.; Tiano, S. M.; Coffey, B.; Tenney, S. M.; Hayes, D.; Caram, J. R. Heteroconfinement in Single CdTe Nanoplatelets. *ACS Nano* **2025**, *19* (3), 3944–3952.
- (26) Anand, A.; Zaffalon, M. L.; Cova, F.; Pinchetti, V.; Khan, A. H.; Carulli, F.; Brescia, R.; Meinardi, F.; Moreels, I.; Brovelli, S. Optical and Scintillation Properties of Record-Efficiency CdTe Nanoplatelets toward Radiation Detection Applications. *Nano Lett.* **2022**, *22* (22), 8900–8907.
- (27) Al-Shnani, F.; Mutyal, C. S.; Rodà, C.; Moreels, I. Fluorescence Quantum Efficiency Enhancement in Size-Controlled 3.5 Monolayer Cadmium Telluride Nanoplatelets. *Chem. Mater.* **2023**, *35* (16), 6258–6265.
- (28) Rugen-Hankey, S. L.; Clayton, A. J.; Barrioz, V.; Kartopu, G.; Irvine, S. J. C.; McGettrick, J. D.; Hammond, D. Improvement to Thin Film CdTe Solar Cells with Controlled Back Surface Oxidation. *Sol. Energy Mater. Sol. Cells* **2015**, *136*, 213–217.
- (29) Bartolo-Pérez, P.; Fariás, M. H.; Castro-Rodríguez, R.; Peña, J. L.; Caballero-Briones, F.; Cauich, W. XPS Analysis of Oxidation States of Te in CdTe Oxide Films Grown by Rf Sputtering with an Ar-NH₃ Plasma. *Superficies Vacio* **2001**, 8–11.
- (30) Zhong, H.; Zhou, Y.; Ye, M.; He, Y.; Ye, J.; He, C.; Yang, C.; Li, Y. Controlled Synthesis and Optical Properties of Colloidal Ternary Chalcogenide CuInS₂ Nanocrystals. *Chem. Mater.* **2008**, *20* (20), 6434–6443.
- (31) Shendre, S.; Delikanli, S.; Li, M.; Dede, D.; Pan, Z.; Ha, S. T.; Fu, Y. H.; Hernández-Martínez, P. L.; Yu, J.; Erdem, O.; Kuznetsov, A. I.; Dang, C.; Sum, T. C.; Demir, H. V. Ultrahigh-Efficiency Aqueous Flat Nanocrystals of CdSe/CdS@Cd_{1-x}Zn_xS Colloidal Core/Crown@alloyed-Shell Quantum Wells. *Nanoscale* **2019**, *11* (1), 301–310.
- (32) Tenne, R.; Pedetti, S.; Kazes, M.; Ithurria, S.; Houben, L.; Nadal, B.; Oron, D.; Dubertret, B. From Dilute Isovalent Substitution to Alloying in CdSeTe Nanoplatelets. *Phys. Chem. Chem. Phys.* **2016**, *18* (22), 15295–15303.
- (33) Kelestemur, Y.; Dede, D.; Gungor, K.; Usanmaz, C. F.; Erdem, O.; Demir, H. V. Alloyed Heterostructures of CdSe α S_{1-x} Nanoplatelets with Highly Tunable Optical Gain Performance. *Chem. Mater.* **2017**, *29* (11), 4857–4865.
- (34) De Mello, J. C.; Wittmann, H. F.; Friend, R. H. An Improved Experimental Determination of External Photoluminescence Quantum Efficiency. *Adv. Mater.* **1997**, *9* (3), 230–232.
- (35) Landolt, H.; Börnstein, R. *Numerical Data and Functional Relationships in Science and Technology*; Springer: Berlin, 1961.
- (36) Xu, W.; Gan, L.; Wang, R.; Wu, X.; Xu, H. Surface Adsorption and Vacancy in Tuning the Properties of Tellurene. *ACS Appl. Mater. Interfaces* **2020**, *12* (16), 19110–19115.
- (37) Gossé, S. Tellurium Oxides: Thermodynamics and Phase Relations in the Te–O System. *J. Phase Equilib. Diffus.* **2025**, *46* (1), 20–30.
- (38) Xiang, X.; Tong, Y.; Gehrke, A.; Dunham, S. T. Point Defects in CdTe and CdTeSe Alloy: A First Principles Investigation with DFT + U. *Phys. Rev. Mater.* **2024**, *8* (8), 084602.
- (39) Kresse, G.; Furthmüller, J. Efficient Iterative Schemes for Ab Initio Total-Energy Calculations Using a Plane-Wave Basis Set. *Phys. Rev. B* **1996**, *54* (16), 11169–11186.
- (40) Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996**, *77* (18), 3865–3868.
- (41) Blöchl, P. E. Projector Augmented-Wave Method. *Phys. Rev. B* **1994**, *50* (24), 17953–17979.
- (42) Grimme, S. Semiempirical GGA-type Density Functional Constructed with a Long-range Dispersion Correction. *J. Comput. Chem.* **2006**, *27* (15), 1787–1799.