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Highly Luminescent and Stable CsPbI3 Perovskite Nanocrystals with Sodium Dodecyl Sulfate Ligand Passivation for Red Light-Emitting Diodes

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Abstract

CsPbI₃ perovskite nanocrystals (NCs) have recently emerged as promising materials for optoelectronic devices due to their superior properties. However, the poor stability of the CsPbI₃ NCs induced by easy ligand desorption represents a key issue limiting their practical applications. Herein, we report stable and highly luminescent black-phase CsPbI₃ NCs passivated by novel ligands of sodium dodecyl sulfate (SDS). Theoretical calculation results reveal a stronger adsorption energy of SDS molecules at CsPbI₃ surface than that of commonly used oleic acid. As a result, the defect formation caused by the ligand loss during the purification process is greatly suppressed. The optimized SDS-CsPbI₃ NCs exhibit significantly reduced surface defects, much enhanced stability and superior photoluminescence efficiency. The red perovskite light-emitting diodes based on the SDS-CsPbI₃ NCs demonstrate an external quantum efficiency of 8.4%, which shows a fourfold improvement compared to the devices based on the oleic acid modified CsPbI₃ NCs.

TOC Graphic:
Colloidal all-inorganic halide perovskite (CsPbX₃, X = Cl, Br, I) nanocrystals (NCs) are emerging as promising candidates for optoelectronic applications owing to their outstanding material properties¹-⁵. Among various halide perovskite NCs, CsPbI₃ NCs have demonstrated a wide range of applications in solar cells, light-emitting diodes (LEDs), and photodetectors⁶-⁷. However, due to the ionic structure and highly labile ligand bonding, the CsPbI₃ NCs easily transform into non-perovskite orthorhombic (δ) phase with an indirect band gap of 2.82 eV in the ambient conditions ⁸-⁹. The degradation process could be greatly accelerated by stress factors of moisture, heat, or ultraviolet (UV) illumination. Although the surface ligands of oleic acid (OA) and oleylamine (OAm) were commonly used for the synthesis of CsPbI₃ NCs, they can be easily stripped off during the subsequent isolation/purification process due to their dynamic ligand bonding nature at the surface of the NCs ¹⁰-¹¹. The ligand loss usually causes under-coordinated atoms and traps at the surface of as-purified NCs, which not only induce detrimental nonradiative recombination paths, but also speed up the phase transformation to δ-CsPbI₃.

A range of useful methods have been explored to eliminate surface defects and improve the stability of CsPbI₃ NCs, such as constructing CsPbI₃/PbSe heterostructured nanocrystals¹², adopting PbI₂/GeI₂ dual-source iodine synthetic approach¹³, decorating with super-hydrophobic frameworks¹⁴, alloying with transition metal to partially replace Pb¹⁵-¹⁹, and forming hybrid structure through epitaxial growth²⁰. On the other hand, the under-coordinated Pb⁰ is regarded as the main source of surface trap states, which can be passivated by ligands with stronger
binding energy to NC surface, leading to the improvements of stability and photoluminescence quantum yield (PLQY) of the resulting NCs\textsuperscript{21}. For instance, Shen and co-workers achieved CsPbI\textsubscript{3} NCs with enhanced stability through trioctylphosphine (TOP) passivation\textsuperscript{22}. Tian and co-workers proposed a ligand exchange strategy using aminoethanethiol (AET), which passivates the surface traps of NCs and prevents penetration of water molecules, leading to an enhanced PLQY and stability\textsuperscript{23}. Despite the useful methods, the stability of the CsPbI\textsubscript{3} NCs needs to be further improved for their practical applications, and the detailed mechanisms behind the performance enhancements upon ligand modulations also needs to be clearly elucidated.

In this work, we introduce a surfactant of sodium dodecyl sulfate (SDS) during the synthesis as the surface ligand to in-situ passivate the surface defects of CsPbI\textsubscript{3} NCs. The experimental measurements and theoretical calculations are combined to reveal how the SDS influences the optical performance and stability of CsPbI\textsubscript{3} NCs. We found that the SDS molecules possess stronger adsorption energy on the surface of CsPbI\textsubscript{3} than that of OA ligands, which ensures notably enhanced stability of the SDS-CsPbI\textsubscript{3} NCs. The PLQY of SDS-CsPbI\textsubscript{3} NCs reaches up to 96\% owing to the greatly reduced trap states through in-situ SDS passivation during the synthesis. Moreover, we demonstrated notably improved device performance of red-remitting perovskite LEDs (PeLEDs) based on the SDS-CsPbI\textsubscript{3} NCs, verifying the effectiveness of this method in modulating the surface properties of the NCs.
The CsPbI₃ NCs were synthesized using a hot-injection method, according to the previous report with minor modifications². The SDS-CsPbI₃ NCs were obtained by incorporating SDS into the lead precursor solution (details in the Experimental Section) before the injection of the cesium olate. Figure S1 shows the photographs of the crude solutions of the as-synthesized CsPbI₃ NCs and SDS-CsPbI₃ NCs under daylight and UV-irradiation, which exhibit dark-red and vivid red color, respectively. Figure 1 a-d show the transmission electron microscopy (TEM) images and high-resolution TEM (HRTEM) images of the samples. All the NCs synthesized with different feeding molar ratios of SDS/PbI₂ show similar cubic shapes. However, the NCs demonstrate a more regular and uniform shape with the increase of the feeding amount of SDS. The average sizes of the samples decreased from 12.1 to 10.4 nm (Figure S2) with the molar ratios of SDS to PbI₂ increase from 0 to 0.6. The results suggest that the surfactant SDS restricts the growth of perovskite nanocrystals, leading to the formation of small-size CsPbI₃ NCs with enhanced quantum confinement effects. All of the samples show the same lattice spacing of 3.09 Å, which corresponds to the (220) crystal plane in γ-CsPbI₃. Selected area electron diffraction (SAED) patterns of CsPbI₃ NCs and SDS-CsPbI₃ NCs verify good crystallinity of both CsPbI₃ NCs and SDS-CsPbI₃ NCs (Figure S3). The high-angle annular dark-field scanning transmission microscopy (HAADF–STEM) image and the corresponding EDS mapping images further confirm the uniform distribution of Cs, Pb, and S elements in the SDS-CsPbI₃ NCs (Figure S4). We present X-ray diffraction (XRD) characterization results of different CsPbI₃ NCs in Figure 1e. All XRD patterns match well
with the $\gamma$-phase of CsPbI$_3$, revealing that incorporating SDS molecules has negligible influence on the perovskite structures. However, when a large amount of SDS was added (molar ratio of SDS/PbI$_2$ = 0.6), the XRD patterns show obviously decreased intensity for the main diffraction peaks. At the same time, the full widths at half maximum (FWHM) of the diffraction peak at around 28° increases from 0.74, to 0.83, 0.89, and 1.25 degree as the SDS to PbI$_2$ ratio increased from 0 to 0.2, 0.4, and 0.6, respectively, indicating that excessive SDS reduces the crystallinity of CsPbI$_3$ NCs. We anticipate that this is due to the strong binding energy between SDS and Pb$^{2+}$ and the excessive SDS molecules would slow down the construction of the PbI$_6^{4-}$ octahedra during the synthesis of CsPbI$_3$ NCs.

Fourier-transform infrared (FTIR) spectroscopy was conducted to verify the binding mode of the ligands on the surface of NCs (Figure 1f). We observe that binding characteristic peaks belonging to OA and OAm remain in both CsPbI$_3$ NCs and SDS-CsPbI$_3$ NCs. However, the two additional peaks at 1260 and 1095 cm$^{-1}$ corresponding to the vibrational signals of chemical bonds of S=O and S-O in SDS are only observed for SDS-CsPbI$_3$ NCs$^{25}$. The FTIR spectrum of the SDS-CsPbI$_3$ NCs reveals an increased stretching frequency (10 cm$^{-1}$) of the S=O and S-O compared to that of pure SDS (Figure 1g). The increase of S=O and S-O stretching wavenumber in SDS-CsPbI$_3$ NCs could be reasonably ascribed to the decreased spatial symmetry of the SO$_3^-$ group after interacting with the perovskite NCs. This would induce harder symmetric stretching vibration in the SO$_3^-$ group, which is similar to the observations in the sulfobetaine zwitterions modified CsPbI$_3$.$^{26}$ The binding mode of ligands on the surface of
CsPbI3 NCs was demonstrated by the X-ray photoelectron spectroscopy (XPS) measurement. **Figure S5a** displays the survey XPS spectra and high-resolution XPS of S-2\textit{p} and Pb-4\textit{f} regions of CsPbI3 NCs and SDS-CsPbI3 NCs. We observed a new peak with the binding energy at ~169 eV corresponding to the S-2\textit{p} core level appears in SDS-CsPbI3 NCs, which manifests the presence of sulfur on the surface of SDS-CsPbI3 NCs (**Figure S5b**). The Pb-4\textit{f} core levels (143.2, 138.1 eV) of SDS-CsPbI3 NCs shift to higher binding energy compared to those (142.9, 137.8 eV) of CsPbI3 NCs (**Figure 1h**), which can be explained by the increased binding energies between SDS and the Pb atoms of the SDS-CsPbI3 NCs. In addition, the Pb-4\textit{f} peaks of CsPbI3 NCs can be fitted with two peaks, where the signals with high and low binding energies are assigned to Pb-I (142.9, 137.8 eV) and Pb$^0$ (~141.5 eV and 136.5 eV) associated with uncoordinated lead on the surface, respectively. The Pb$^0$ signal indicates the existence of surface defects of NCs\textsuperscript{12}. On the contrary, the Pb-4\textit{f} peaks of SDS-CsPbI3 NCs demonstrate negligible signals of Pb$^0$, which is expected to reduce surface defects and suppress nonradiative recombination of SDS-CsPbI3 NCs.

The UV–vis absorption and PL spectra of CsPbI3 NCs prepared with different contents of SDS are compared in **Figures 2a** and **2b**. The first excitonic absorption and the PL peaks of NCs show a bit blueshift with the increasing contents of SDS due to the quantum confinement effect, which agrees well with the decreased sizes observed in the TEM results. The PLQYs of the samples prepared with different feeding amounts of SDS were determined using a fluorescence spectrometer equipped with an integrating sphere with excitation wavelength at
365 nm, and the PLQY measurement results of the samples in hexane solution are shown in 
**Figure S6**. The intensity of the PL spectra is observed to rise first and then decrease with the increasing amount of SDS, corresponding to an improved PLQY from 62.5% for CsPbI3 NCs to 96.5% for SDS-CsPbI3 NCs (SDS/PbI2 = 0.4), and then reduced to 81.6% (SDS/PbI2 = 0.6) owing to the poor crystallinity of the NCs, as discussed in the XRD section. The PLQYs of thin films assembled from CsPbI3 and SDS-CsPbI3 NCs (SDS/PbI2 = 0.4) were measured to be 47.3% and 66.4%, respectively (**Figure S7**). The lower PLQYs of the assembled films are possibly due to the aggregation of the NCs and newly introduced defects during the film formation27-28. Compared with the CsPbI3 NCs, the improved PLQY of SDS-CsPbI3 NCs both in film and solution indicate the suppressed non-radiative recombination.

To further investigate the effects of SDS on CsPbI3 NCs, time-resolved PL (TRPL) decay measurements were conducted under an excitation fluence of $1.2 \times 10^{10}$ photons/cm$^2$/pulse (**Figure 2c**), where the carrier dynamics is dominated by single neutral excitons29. The PL decay curves were fitted by bi-exponential decay functions of $A_1 e^{-t/\tau_1} + A_2 e^{-t/\tau_2}$, where $A_1$ and $A_2$ are the amplitudes of shorter lifetime ($\tau_1$) and longer lifetime ($\tau_2$), respectively. The shorter lifetime of around 20 ns is ascribed to surface-related recombination, and the intrinsic recombination of the NCs contributes to the longer lifetime of around 60 ns30-33. The average PL lifetime calculated by $(A_1 \tau_1^2 + A_2 \tau_2^2) / (A_1 \tau_1 + A_2 \tau_2)$ increased from 30.8 ns for the CsPbI3 NCs to 43.1 ns for the SDS-CsPbI3 NCs (see details in **Table S1**), which could originate from the inhibited non-radiative deep surface defects30-33. Notably, though the PLQY of SDS-CsPbI3
NCs is near-unity, the time-resolved PL spectrum still exhibits two-channel decay. It implies that there would be another radiative channel convoluted in the shorter lifetime, which possibly relates to the radiative recombination of shallow surface states\textsuperscript{34}.

We further implemented transient absorption (TA) spectroscopy to gain more insights on the carrier dynamics in the solution of CsPbI\textsubscript{3} NCs and SDS-CsPbI\textsubscript{3} NCs at higher pump fluences of 3.2×10\textsuperscript{13} photons/cm\textsuperscript{2}/pulse. The TA images from 480 nm to 720 nm are illustrated in Figure 2\textsuperscript{d} and Figure 2\textsuperscript{e}, respectively. The negative responses at around 660 nm in both TA images coincide with the exciton absorption position in the steady-state UV–vis absorption spectra, suggesting their properties of ground states\textsuperscript{35}. Decays of the negative responses are plotted in Figure 2\textsuperscript{f} for the CsPbI\textsubscript{3} NCs and SDS-CsPbI\textsubscript{3} NCs, and fitted by a bi-exponential function with a shorter lifetime of 10s ps and a longer lifetime of around 2 ns (see details in Table S2). The shorter lifetime originates from Auger recombination of biexcitons, where the energy of single neutral exciton transfers to another electron or hole without photon emission\textsuperscript{36}. In contrast to radiative recombination of single neutral excitons with an average PL decay lifetime of around 40 ns, the longer lifetime of around 2 ns could relate to the radiative recombination of exciton complexes (multi-excitons or charged excitons)\textsuperscript{37-38}. Considering the positive correlation between the radiative recombination of exciton complexes and single neutral excitons\textsuperscript{38}, the increase of longer lifetime from 1.9 ns for the CsPbI\textsubscript{3} NCs to 2.4 ns for the SDS-CsPbI\textsubscript{3} NCs (Table S2) indicates that the average lifetime for radiative recombination of single
neutral excitons increases during the process of surface treatment. The result is consistent with increased average PL lifetime in TRPL measurement and enhanced PLQY of SDS-CsPbI₃ NCs.

The stability of the SDS-CsPbI₃ NCs was greatly improved in comparison with that of CsPbI₃ NCs. Figure 3a illustrates the stability of the samples against water (2 mL of hexane NCs solution and 1 mL of water were added in a cuvette). The red emission of CsPbI₃ NCs became very weak after 10 min and completely disappeared in 20 min. On the contrary, the bright red emission of SDS-CsPbI₃ NCs was maintained, and above 70% of the initial PL intensity was reserved after water treatment for 40 min (Figure S8a). The PL properties of the CsPbI₃ NCs and SDS-CsPbI₃ NCs (SDS/PbI₂ = 0.4) in hexane were also monitored (Figure 3b). The SDS-CsPbI₃ NCs maintained 80% of the original PL intensity after 30 days, while the CsPbI₃ NCs show almost no PL emission after 12 days. The thermal-stability of SDS-CsPbI₃ NCs is also increased (Figure 3c). At high temperatures (above 110 ℃), the SDS-CsPbI₃ NCs can maintain 40% of their original PL intensity while the relative PL intensity rapidly dropped to zero at the same temperature. The ambient stability of the NCs was investigated via monitoring the XRD patterns of the film samples stored in ambient conditions (30 ℃ and 80% relative humidity) (Figure 3d, e). The CsPbI₃ NCs show a fast phase transformation to δ-phase after 5 days, while the SDS-CsPbI₃ NCs film well maintains their γ-phase under the same storage conditions. We further investigated the photo-stability of CsPbI₃ NCs and SDS-CsPbI₃ NCs in the colloidal solutions under a sustained UV-light (365 nm, 16 W) irradiation at room temperature (Figure S8b). The PL intensity of CsPbI₃ NCs was completely quenched within 15 h, while the SDS-
CsPbI₃ NCs maintained about 70% of the initial PL intensity under the UV-light irradiation for 30 hours. The obvious PL quenching of the CsPbI₃ NCs under UV illumination probably results from the photoinduced desorption of surface ligands and the introduced carrier-trapping defects, which is consistent with the observation in the previous work⁴⁹.

To get a deep insight into the improved PLQY and stability, density functional theory (DFT) calculations were performed to investigate the binding nature of SDS and OA on the NCs surface. The model CsPbI₃ NCs were assumed to be covered with Pb and I atoms (a PbI₂-rich surface)⁴⁰, as shown in Figure 3f. In both cases, Pb atoms are the preferred adsorption sites for the carboxylic group of OA and a sulfonic acid group of SDS. The charge redistribution mainly happens around the bonding region of ligand attachment. It also can be found that the bonding orbital regions of SDS adsorption are significantly larger than that of OA adsorption. Thus, the NCs surface passivated with a sulfonic acid group of SDS shows a much larger binding energy (Eₜₐₜ, 1.62 eV) than that of a carboxylic-capped surface using OA ligand (0.85 eV). The weak binding energy between OA and CsPbI₃ NCs easily resulted in the desorption of the surface ligands, introducing additional surface defects and a fast PL quenching. The presence of SDS ligands with strong binding affinity can preserve the surface properties of the NCs, which leads to high-quality SDS-CsPbI₃ NCs with fewer surface defects, higher PLQY, and better phase stability.

It is well known that insufficient ligands on NCs surface may lead to low colloidal stability and severe aggregation, while excessive ligands on the NCs surface act as the insulating layer
deteriorating performance of the resulting optoelectronic devices. And hence, proper purification of the NCs is necessary for their practical device applications. Owing to the strong binding affinity of SDS on the surface of CsPbI$_3$ NCs, the SDS-CsPbI$_3$ NCs are expected to exhibit higher stability against multistep purification than conventional CsPbI$_3$ NCs. We purified the CsPbI$_3$ NCs and SDS-CsPbI$_3$ NCs by hexane/ethyl acetate for different cycles (details in the Experiment Section) and the TEM images and PL spectra of the samples are presented in Figure S9. It was observed that, after three cycles of purification, CsPbI$_3$ NCs displayed serious aggregation (Figure S9a-c) and very weak PL intensity (Figure S9g). As a comparison, SDS-CsPbI$_3$ NCs exhibited improved stability during the same purification process, with their cubic shape maintained after being washed three times (Figure S9d-f). A negligible decrease was also observed in the PL intensity after purification (Figure S9h).

To evaluate the potential applications of the SDS-CsPbI$_3$ NCs in optoelectronic devices, both types of NCs were adopted as light emitters for PeLEDs. The PeLEDs were fabricated based on a device structure of ITO/ZnO/polyethyleneimine (PEI)/NCs/4,4',4″-tris(carbazol-9-yl)-triphenylamine (TCTA)/MoO$_3$/Al (Figure 4a), and the energy diagrams of the function layers are shown schematically in Figure 4b. The energy level of perovskite NCs was given according to the results in previous work on CsPbI$_3$ NCs. Apart from the TCTA and MoO$_3$/Al, which were deposited in a vacuum chamber, all the other layers were solution-processed via spin-coating and annealing on pre-patterned ITO substrates. The luminance versus driving voltage and external quantum efficiency (EQE) versus current density curves for the PeLEDs are...
presented in Figures 4c and 4d, respectively. And EQE histograms of devices based on CsPbI₃
NCs and SDS-CsPbI₃ NCs are given in Figures S10. Obviously, in the whole voltage range,
the PeLEDs based on SDS-CsPbI₃ NCs show improved luminance and EQE than those of the
CsPbI₃ NCs. The maximum luminance and EQE of the optimized PeLEDs based on SDS-
CsPbI₃ NCs are 830 cd m⁻² and 8.4%, respectively, which are both improved compared with
those using CsPbI₃ NCs with a maximum luminance of 320 cd m⁻² and a peak EQE of 2.1%.
The PeLEDs based on SDS-CsPbI₃ NCs exhibit stable electroluminescence (EL) spectra at
elevated driving voltages (Figure 4e), corresponding to Commission Internationale de
l’Eclairage (CIE) coordinates of (0.730, 0.269), which presents saturated red color and high
color purity (Figure 4f).

In summary, we have demonstrated a facile in-situ strategy for passivating the surface defects
of CsPbI₃ NCs with a novel surfactant of sodium dodecyl sulfate. The theoretical calculations
and experimental results reveal a strong binding affinity of the sulfonic acid group on the
surface of the CsPbI₃ NCs, which preserves the surface properties of the NCs during the
purification processes. As a result of the efficient defect passivation, the SDS-CsPbI₃ NCs
exhibit greatly enhanced stability and improved PLQY of nearly 100%. The resulting PeLEDs
based on the SDS-CsPbI₃ NCs demonstrated better device performance than that using the
CsPbI₃ NCs. This work demonstrated a facile strategy to eliminate the notorious limitation of
poor stability and low PLQY of CsPbI₃ NCs for applications in optoelectronic devices.
ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI:

Experimental and computational details (PDF)

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Notes

The authors declare no competing financial interest.

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Figure 1. (a-d) TEM and HRTEM (inset) images of CsPbI$_3$ NCs with different feeding molar rates of SDS to PbI$_2$ (0, 0.2, 0.4, 0.6). (e) XRD patterns of the different CsPbI$_3$ NCs. (f) FTIR spectra of CsPbI$_3$ NCs, SDS-CsPbI$_3$ NCs (SDS/PbI$_2$ = 0.4), and pure SDS. (g) Comparison of S=O and S-O vibration mode in FTIR of pure SDS and SDS-CsPbI$_3$ NCs (SDS/PbI$_2$ = 0.4). High-resolution XPS spectra of (h) Pb-4f of CsPbI$_3$ NCs and SDS-CsPbI$_3$ NCs (SDS/PbI$_2$ = 0.4).
Figure 2. (a) Absorption spectra, (b) PL spectra (excitation at 365 nm), and (c) Time-resolved photoluminescence decays for excitonic luminescence of CsPbI$_3$ NCs and SDS-CsPbI$_3$ NCs (SDS/PbI$_2$ = 0.4). TA spectra of the (d) CsPbI$_3$ NCs and (e) SDS-CsPbI$_3$ NCs recorded at different delay times. (f) TA comparisons between CsPbI$_3$ NCs and SDS-CsPbI$_3$ NCs (SDS/PbI$_2$ = 0.4).
Figure 3. (a) Photographs showing the resistance of different samples against water treatment for CsPbI$_3$ NCs and SDS-CsPbI$_3$ NCs (SDS/PbI$_2$ = 0.4). (b) Normalized PL intensity as a function of aged days in air for CsPbI$_3$ NCs and SDS-CsPbI$_3$ NCs (SDS/PbI$_2$ = 0.4) in hexane (the inset shows the photographs of CsPbI$_3$ NCs and SDS-CsPbI$_3$ NCs in hexane under UV-irradiation after aged for 0 and 30 days). (c) Temperature dependent PL behavior of the peak emission intensity for different samples. Compared XRD patterns of (d) CsPbI$_3$ NCs and (e) SDS-CsPbI$_3$ NCs (SDS/PbI$_2$ = 0.4) films stored in air (30 °C, 80% R.H.) for 0 and 5 days (the inset shows the corresponding photographs of NCs films under UV-irradiation). (f) DFT calculated binding energy ($E_{\text{be}}$) of OA and SDS ligands on the optimized CsPbI$_3$ NCs surfaces.
Figure 4. (a) Device structure of PeLED. (b) Band alignment of each functional layer. (c) Current density and luminance versus driving voltage curves for PeLED based on CsPbI$_3$ NCs and SDS-CsPbI$_3$ NCs. (d) EQEs of PeLED based on different NCs at different current densities. (e) EL spectra at various driving voltages. (f) The corresponding CIE coordinate for the EL spectrum of SDS-CsPbI$_3$ NCs-based PeLED at an applied voltage of 7.0 V.