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Supplementary information

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Highly efficient emission and high-CRI warm white light-emitting diodes from ligand-modified $CsPbBr_3$ quantum dots

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Table S1 | The binding energies of OA and DA molecules with the CsBr-terminated $CsPbBr_3$ surface. The structural models are shown in Fig. S1. The energy gaps are also shown.

	Binding energy (eV)	Energy gap (eV)
OA on pristine CsBr	–0.127	2.96
DA on pristine CsBr	–0.136	2.99
OA on CsBr with a Br-vacancy	–0.933	1.65
DA on CsBr with a Br-vacancy	–1.135	2.83
CsBr surface, pristine	–	3.01
CsBr surface, with a Br vacancy	–	2.31
OA	–	4.64
DA	–	5.20

Evaluation of the computational convergence and numerical fidelity. A strict comparison of the molecular binding energies requires well-converged structural relaxations, which is usually quite difficult because of the open boundary at the surface. Fig. S1 shows the structural relaxation convergence of the four adsorption models (Fig. S1) and two reference surface structures (i.e., the pristine CsBr-terminated surface and the CsBr surface with a Br vacancy, both without molecules adsorption). Several thousands of ionic steps are needed to converge the total energy to a threshold of 0.02 eV/Cell, and Fig. S1 shows the last 50 steps. Clearly, the first four structures (Fig. S1(a, b, c, d)) are well converged, which validates the fidelity of relative stability of DA/OA adsorbed on the pristine CsBr-surfaces. The last two structures (Fig. S1(e, f)) are much more difficult to converge, which show energetic oscillations around 0.05 eV/Cell. Our discussion on the relative stability of DA/OA is still correct though, since the energy difference between the two models has a much larger value of 0.202 eV.

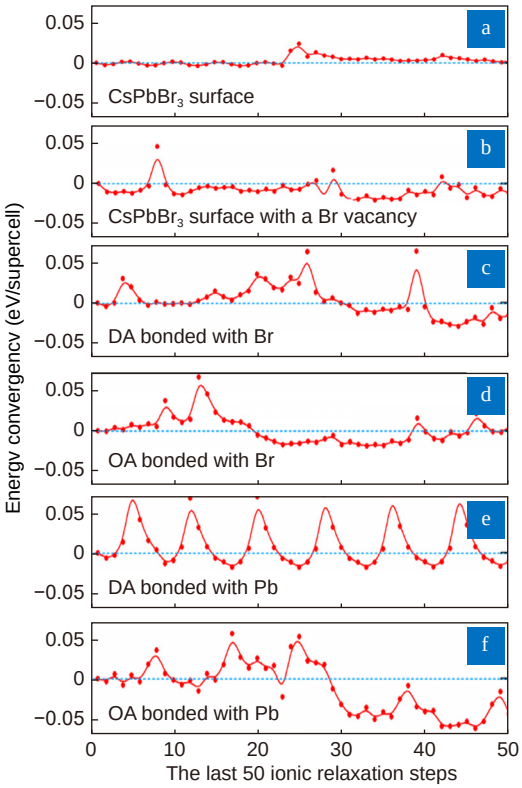

Fig. S1 | The energy convergence of the structural relaxation. Several thousands of ionic steps are performed and here only shows the last 50 steps.

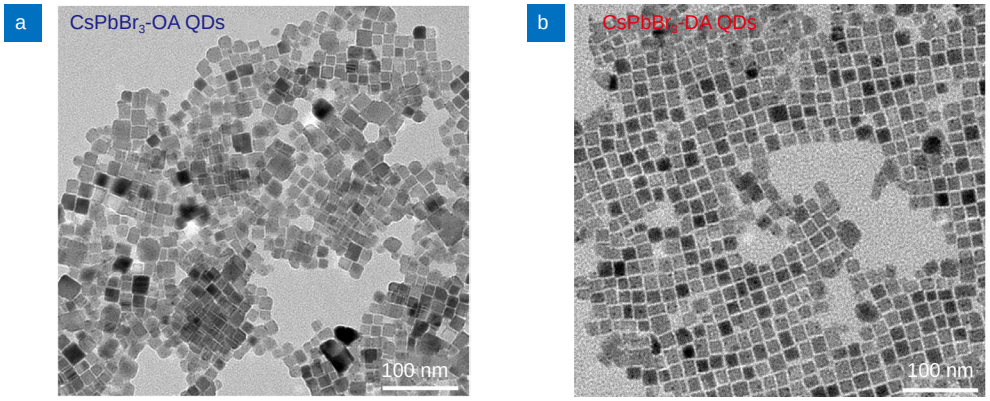

Fig. S2 | Low resolution TEM images of (**a**) $CsPbBr_3$-OA QDs and (**b**) $CsPbBr_3$-DA QDs.

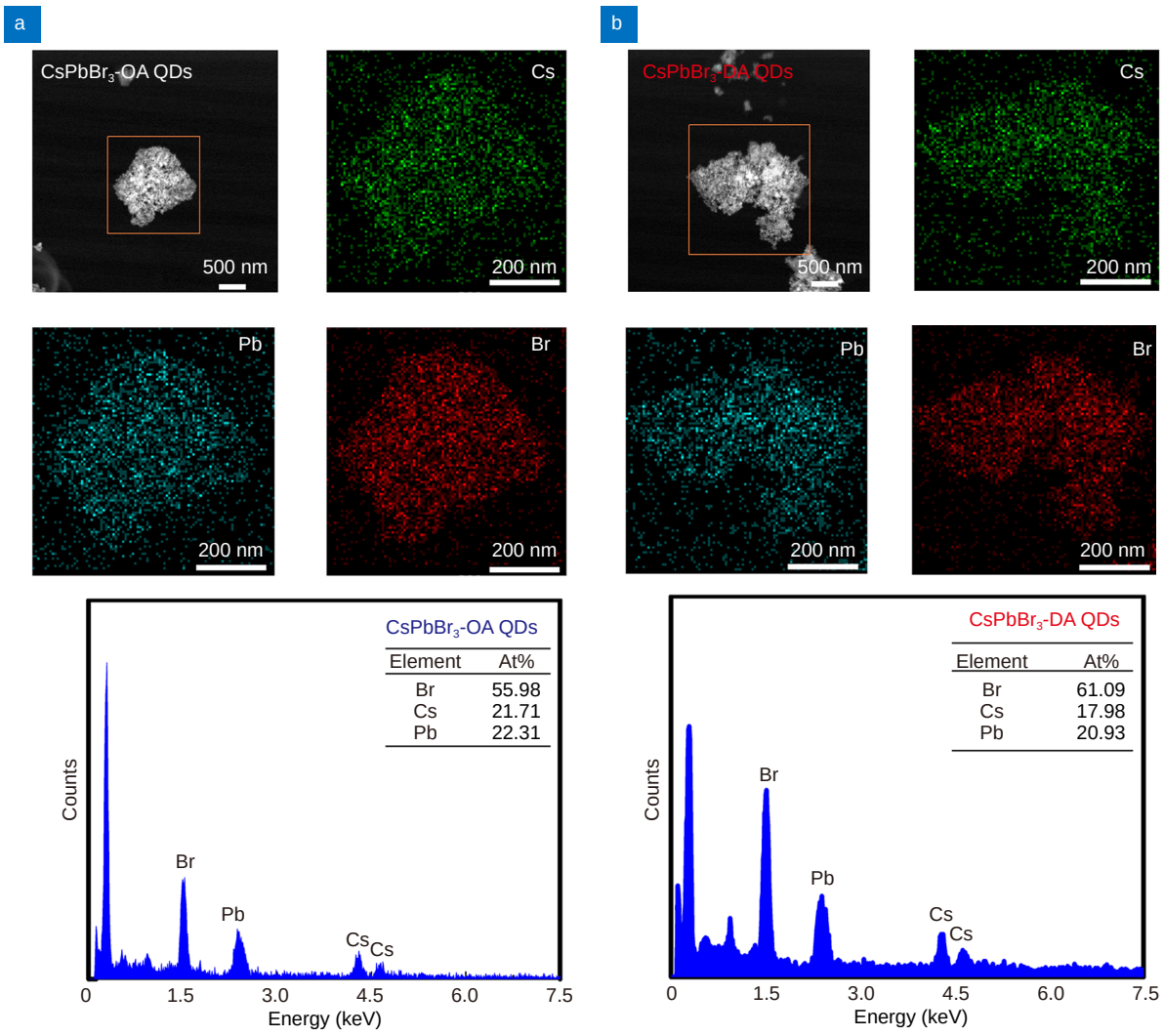

Fig. S3 | EDX mapping of $CsPbBr_3$ QDs including the elements of Cs, Pb and Br for (**a**) CsPbBr3-OA QDs and (**b**) $CsPbBr_3$-DA QDs.

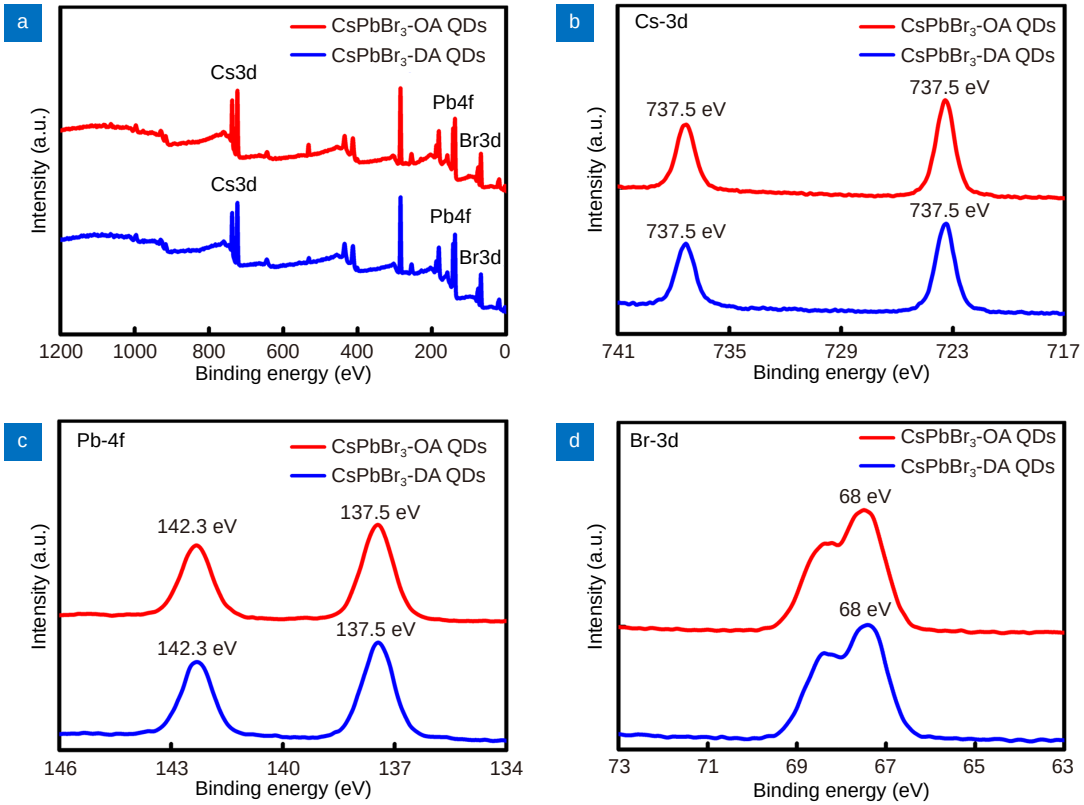

Fig. S4 | (**a**) XPS survey spectrum of $CsPbBr_3$ QDs. (**b**) Cs-3d spectrum. (**c**) Pb-4f spectrum (**d**) Br-3d spectrum. All peaks were calibrated using C 1s (284.8 eV).

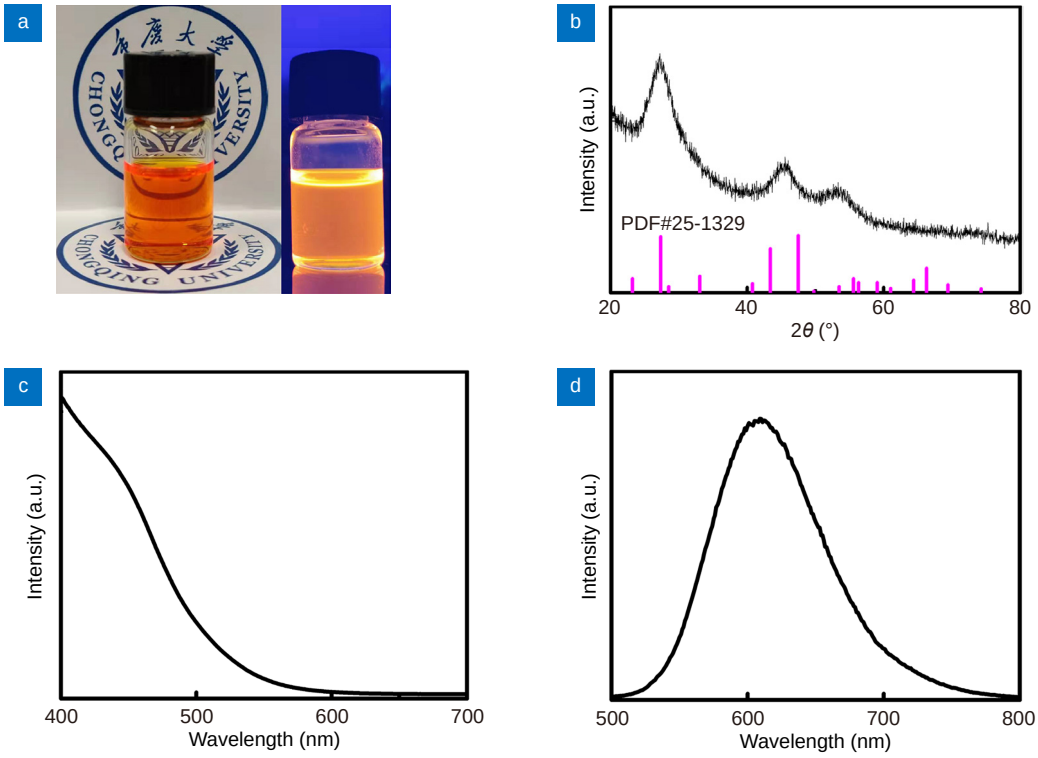

Fig. S5 | (**a**) Photographs of AgInZnS QDs under daylight and UV light. (**b**) XRD pattern, (**c**) Absorption spectra, (**d**) PL spectra of AgInZnS QDs.

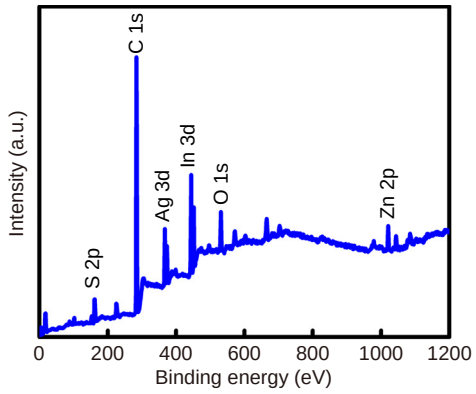

Fig. S6 | XPS survey of Ag-In-Zn-S QDs.

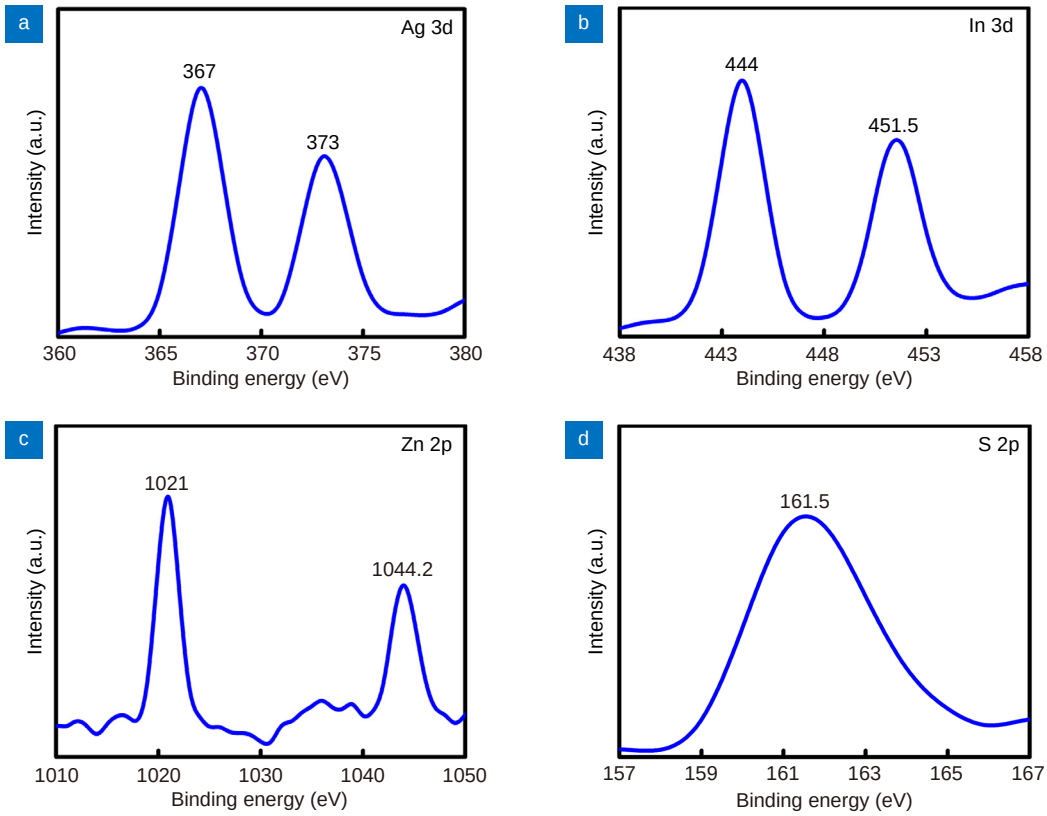

Fig. S7 | High-resolution XPS spectra of AgInZnS QDs. (**a**) Ag 3d, (**b**) In 3d, (**c**) Zn 2p, (**d**) S 2p

Table S2 | Optical parameters of $CsPbBr_3$-OA QDs WLEDs with the increased driving voltage.

Voltage (V)	CRI	CCT (*K*)	CIE coordinates (*X*, *Y*)
2.50	**85**	**5182**	**(0.34, 0.42)**
2.56	**84**	**5211**	**(0.34, 0.39)**
2.62	**84**	**5659**	**(0.33, 0.36)**
2.68	**83**	**6728**	**(0.31, 0.33)**
2.74	**82**	**8938**	**(0.29, 0.29)**
2.80	**81**	**14739**	**(0.27, 0.26)**

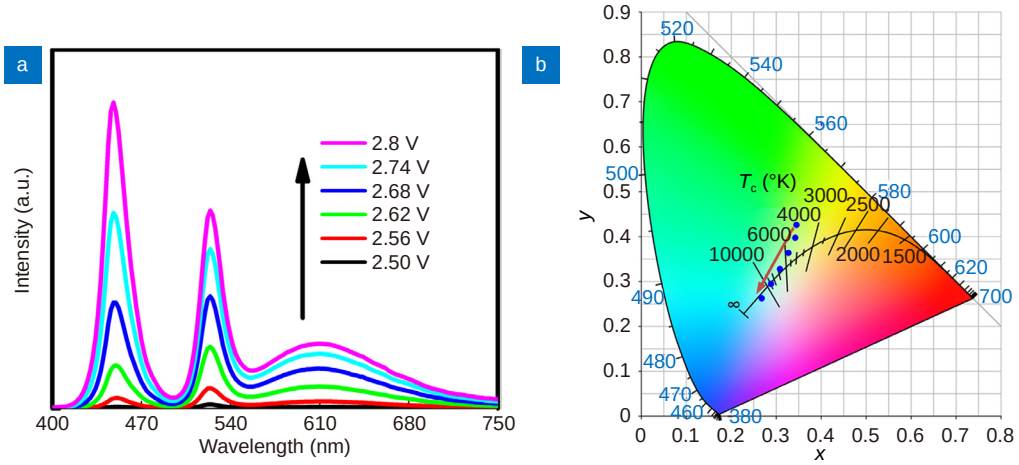

Fig. S8 | (**a**) EL spectra and (**b**) CIE color coordinates of $CsPbBr_3$-OA QDs WLEDs with the change of driving voltage.

Table S3 | Optical parameters of $CsPbBr_3$-DA QDs WLEDs with the increased driving voltage.

Voltage (V)	CRI	CCT (*K*)	CIE coordinates (*X*, *Y*)
2.50	**93**	**2651**	**(0.47, 0.43)**
2.56	**93**	**2780**	**(0.46, 0.43)**
2.62	**93**	**2914**	**(0.45, 0.42)**
2.68	**92**	**3140**	**(0.43, 0.41)**
2.74	**92**	**3425**	**(0.41, 0.39)**
2.80	**90**	**3768**	**(0.39, 0.37)**

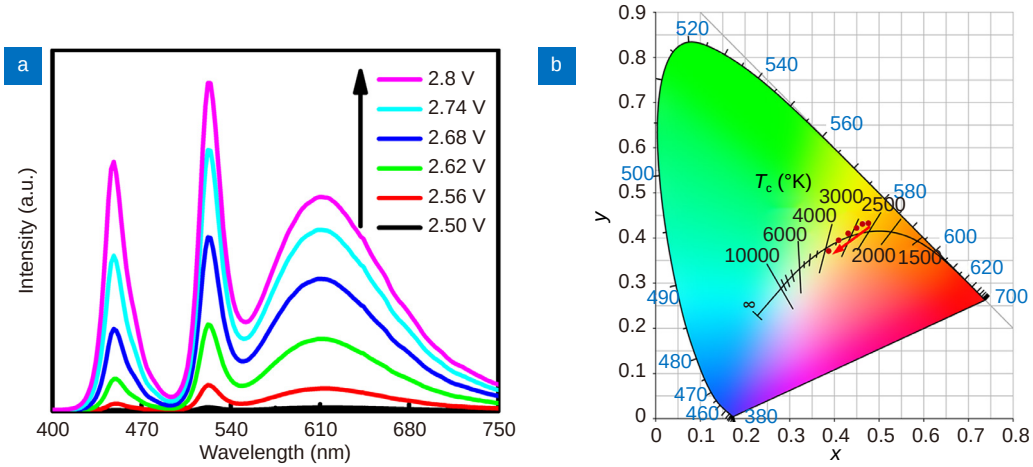

Fig. S9 | (**a**) EL spectra and (**b**) CIE color coordinates of $CsPbBr_3$-DA QDs WLEDs with the change of driving voltage.

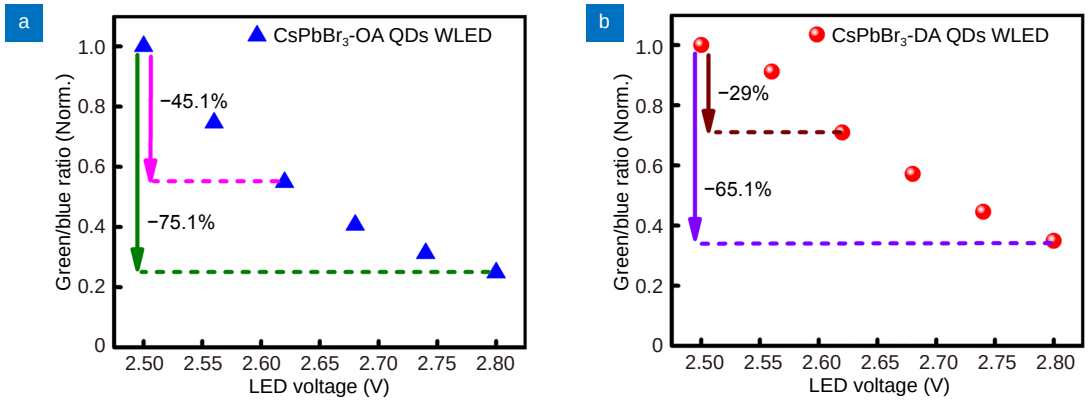

Fig. S10 | The decrease in green-to-blue intensity ratio at increasing voltage.