

Supporting Information

Enhanced charge transport from Pd-doping in CsPbBr₃ quantum dots for efficient photoelectrocatalytic water splitting

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[PLEASE NOTE: this document contains an updated Table S2; it replaced the original version on 17th September 2024]

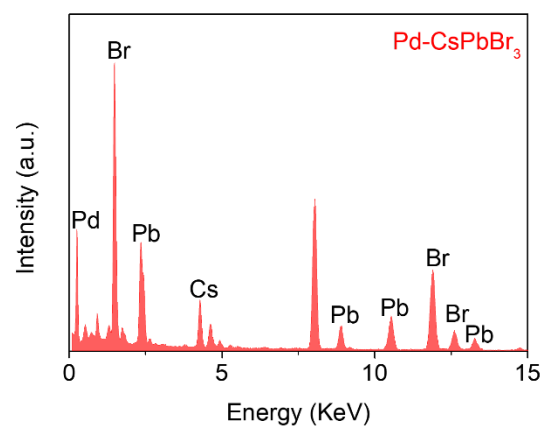


Figure S1 EDS of Pd-CsPbBr₃ QDs

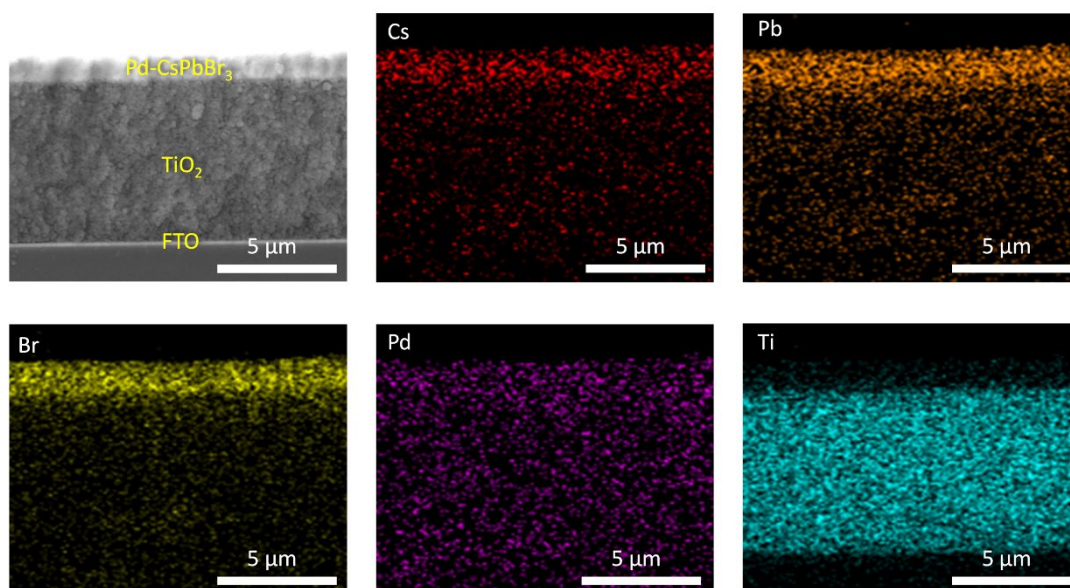


Figure S2. The cross-sectional SEM and EDS images of Pd-CsPbBr₃ QDs based device.

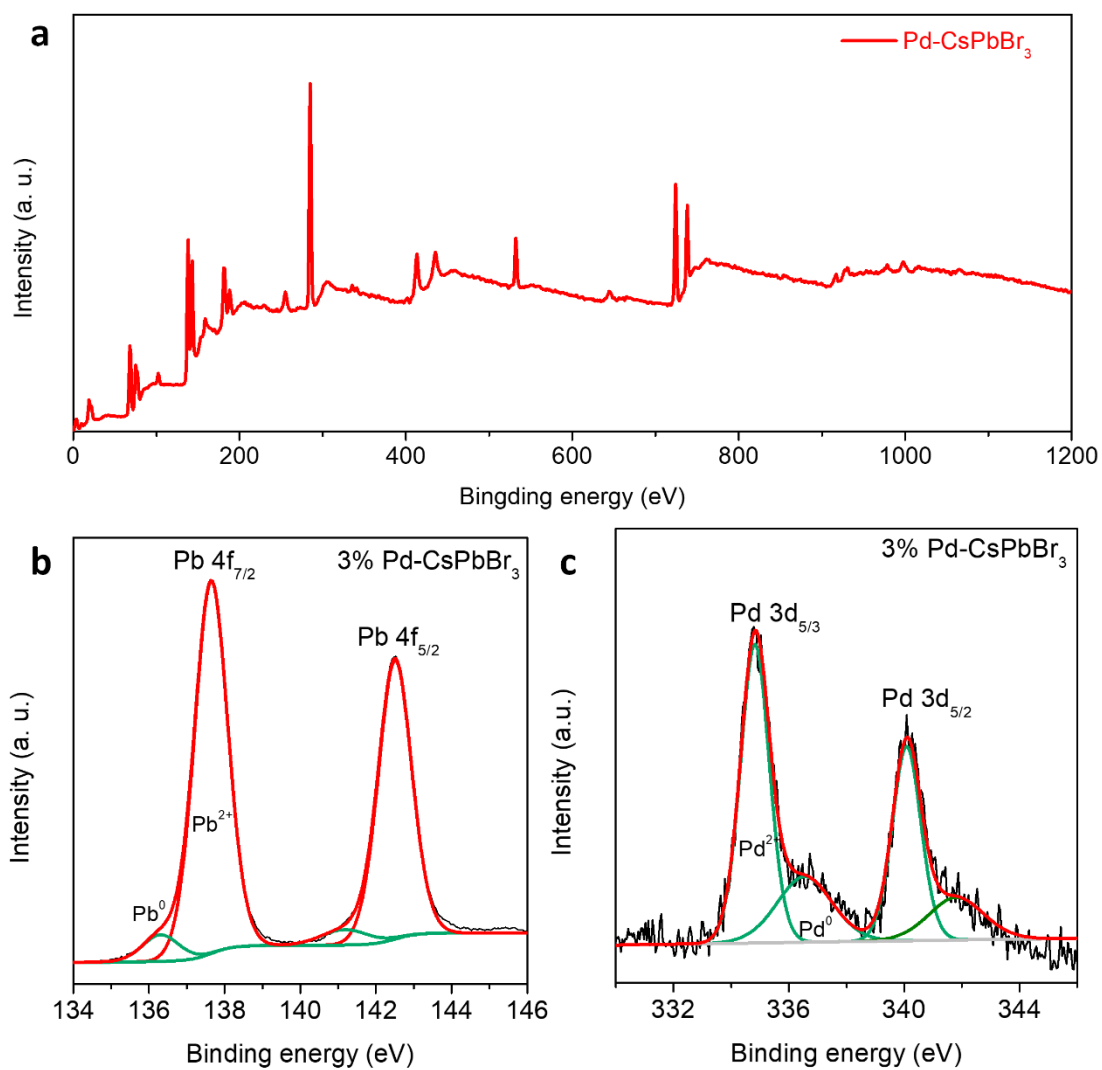


Figure S3. (a) The survey XPS spectrum of Pd-CsPbBr₃ QDs. The XPS (b) Pb 4f and Pd 3d spectrum of 3% Pd-CsPbBr₃ QDs.

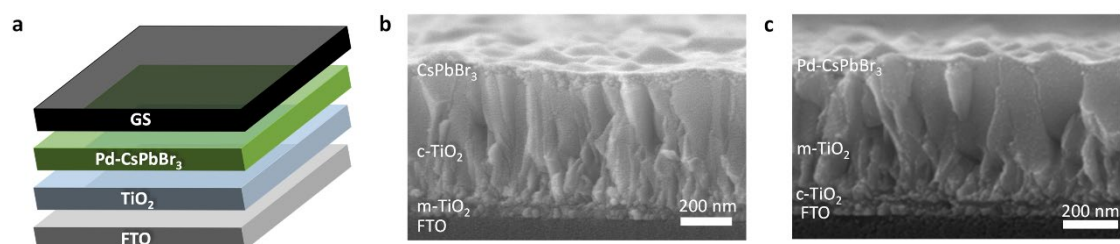


Figure S4. (a) The schematic of Pd-CsPbBr₃ QDs based device layer by layer. The cross-sectional EDS of the (b) CsPbBr₃ and (c) Pd-CsPbBr₃ QDs.

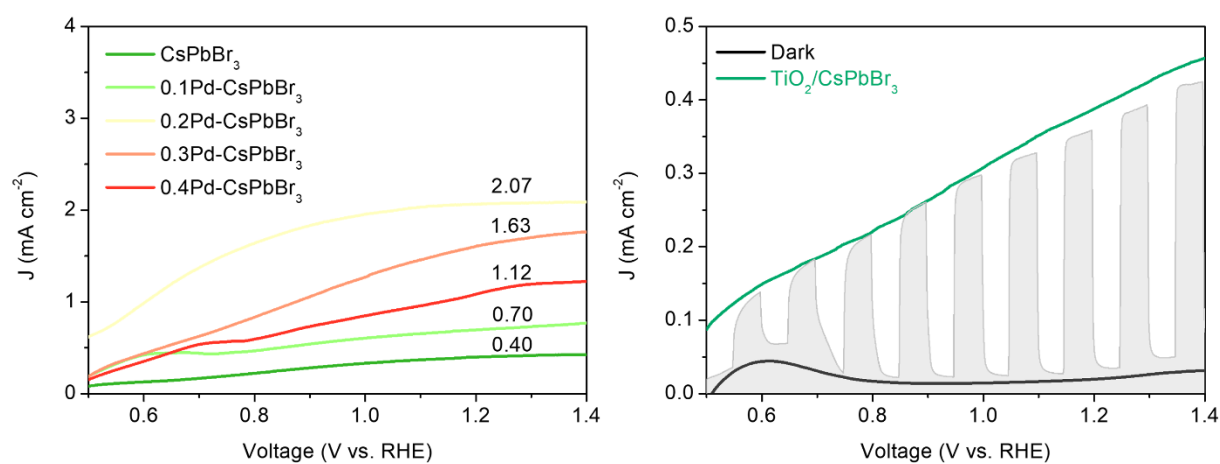


Figure S5. LSV of the Pd-CsPbBr₃ QDs based photoanode with different concentrations of Pd doping. The chopped plot of the CsPbBr₃ QDs based device.

Table S1. The cross-sectional element EDS mapping of Pd-CsPbBr₃ QDs based device.

Element	Weight percentage	Wt % Sigma
O	38.55	0.43
Ti	36.95	0.35
Pb	4.59	0.32
Br	12.89	0.20
Pd	2.60	0.22
Cs	4.42	0.35

Table S2. The Pd/Pb ratio versus dopant concentration of Pd-CsPbBr₃ QDs determined by ICP-OES.

Element	Pd	Cs	Pb	Br
W (%)	0.09	19.02	33.03	8.40

Table S3. High-resolution XPS peak positions of Cs, Br and Pb elements in CsPbBr₃ and Pd-CsPbBr₃ QDs.

Sample	Cs (eV)		Br (eV)		Pb (eV)	
	Cs	Cs	Br	Br	Pb	Pb
	3d _{5/3}	3d _{3/2}	3d _{5/3}	3d _{3/2}	4f _{7/2}	4f _{5/2}
CsPbBr ₃	722.0	735.9	66.2	67.3	136.4	141.3
Pd-CsPbBr ₃	722.0	735.9	66.2	67.3	136.6	141.5

Table S4. The corresponding band energy parameters of Pd-CsPbBr₃ and Pd-CsPbBr₃ QDs.

Sample	E _{GB} (eV)	E _F (eV)	E _{VB} (eV)	E _{CB} (eV)
CsPbBr ₃	2.35	-3.95	-5.95	-3.6
Pd-CsPbBr ₃	2.30	-4.02	-5.79	-3.49

Table S5. Fitted parameters of TRPL decay curves in perovskite films with using Pd-CsPbBr₃ and Pd-CsPbBr₃ QDs.

ETLs	A ₁	τ ₁ [ns]	A ₂	τ ₂ [ns]	τ [ns]
CsPbBr ₃	486.90	5.26	1304.30	0.91	3.87
Pd-CsPbBr ₃	899.99	2.28	396.35	13.38	10.28

The TRPL decay was fitted by a bi-exponential decay function with below equation:

$$PL_{intensity} = A_1 e^{\frac{-t}{\tau_1}} + A_2 e^{\frac{-t}{\tau_2}}$$

where A_1 and A_2 are time-independent coefficients of amplitude fraction for each decay component, τ_1 and τ_2 are decay time of a fast and slow component, respectively.