

Supplementary Information

Self-Assembled Molecules as Selective Contacts in CsPbBr₃ Nanocrystal Light Emitting Diodes

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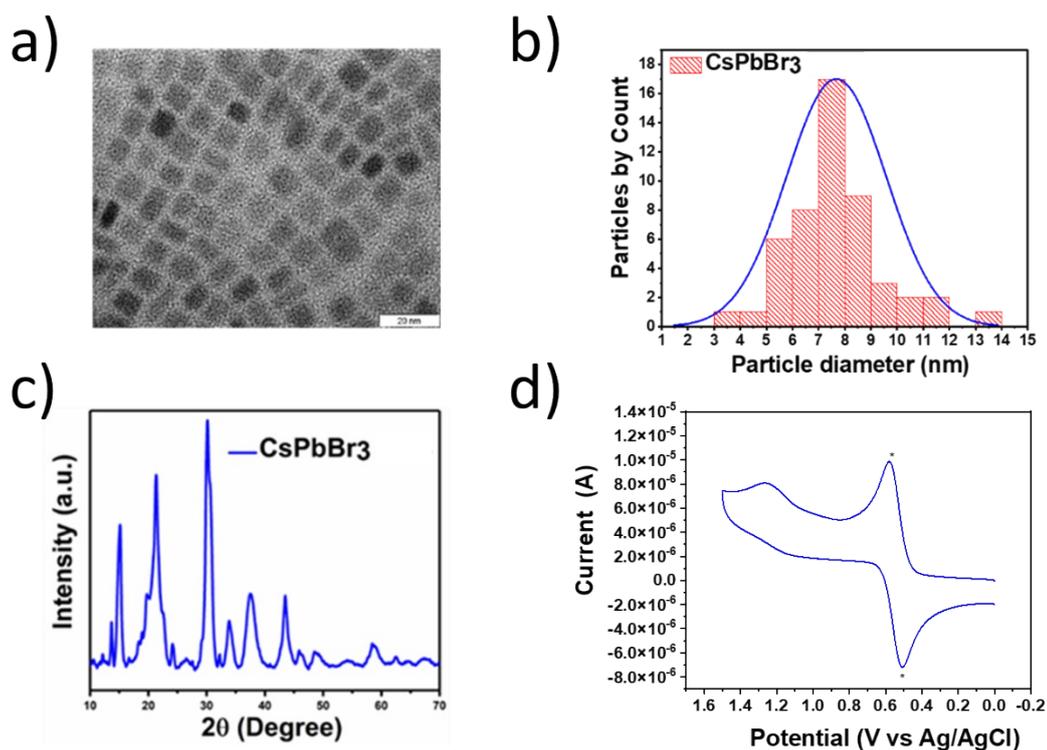


Figure S1. a) TEM images of the CsPbBr₃ nanocrystals (NCs) prepared in solution, b) histogram showing the particle size distribution as measured by TEM, c) XRD pattern of the CsPbBr₃ NCs prepared in solution, and d) cyclic voltammogram of the MHP NCs measured in toluene and 0.1 M TBAPF₆ using ferrocene as internal reference (the corresponding signals are marked by *).

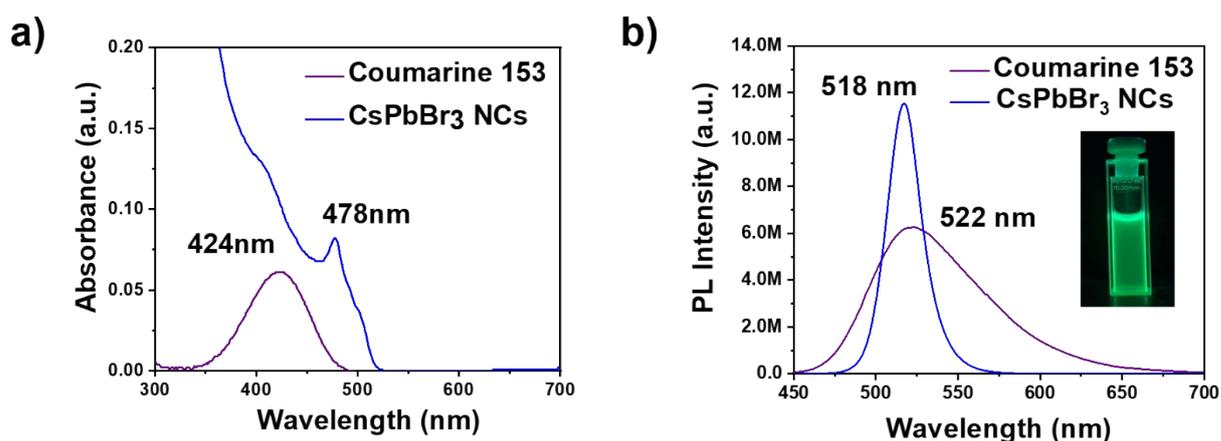


Figure S2. UV-vis absorption (a) and fluorescence spectra (b) of the CsPbBr₃ NCs in toluene solution and the solution of Coumarine 153 used as reference. The excitation wavelength was 424 nm.

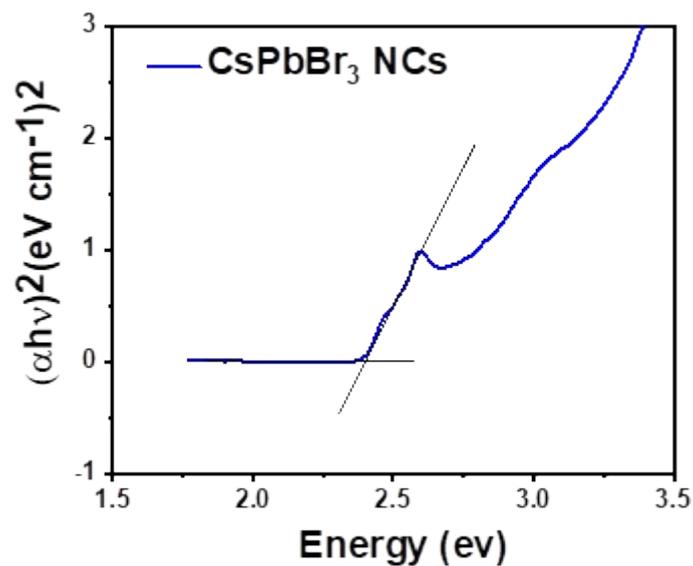


Figure S3. Tauc plot of the CsPbBr₃ NCs in toluene solution.

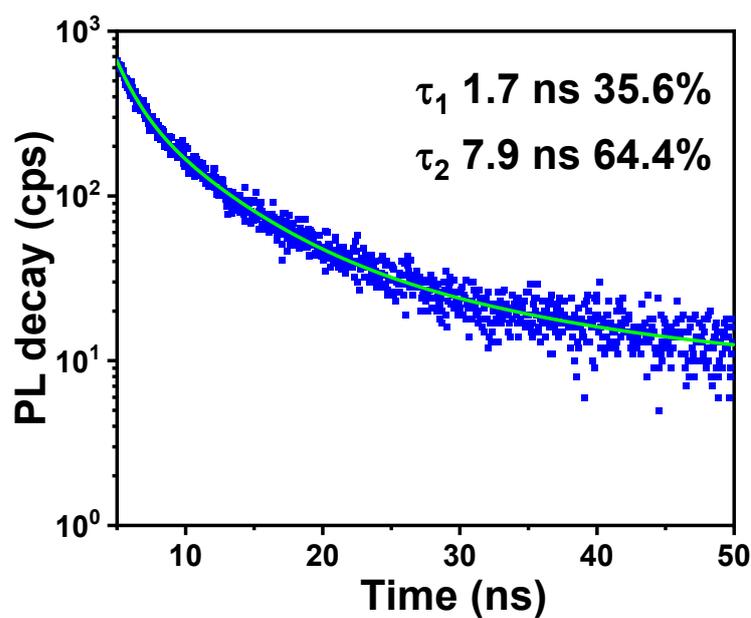


Figure S4. Photoluminescence decay with time of the CsPbBr₃ NCs in solution after excitation at 470 nm. The solid line represents the exponential fitted decay whose fitting parameters are indicated in the legend.

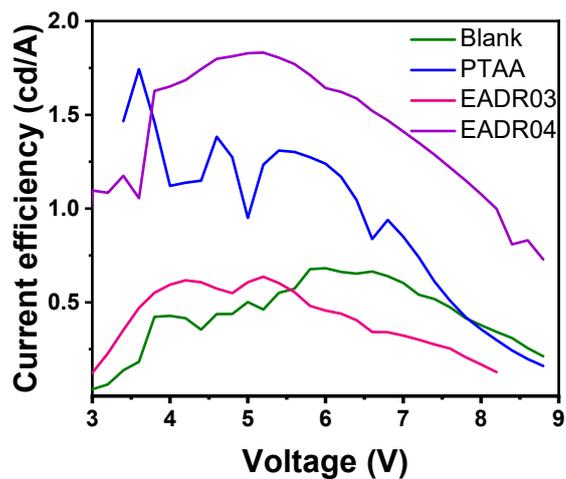


Figure S5. Current efficiency vs. applied bias for the PeLEDs prepared with different HTMs.

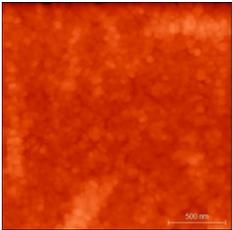
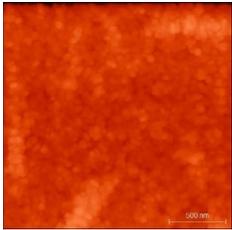
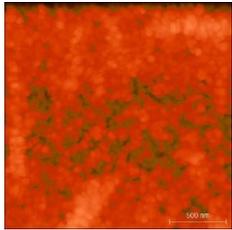
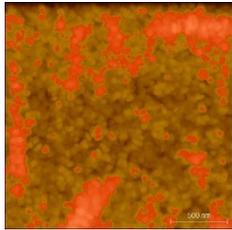
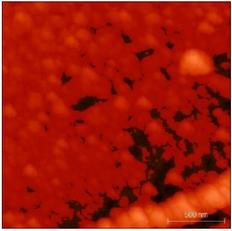
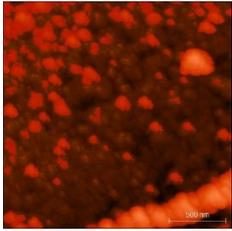
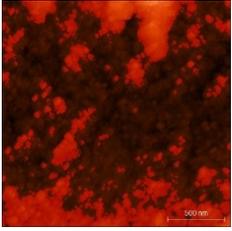
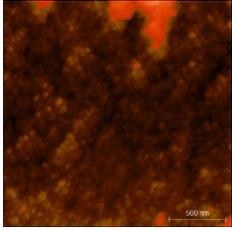
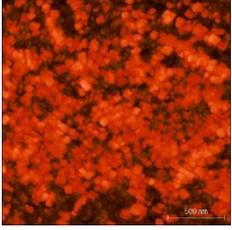
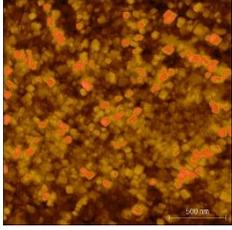
Sample	Threshold 15 nm	Threshold 25 nm	Threshold 40 nm	Threshold 50 nm
BLANK				
PTAA			-----	-----
EADR03			-----	-----
EADR04			-----	-----

Figure S6. Threshold image analysis of the AFM images of the films of ITO/HTM/CsPbBr₃ NCs where HTM is blank, PTAA, **EADR03**, and **EADR04**. The red colour correspond to the masked regions whose heigh is higher than the threshold value indicated at the top of each column.

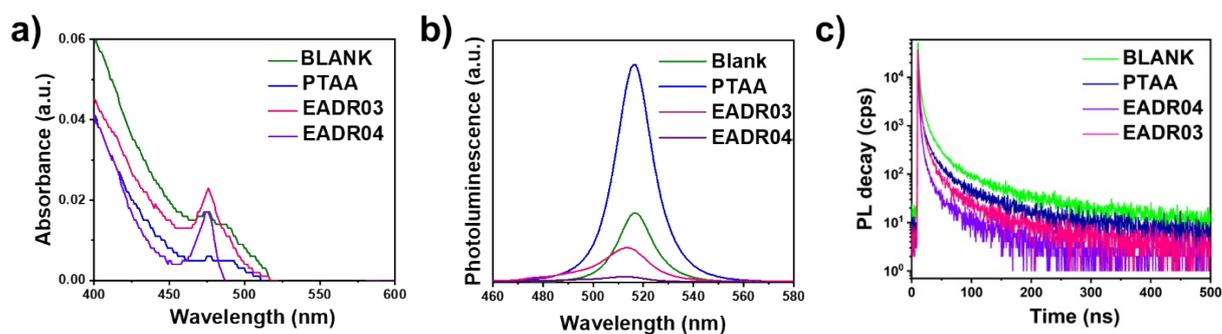


Figure S7. Optical characterization of the films made of ITO/HTMs/CsPbBr₃ NCs: (a) UV-VIS absorption spectra, (b) Steady-state fluorescence spectra of the samples covered with PMMA, and (c) Fluorescence time decay of the samples measured after excitation at 470 nm.

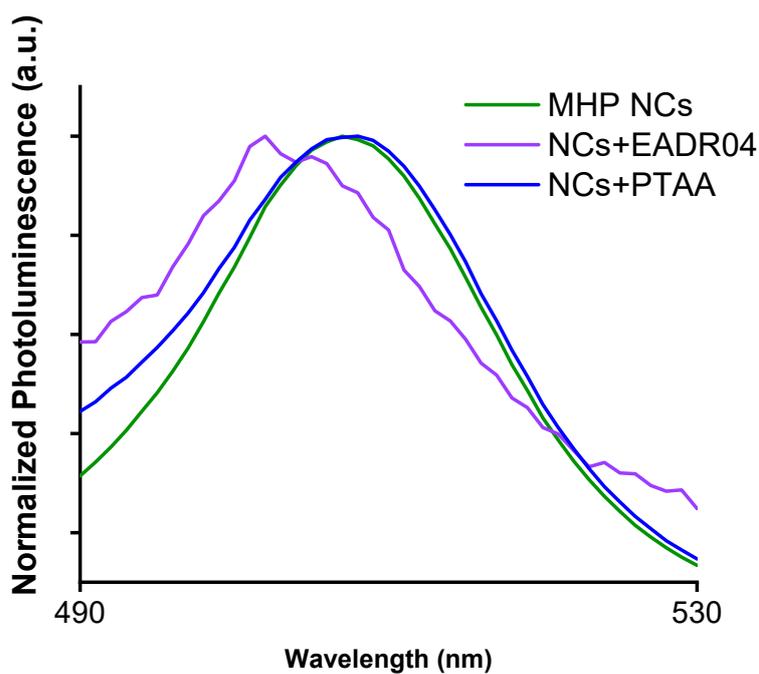


Figure S8. Steady-state fluorescence spectra of the solutions of MHP NCs, MHP NCs mixed with PTAA and MHP NCs mixed with **EADR04**.

REFERENCES

(1) Aktas, E.; Phung, N.; Köbler, H.; González, D. A.; Méndez, M.; Kafedjiska, I.; Turren-Cruz, S. H.; Wenisch, R.; Lauermann, I.; Abate, A.; Palomares, E. Understanding the Perovskite/Self-Assembled Selective Contact Interface for Ultra-Stable and Highly Efficient p-i-n Perovskite Solar Cells. *Energy Environ. Sci.* **2021**, *14* (7), 3976–3985. <https://doi.org/10.1039/d0ee03807e>.