

Supporting information

Construction 3D and 2D perovskites with N-methylpropane-1,3-diammonium as organic cation and superior interlayer charge transport in the 3D perovskite single crystal photodetector

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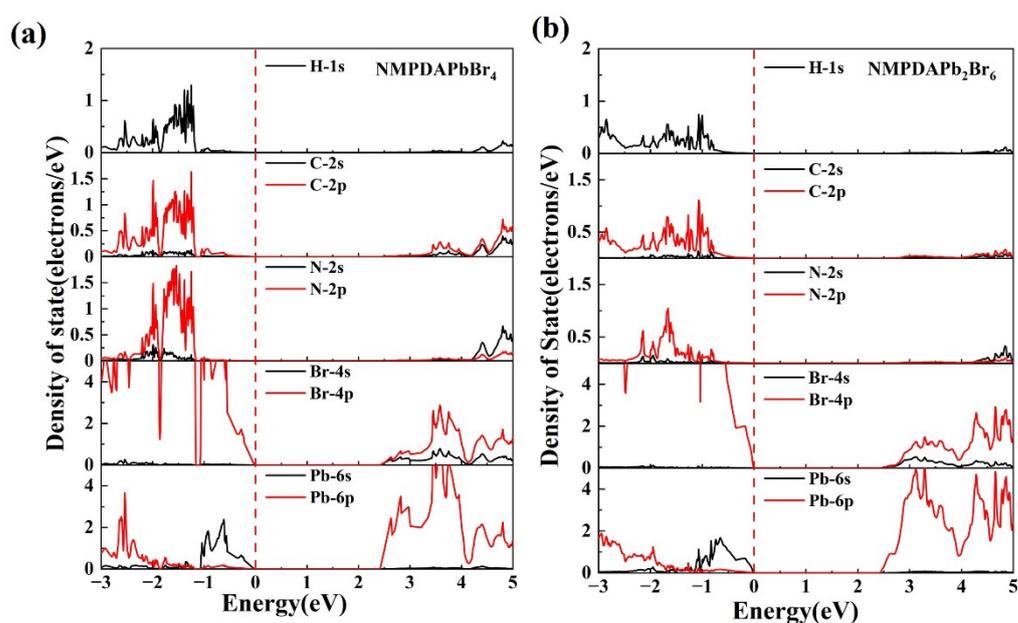


Fig. S1 PDOS of (a) (NMPDA)PbBr₄ and (b) (NMPDA)Pb₂Br₆. Using PBE+DFT-D3 method.

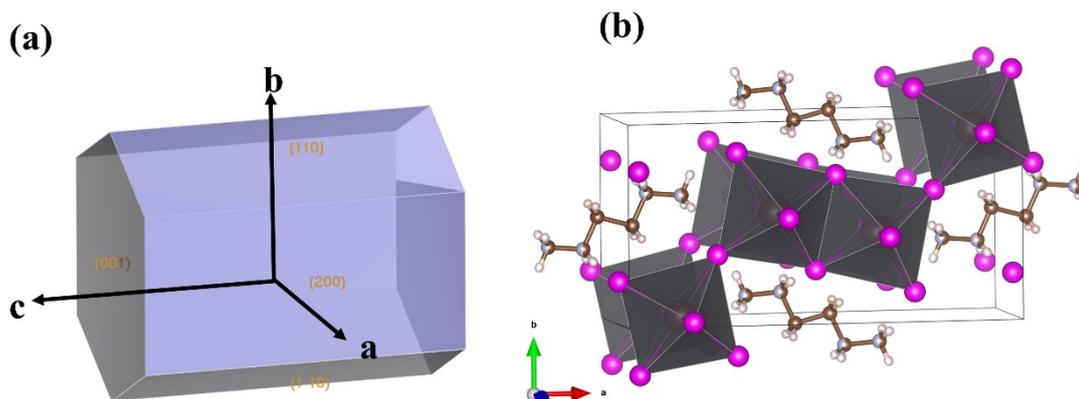


Fig. S2 (a) The calculated crystal morphology of (b) NMPDAPbBr₆ crystal structure.

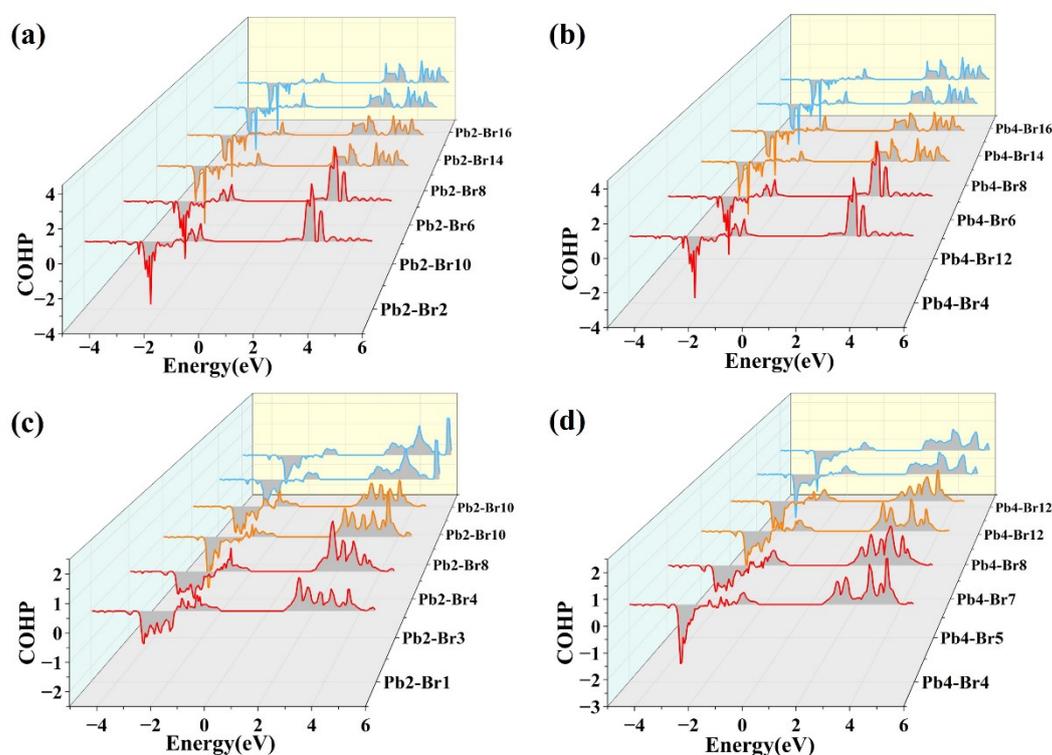


Fig. S3 Analysis of the bonding and antibonding states in the Pb-Br bonds formed by Br atoms coordinated to Pb2 and Pb4 in (NMPDA)PbBr₄ and (NMPDA)Pb₂Br₆, respectively. The six Pb-Br bonds surrounding (a) Pb2 and (b) Pb4 in (NMPDA)PbBr₄. The six Pb-Br bonds surrounding (c) Pb2 and (d) Pb4 in (NMPDA)Pb₂Br₆. COHP > 0 corresponds to the antibonding state, while a COHP < 0 corresponds to the bonding state.

Table S1: The Br–Pb–Br bond angles in (NMPDA)PbBr₄ and (NMPDA)Pb₂Br₆ after optimization using the PBE + DFT-D3 method

(NMPDA)PbBr ₄	(°)	(NMPDA)Pb ₂ Br ₆	(°)
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Br10-Pb2-Br14	95.1288	Br10-Pb2-Br4	91.4111
Br10-Pb2-Br6	95.1571	Br10-Pb2-Br3	90.5994
Br10-Pb2-Br8	83.5725	Br10-Pb2-Br1	88.6431
Br10-Pb2-Br16	87.3037	Br10-Pb2-Br8	89.1460
Br2-Pb2-Br14	95.7664	Br10-Pb2-Br4	91.4113
Br2-Pb2-Br6	84.6100	Br10-Pb2-Br3	90.5996
Br2-Pb2-Br8	85.5220	Br10-Pb2-Br1	88.6430
Br2-Pb2-Br16	93.0133	Br10-Pb2-Br8	89.1459
Br14-Pb2-Br6	88.7521	Br4-Pb2-Br3	89.5225
Br14-Pb2-Br16	90.8232	Br4-Pb2-Br8	101.3519
Br8-Pb2-Br6	89.2426	Br1-Pb2-Br3	85.6722
Br8-Pb2-Br16	91.2432	Br1-Pb2-Br8	83.4534

Note: The blue font in the table represents the axial Br–Pb–Br bond angles, while the black font denotes the equatorial Br–Pb–Br bond angles.

Table S2: Performance Comparison of various Perovskite-based Photodetectors

Materials	Wavelength & Power	R(mA/W)	D_{shot}^* (Jones)	References
(AMP)MAPb ₂ I ₇	532nm/0.4mWcm ⁻²	0.16	4.95×10^{10}	1
(BA) ₂ PbBr ₄	447nm/0.5μWcm ⁻²	0.38	9.01×10^{10}	2
(BDA)PbI ₄	532nm/99.94mWcm ⁻²	0.15	5.27×10^8	3
(PEA) ₂ PbBr ₄	380nm/2 × 10 ⁻⁴ mWcm ⁻²	8.26	2×10^{12}	4
(NMPDA)Pb ₂ Br ₆	365nm/0.15 mWcm ⁻²	8.47	6.34×10^{11}	This work

References

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