

Supplementary Materials for **Molecular behavior of zero-dimensional perovskites**

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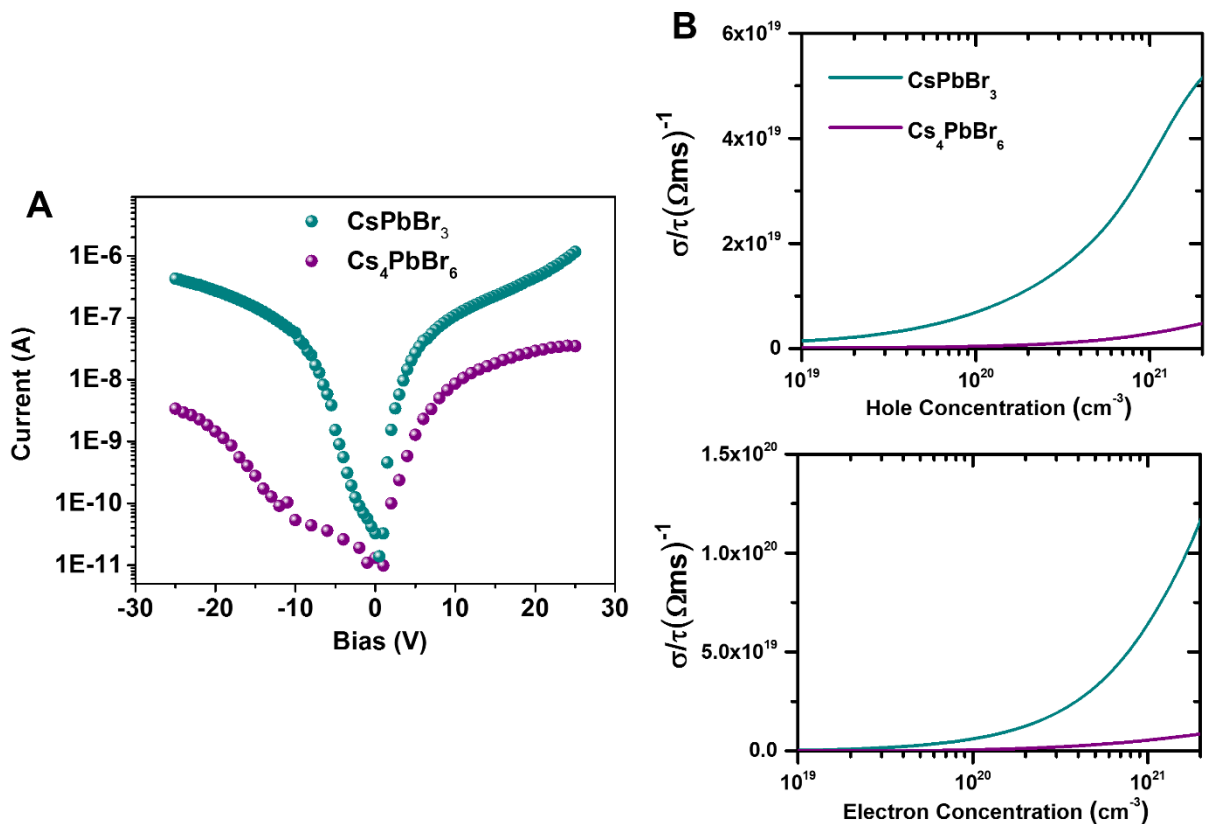


fig. S1. Experimental and calculated electrical conductivity of CsPbBr₃ and Cs₄PbBr₆. (A) current-voltage curves in dark of CsPbBr₃ and Cs₄PbBr₆ thin films; (B) calculated electrical conductivity (σ/τ) as a function of carrier concentration of 3D CsPbBr₃ and 0D Cs₄PbBr₆ at 300 K.

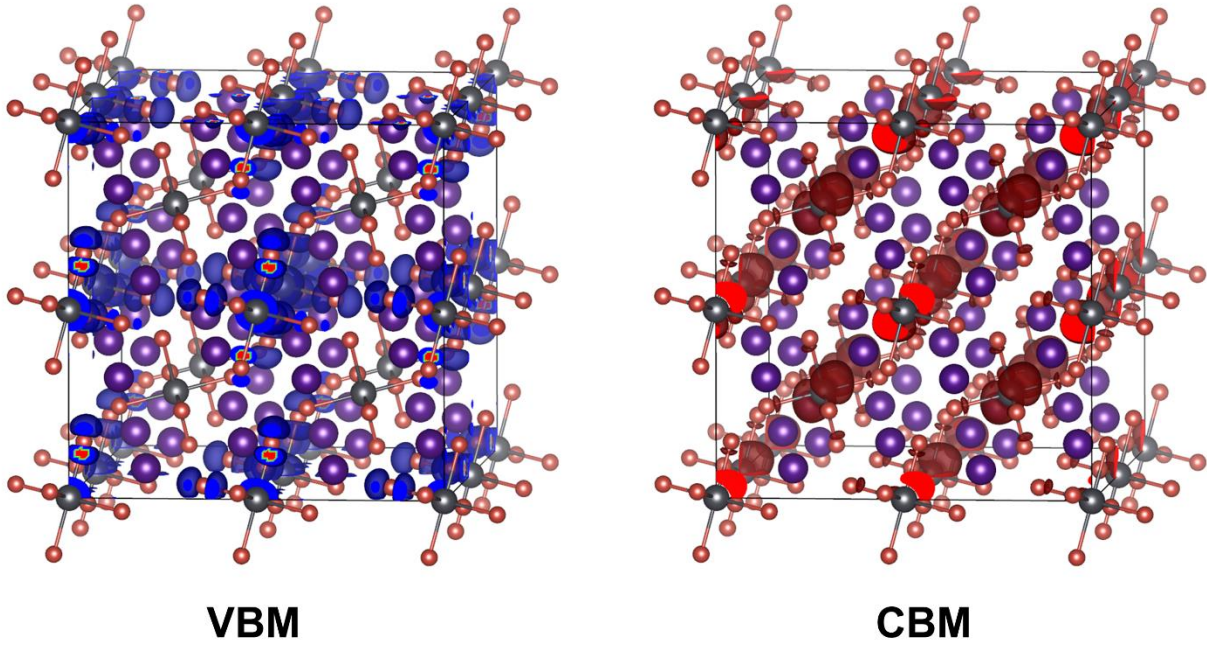


fig. S2. Charge density descriptions of Cs₄PbBr₆ supercell. Charge density descriptions of the valence band maximum (VBM) and conduction band minimum (CBM) for a 2×2×2 Cs₄PbBr₆ supercell.

table S1. Calculated charge transfer parameters and mobility of the Cs₄PbBr₆ crystal.

| Charge Carriers | Pathway | Electronic Coupling (meV) | Distance (Å) | Charge Transfer Rate (s ⁻¹) | Mobility (cm ² /V·s) |
|-----------------|---------|---------------------------|--------------|---|---------------------------------|
| hole | 1 | 4.40 | 10.0 | 1.69×10 ⁴ | 1.35×10 ⁻⁹ |
| | 2 | 6.41 | 8.62 | 3.57×10 ⁴ | |
| | 3 | 4.08 | 8.77 | 1.45×10 ⁴ | |
| electron | 1 | 244 | 10.0 | 345 | 2.20×10 ⁻¹¹ |
| | 2 | 32.1 | 8.62 | 5.98 | |
| | 3 | 7.05 | 8.77 | 0.29 | |

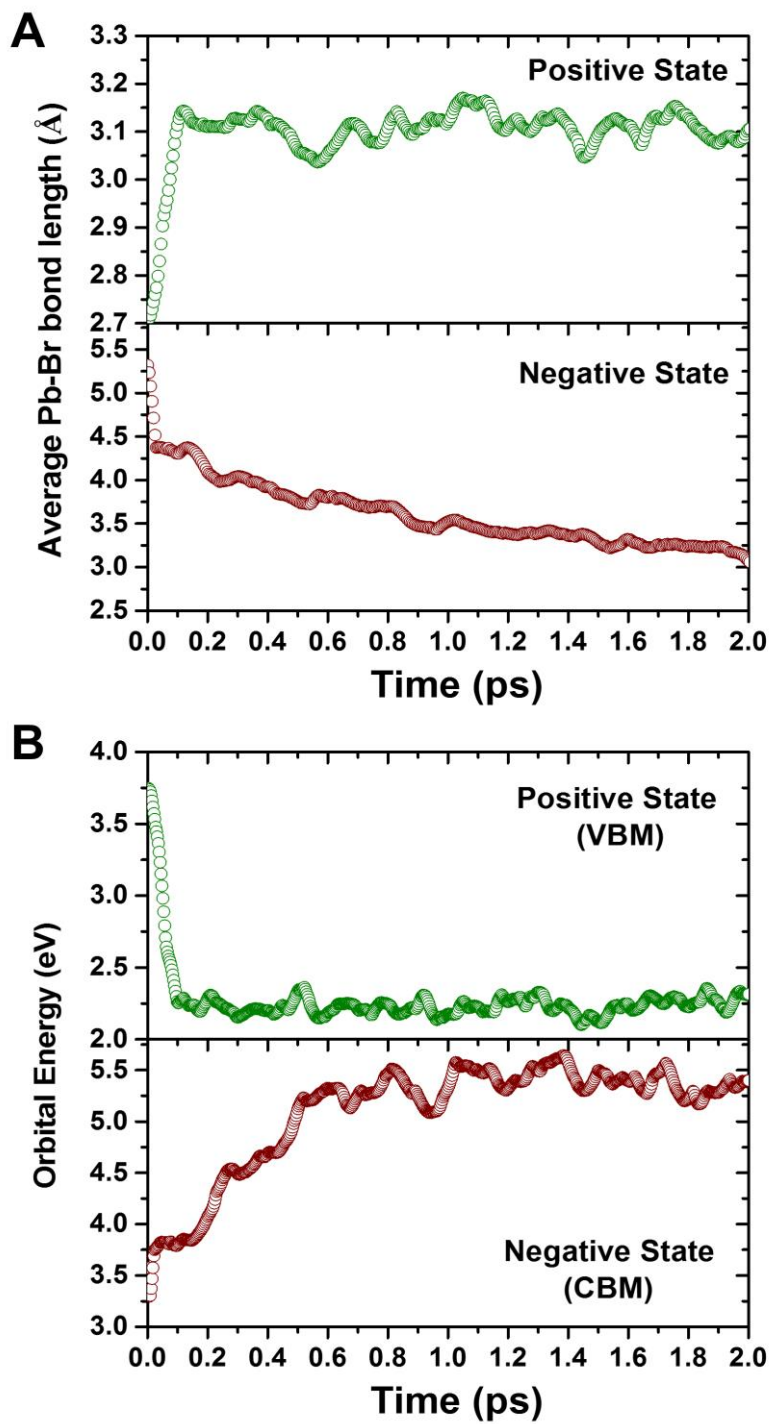


fig. S3. Average Pb–Br bond length and orbital energy evolution. (A) Average Pb-Br bond length evolution in the central $[\text{PbBr}_6]^{4-}$ octahedron and (B) VBM and CBM energy evolution, starting from initial positive and negative polaronic states at 300K.

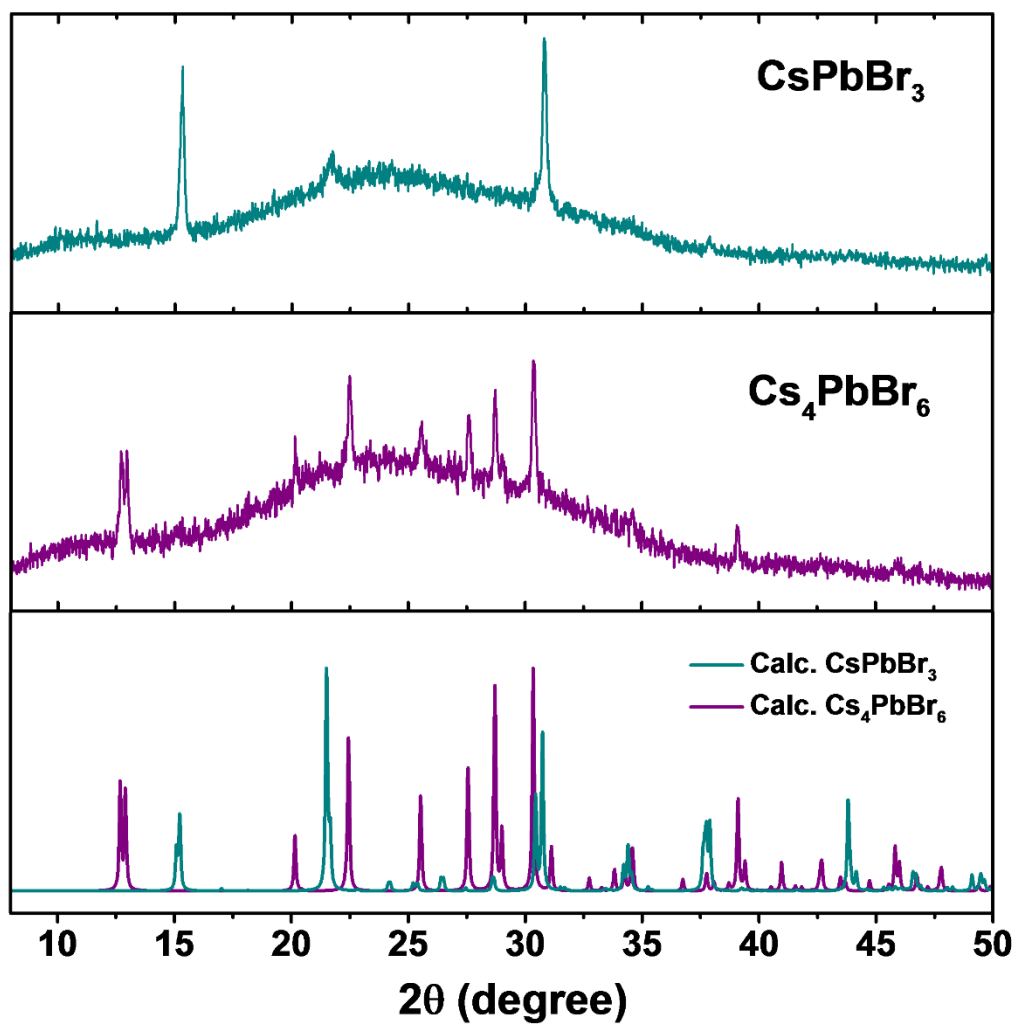


fig. S4. X-ray diffraction patterns of CsPbBr_3 and Cs_4PbBr_6 thin films.