

Structural and Optoelectronic Properties of Two-Dimensional Ruddlesden–Popper Hybrid Perovskite CsSnBr_3

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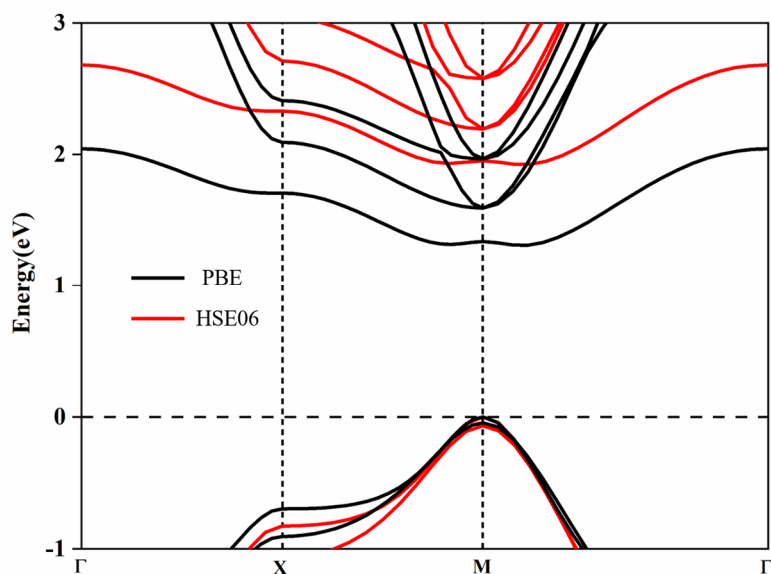


Figure S1. band structure of $\text{Cs}_n\text{Sn}_{n+1}\text{Br}_{3n+2}$ ($n=1$) calculated by PBE (black lines) and HSE06 (red lines) DFT.

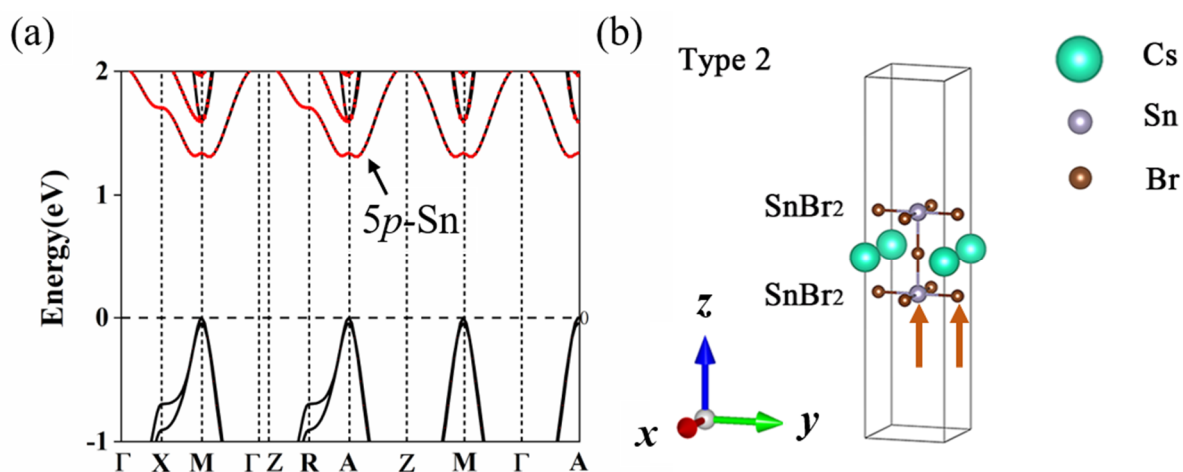


Figure S2. (a) Orbital-projected band structure of $\text{Cs}_n\text{Sn}_{n+1}\text{Br}_{3n+2}$ ($n = 1$). (b) Model of $\text{Cs}_n\text{Sn}_{n+1}\text{Br}_{3n+2}$ ($n = 1$). The arrow points to the Sn and Br atoms in SnBr_2 -terminated surface.

Table S1. All variables use in this work, including variables name and physical meanings.

| variables | physical meanings | variables | physical meanings |
|-----------------|--------------------------------------|-----------------|---|
| a_0 | lattice constant | P | principal value of the integral |
| n | layers | p | momentum transition matrix |
| d | interplanar distance | | dielectric function |
| δ | relative displacements | ω | frequency of light |
| i | layers rumpling | α | absorption coefficient |
| θ | angle degree | \hbar | reduced Planck Constant |
| V | unit volume | e | electron charge |
| ε_1 | real part of the dielectric function | ε_2 | imaginary part of the dielectric function |
| kn | wave function of the conduction band | kn' | wave function of the valence band |