

Supplementary Materials

# A First-Principles Study on the Structural and Carrier Transport Properties of Inorganic Perovskite CsPbI<sub>3</sub> under Pressure

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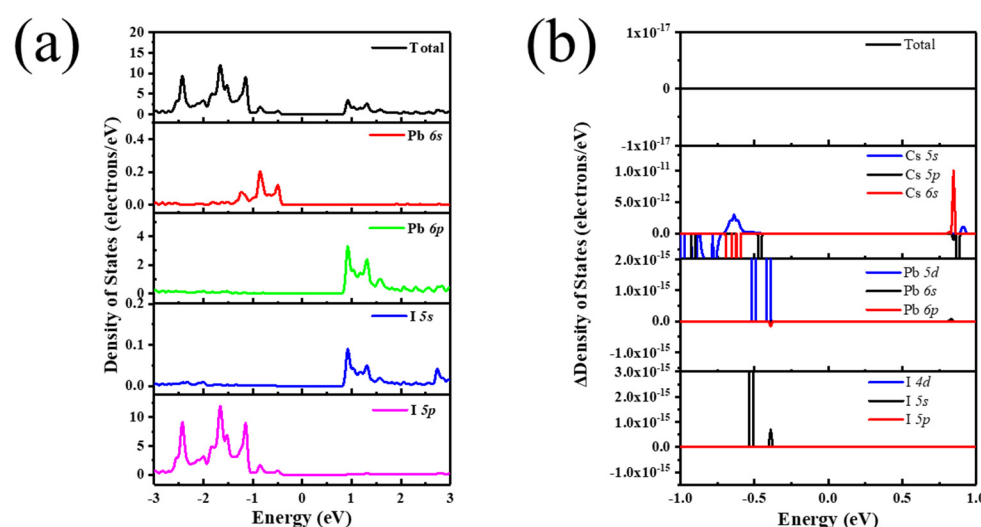
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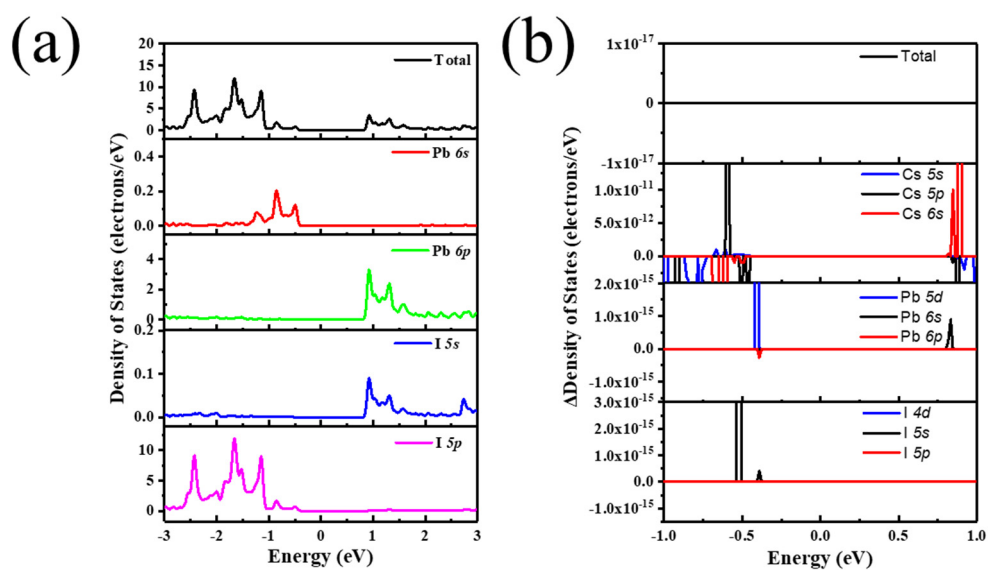
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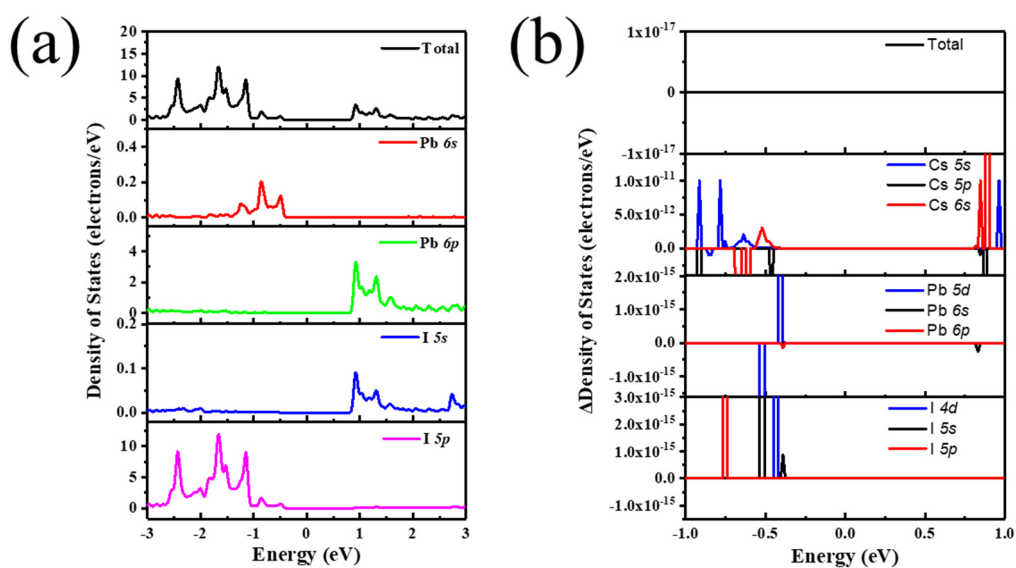
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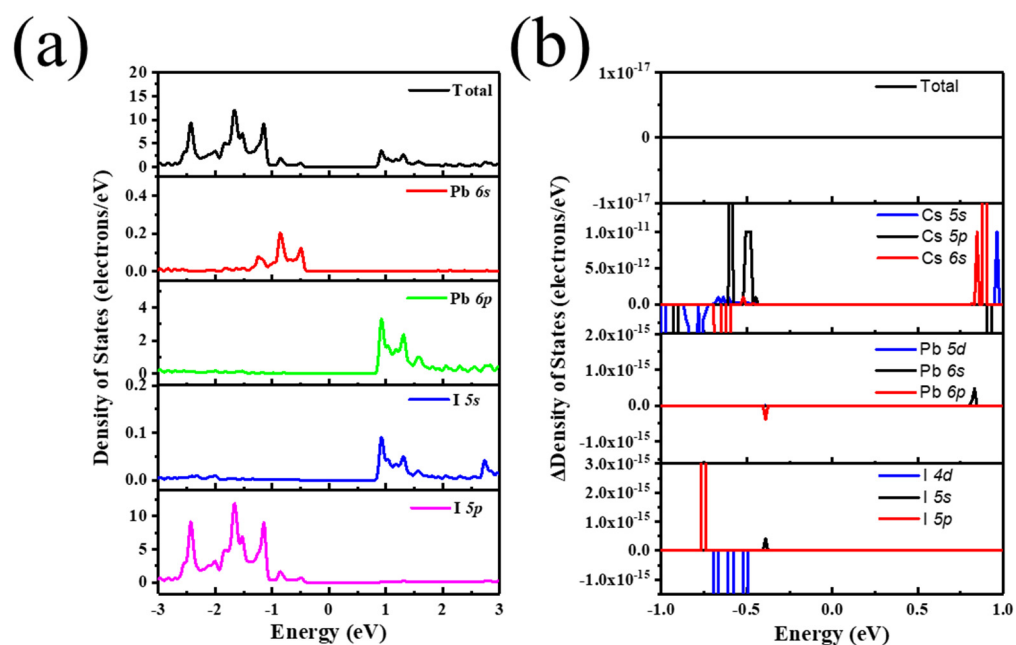
**Figure S1.** The DOS of perovskite CsPbI<sub>3</sub> under different pressure. (a) 2 kPa. (b) The DOS difference between 0 and 2 kPa.



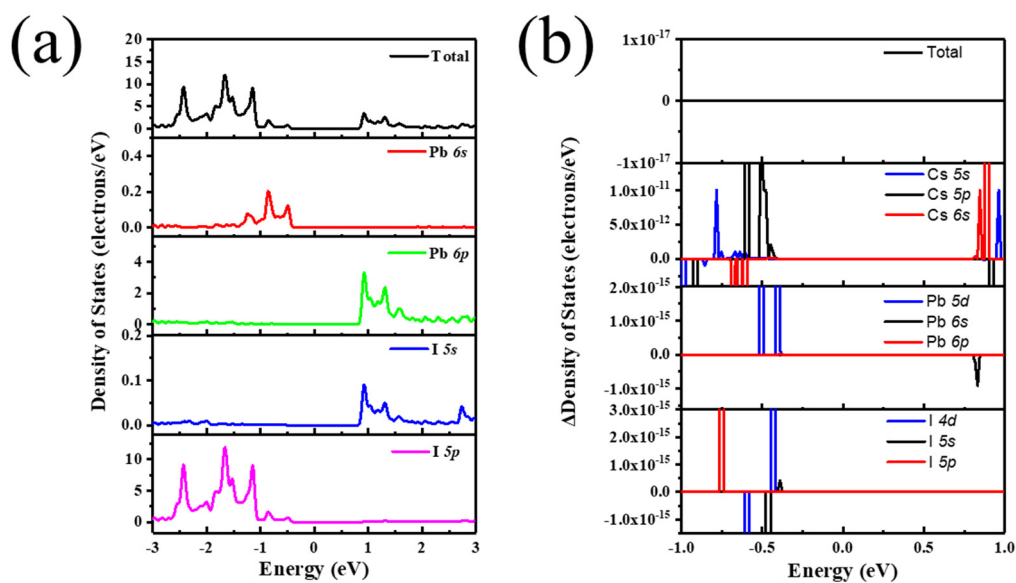
**Figure S2.** The DOS of perovskite CsPbI<sub>3</sub> under different pressure. (a) 4 kPa. (b) The DOS difference between 0 and 4 kPa.



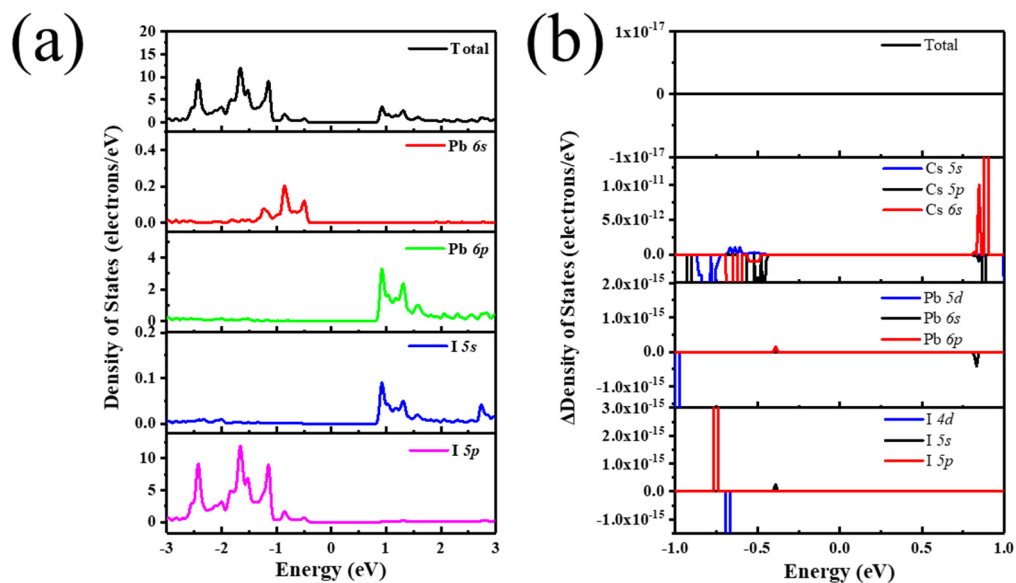
**Figure S3.** The DOS of perovskite CsPbI<sub>3</sub> under different pressure. (a) 6 kPa. (b) The DOS difference between 0 and 6 kPa.



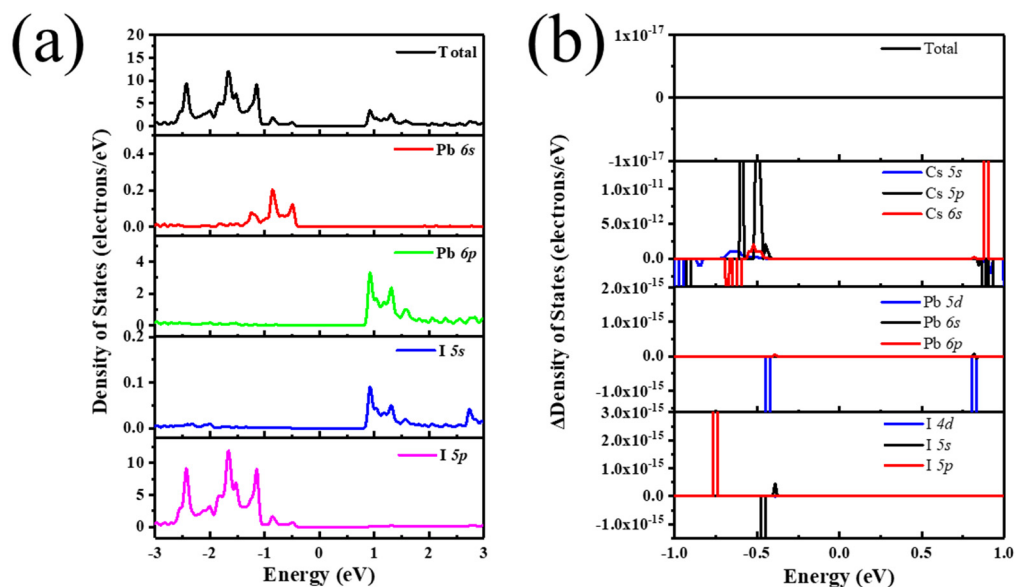
**Figure S4.** The DOS of perovskite CsPbI<sub>3</sub> under different pressure. (a) 8 kPa. (b) The DOS difference between 0 and 8 kPa.



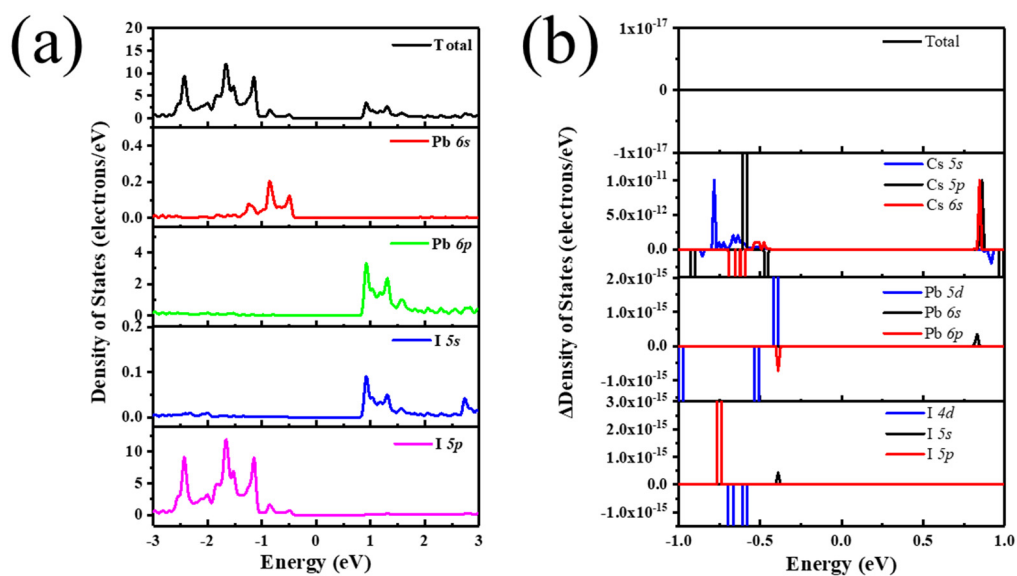
**Figure S5.** The DOS of perovskite CsPbI<sub>3</sub> under different pressure. (a) 12 kPa. (b) The DOS difference between 0 and 12 kPa.



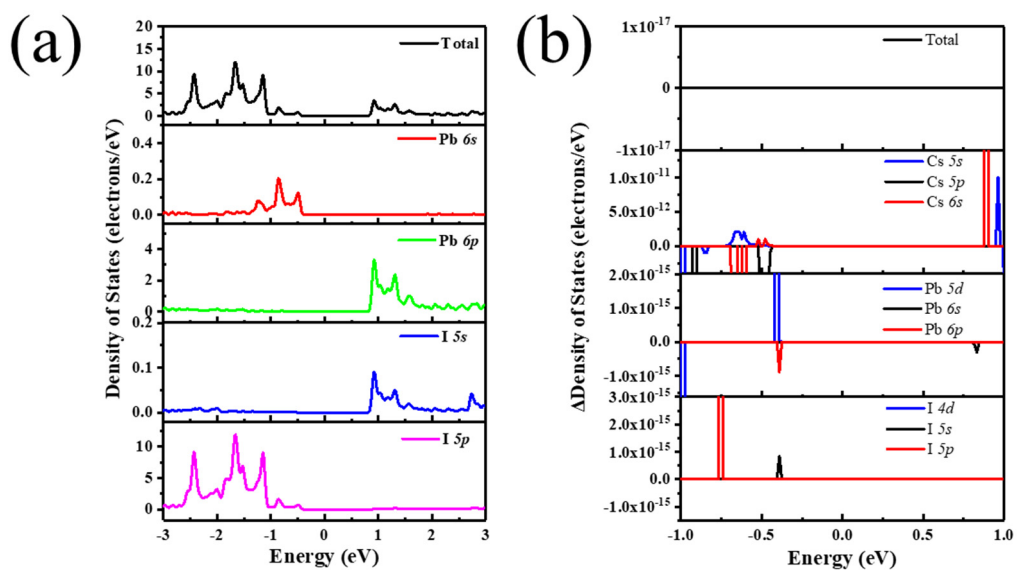
**Figure S6.** The DOS of perovskite CsPbI<sub>3</sub> under different pressure. (a) 14 kPa. (b) The DOS difference between 0 and 14 kPa.



**Figure S7.** The DOS of perovskite CsPbI<sub>3</sub> under different pressure. (a) 16 kPa. (b) The DOS difference between 0 and 16 kPa.



**Figure S8.** The DOS of perovskite CsPbI<sub>3</sub> under different pressure. (a) 18 kPa. (b) The DOS difference between 0 and 18 kPa.



**Figure S9.** The DOS of perovskite CsPbI<sub>3</sub> under different pressure. (a) 20 kPa. (b) The DOS difference between 0 and 20 kPa.

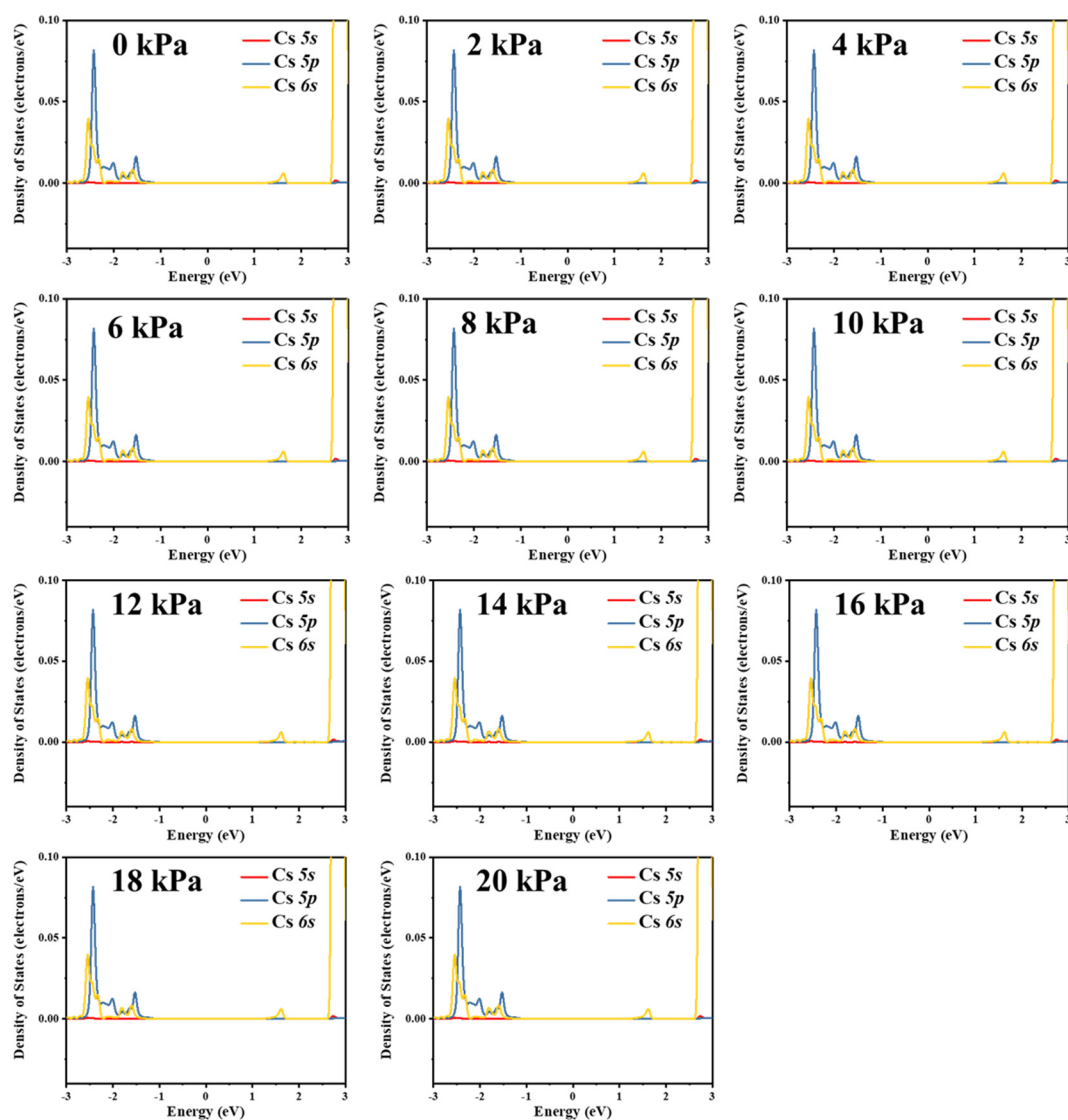


Figure S10. The PDOS of Cs in perovskite CsPbI<sub>3</sub> under different pressure.

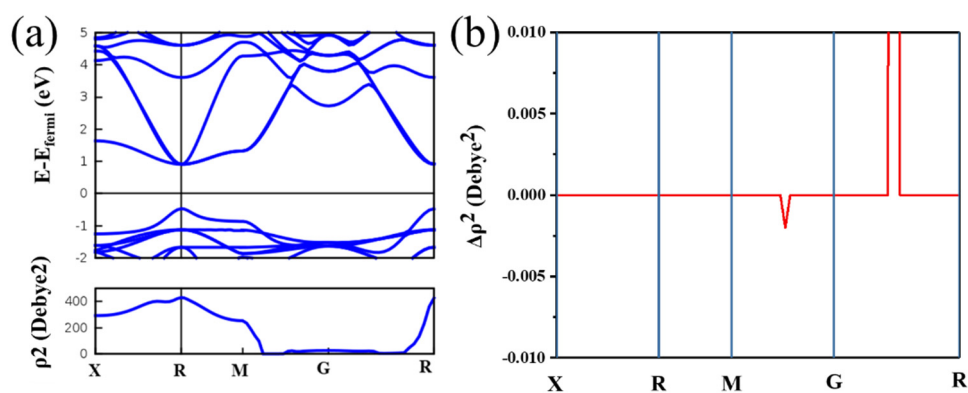
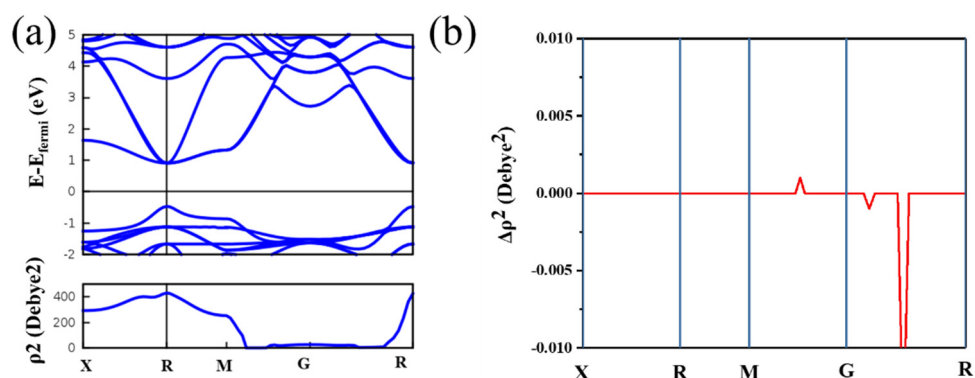
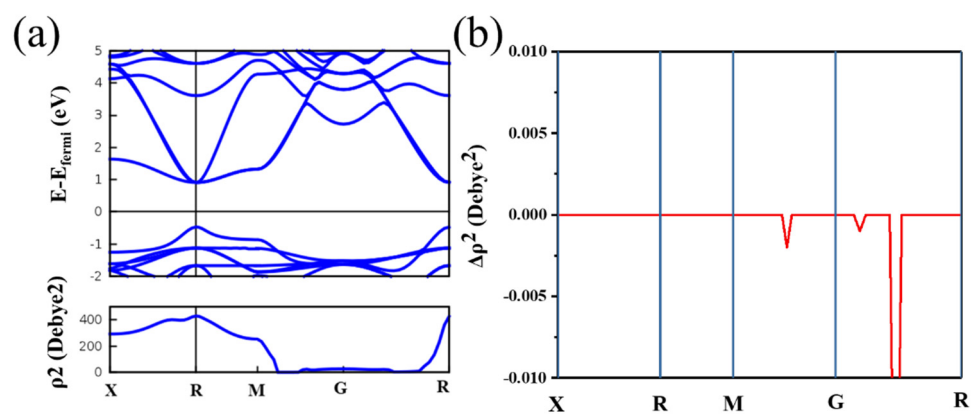


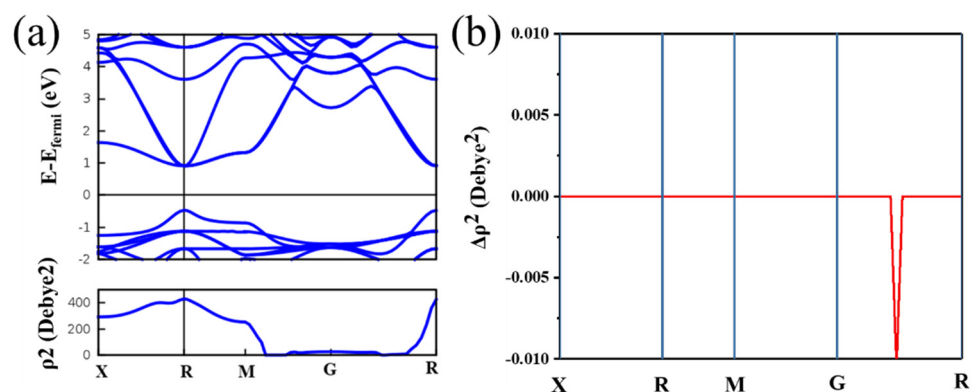
Figure S11. The electronic band structure and transition dipole moment. (a) The upper is electronic band structure and the bottom is transition dipole moment under pressure 2 kPa. (b) The transition dipole moment difference between 0 and 2 kPa.



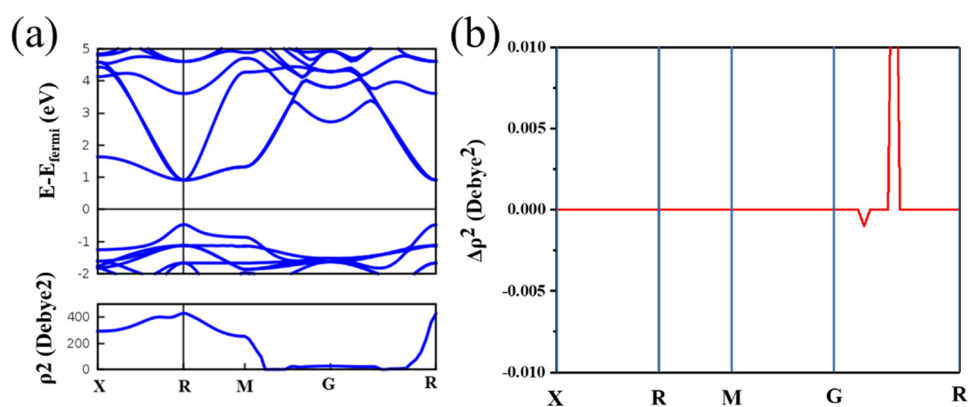
**Figure S12.** The electronic band structure and transition dipole moment. (a) The upper is electronic band structure and the bottom is transition dipole moment under pressure 4 kPa. (b) The transition dipole moment difference between 0 and 4 kPa.



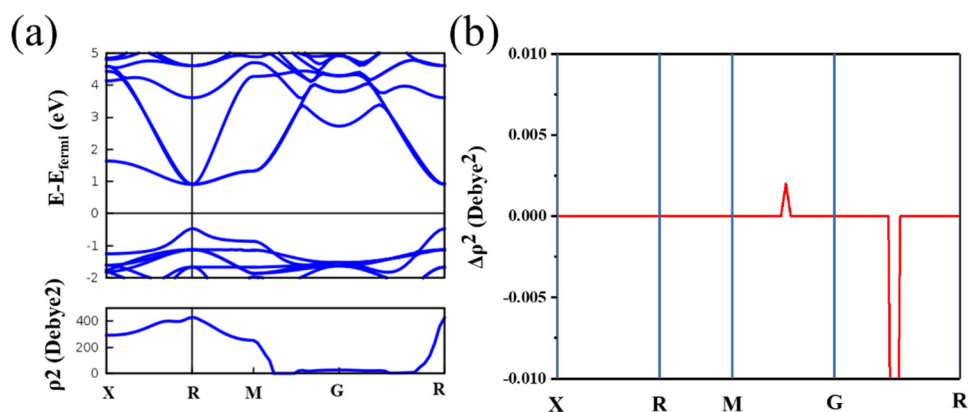
**Figure S13.** The electronic band structure and transition dipole moment. (a) The upper is electronic band structure and the bottom is transition dipole moment under pressure 6 kPa. (b) The transition dipole moment difference between 0 and 6 kPa.



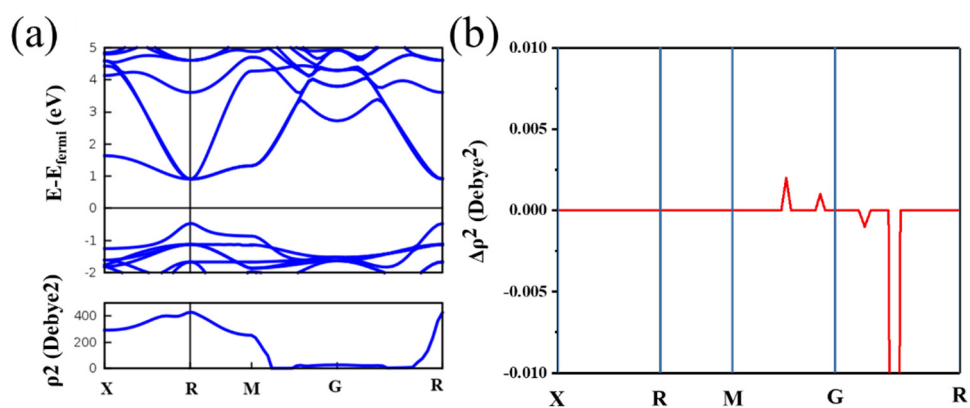
**Figure S14.** The electronic band structure and transition dipole moment. (a) The upper is electronic band structure and the bottom is transition dipole moment under pressure 8 kPa. (b) The transition dipole moment difference between 0 and 8 kPa.



**Figure S15.** The electronic band structure and transition dipole moment. (a) The upper is electronic band structure and the bottom is transition dipole moment under pressure 12 kPa. (b) The transition dipole moment difference between 0 and 12 kPa.

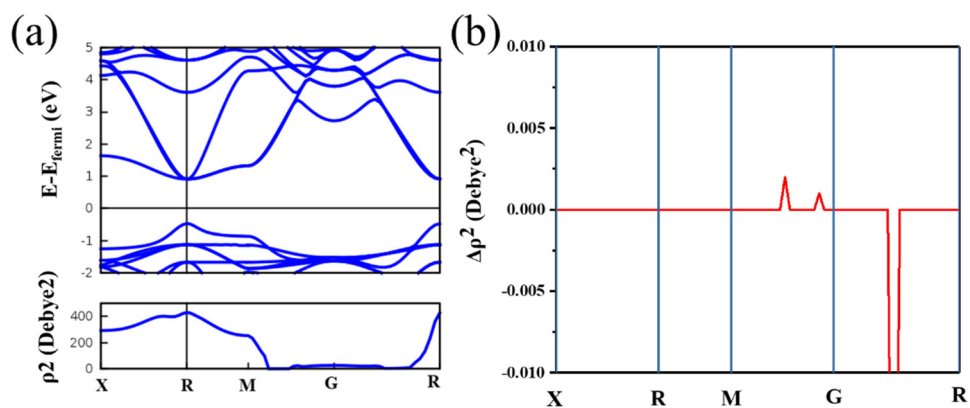


**Figure S16.** The electronic band structure and transition dipole moment. (a) The upper is electronic band structure and the bottom is transition dipole moment under pressure 14 kPa. (b) The transition dipole moment difference between 0 and 14 kPa.

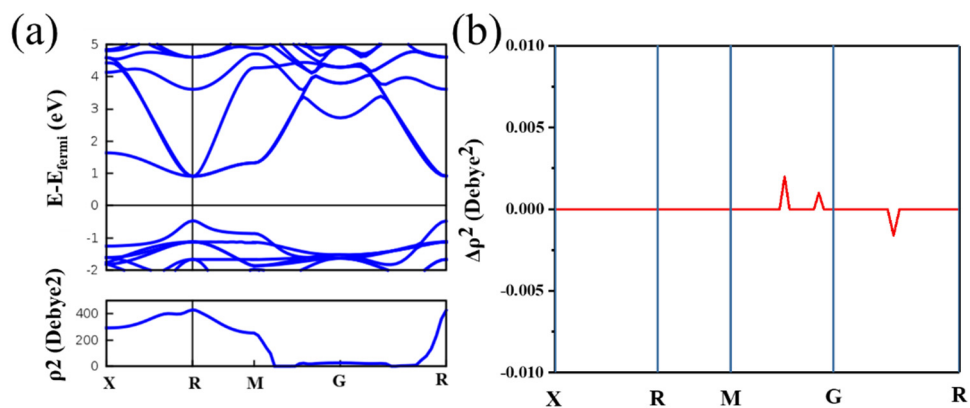


**Figure S17.** The electronic band structure and transition dipole moment. (a) The upper is electronic band structure and the bottom is transition dipole moment under pressure 16 kPa. (b) The transition dipole moment difference between 0 and 16 kPa.

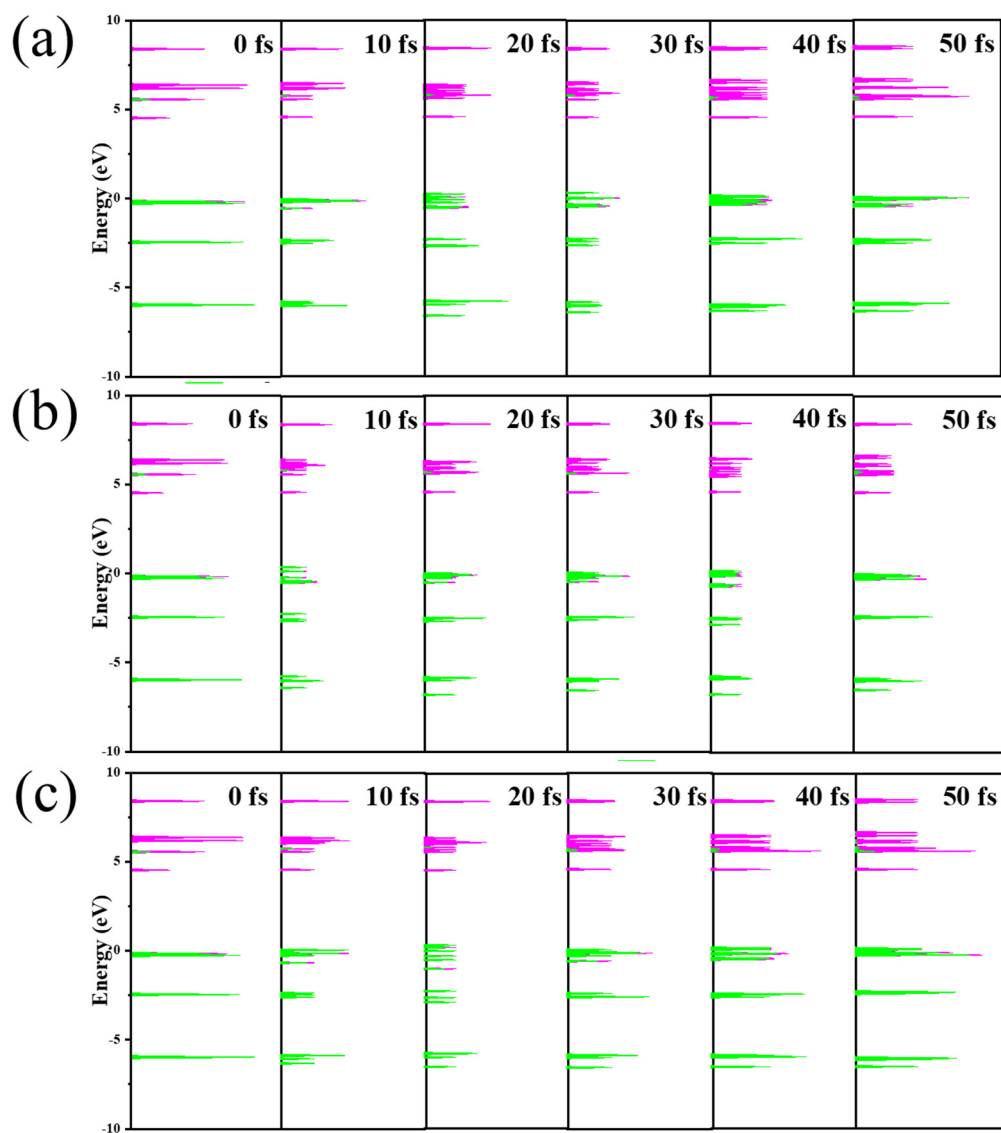




**Figure S18.** The electronic band structure and transition dipole moment. (a) The upper is electronic band structure and the bottom is transition dipole moment under pressure 18 kPa. (b) The transition dipole moment difference between 0 and 18 kPa.



**Figure S19.** The electronic band structure and transition dipole moment. (a) The upper is electronic band structure and the bottom is transition dipole moment under pressure 18kPa. (b) The transition dipole moment difference between 0 and 18 kPa.



**Figure S20.** The evolution of perovskite CsPbI<sub>3</sub> excited carriers under pressure. (a) 0 kPa; (b) 10 kPa; (c) 20 kPa.