

1 **Supporting information for**
2 **“Influence of Sr doping on the photoelectronic properties of CsPbX₃**
3 **(X=Cl, Br, or I): A DFT investigation”**

4 Man Zhang^a, Guangbiao Xiang^a, Yanwen Wu^a, Jing Liu^a, Jiancai Leng^{b*}, Chen
5 Cheng^{a*}, Hong Ma^{a*}

6 ^a Shandong Provincial Key Laboratory of Optics and Photonic Device and Collaborative Innovation
7 Center of Light Manipulations and Applications, School of Physics and Electronics, Shandong
8 Normal University, Jinan 250014, China;

9 ^b School of Electronic and Information Engineering (Department of Physics), Qilu University of
10 Technology (Shandong Academy of Sciences), Jinan 250353, China

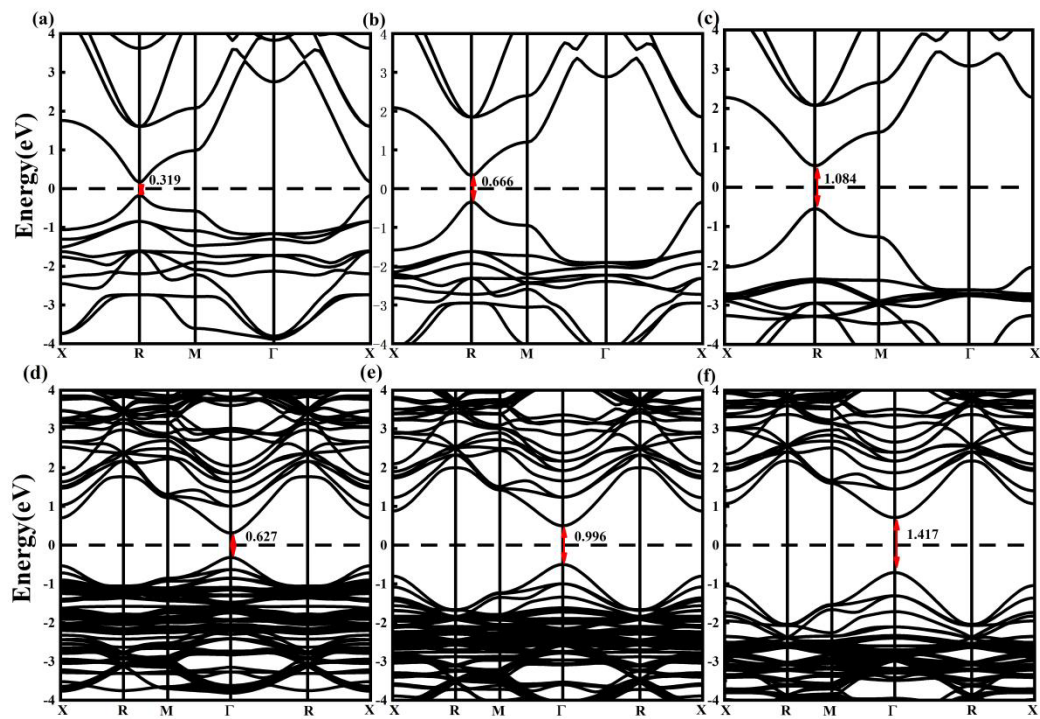
11
12 Corresponding author: jiancaileng@qlu.edu.cn; drccheng@sdnu.edu.cn; mahong@sdnu.edu.cn

13
14
15 **Table S1.** Relating to the energy of formation, the enthalpy of formation of various
16 compounds.

formula	Space group	The formation energy (eV)	formula	Space group	The formation energy (eV)	formula	Space group	The formation energy (eV)
CsI	P4/mbm	-5.411	CsBr	Pm-3m	-6.022	CsCl	Pm-3m	-6.538
PbI ₂	P-3m1	-8.147	PbBr ₂	Pnam	-9.673	PbCl ₂	P42/mnm	-10.764
SrI ₂	pnma	-9.815	SrBr ₂	P4/n2	-11.325	SrCl ₂	Fm-3m	-12.792
CsPbI ₃	Pm-3m	-14.087	CsPbBr ₃	Pm-3m	-15.940	CsPbCl ₃	Pm-3m	-17.624
CsPb _{0.875} Sr _{0.125} I ₃	Pm-3m	-14.225	CsPb _{0.875} Sr _{0.125} Br ₃	Pm-3m	-16.128	CsPb _{0.875} Sr _{0.125} Cl ₃	Pm-3m	-17.849

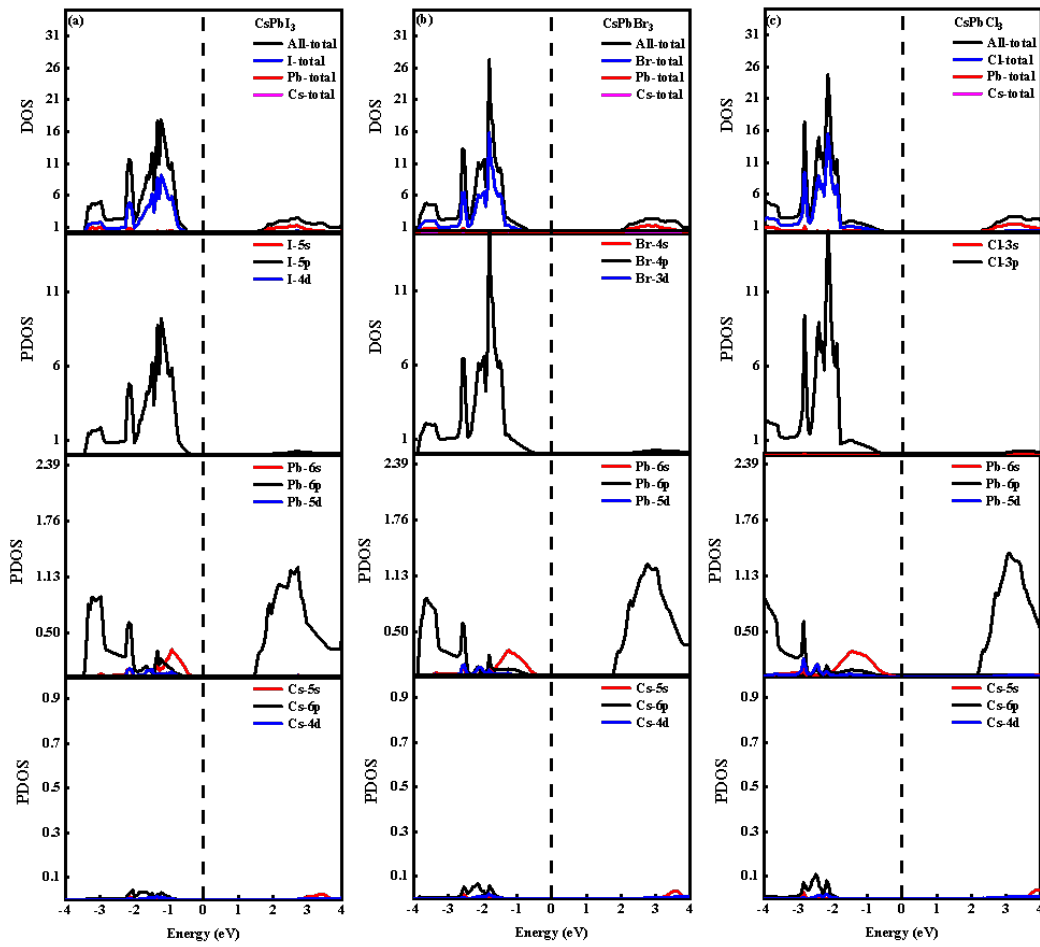
17

18



20

21 **Fig S1.** Energy band calculation with spin-orbit coupling, **(a)** CsPbI₃, **(b)** CsPbBr₃, **(c)**22 CsPbCl₃, **(d)** CsPb_{0.875}Sr_{0.125}I₃, **(e)** CsPb_{0.875}Sr_{0.125}Br₃, and **(f)** CsPb_{0.875}Sr_{0.125}Cl₃.



23

24

25 **Fig S2.** Density distribution of (a) CsPbI₃ (b) CsPbBr₃, and (c) CsPbCl₃

26

27