Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Elastic properties and electronic structures of polymorphic $CsPbI_3$

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Table S1 Lattice parameters of γ-$CsPbI_3$ and δ-$CsPbI_3$ by calculations and experiments in reference. The unit of lattice and density is Å and g/cm^3, respectively. cal represents the calculated values in this work; expt represents the experimental values in the reference (1-4).

Phase	a_{cal}	a_{expt}	a_{expt}	b_{cal}	b_{expt}	b_{expt}	c_{cal}	c_{expt}	c_{expt}	density
γ-$CsPbI_3$	8.68	8.62(1)	8.65(4)	8.82	8.85	8.82	12.53	12.50	12.52	5.02
δ-$CsPbI_3$	10.45	10.46(2)	10.43(3)	4.79	4.80	4.79	17.87	17.79	17.76	5.40

Table S2 The summary of the calculated elastic constants of γ-$CsPbI_3$ and δ-$CsPbI_3$. The maximum and minimum values of shear modulus (G) and Poisson's ratio (ν) are obtained by ELATE software.(5)

properties	quantities	γ-$CsPbI_3$	δ-$CsPbI_3$
Stiffness coefficient Cij (GPa)	C_{11}	33.07	29.81
	C_{22}	34.48	34.43
	C_{33}	45.48	38.38
	C_{44}	6.73	9.27
	C_{55}	6.66	13.51
	C_{66}	17.91	19.32
	C_{12}	18.39	19.81
	C_{13}	7.35	15.38
	C_{23}	7.19	10.66
Bulk modulus K (Gpa)		19.87	21.58
Young's modulus E (Gpa)		(001)43.450 (010)24.034	(001)30.4359 (010)21.2714
Shear modulus G (GPa)	Gmax	(100)<010>18.7230	(100)<010>19.3240
	Gmin	(110)<001>6.6582	(110)<-110>5.8366
Poisson's ratios ν	νmax	<-55-7><5-5-7>0.5727	<010><100>0.6568
	νmin	<55-7><-110>0.0747	<54-3><-54-3>0.0046

Table S3 The elastic constants of γ-$CsPbI_3$ under 3% and 6% strain along <012>.

Elastic constants	γ-$CsPbI_3$(3%)	γ-$CsPbI_3$(6%)
C_{11}	43.125	42.812
C_{22}	26.856	28.624
C_{33}	43.402	43.659
C_{44}	5.343	5.999
C_{55}	7.185	3.301
C_{66}	13.511	4.318
C_{12}	19.686	20.489
C_{13}	19.932	14.527
C_{23}	10.678	1.627
Bulk modulus K (Gpa)	20.9	21.3
Young's modulus E (Gpa)	(001) 34.055	(001) 37.223
Shear modulus G (GPa)	G(max) 13.397 G(min) 5.343	G(max) 14.936 G(min) 3.301
Poisson's ratios v	v(max) 0.5953 v(min) 0.08867	v(max) 0.7588 v(min) 0.2829

Table S4 The surface/volume ratios and bandgaps of γ-$CsPbI_3$ under different strain.

Strain	Surface/Volume($Å^{-1}$)	Eg(eV)
0	0.6169	1.830
1	0.6208	1.828
2	0.6235	1.825
3	0.6257	1.817
4	0.6278	1.788
5	0.6298	1.733
6	0.6318	1.691

Table S5 Comparison of bandgaps obtained within different methods for γ-$CsPbI_3$ and δ-$CsPbI_3$.

	Eg(eV)	
Method	γ-$CsPbI_3$	δ-$CsPbI_3$
PBE	1.83	2.48
PBE+SOC	0.84	1.92
HSE06	2.42	3.22
HSE06+SOC	1.62	2.36

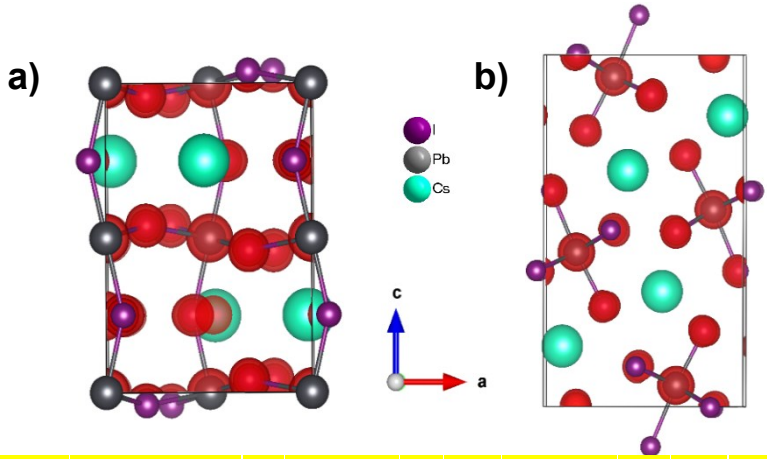

Fig. S1 Charge distributions on γ-$CsPbI_3$ (a) and δ-$CsPbI_3$ (b). The red is the strength of the charge.

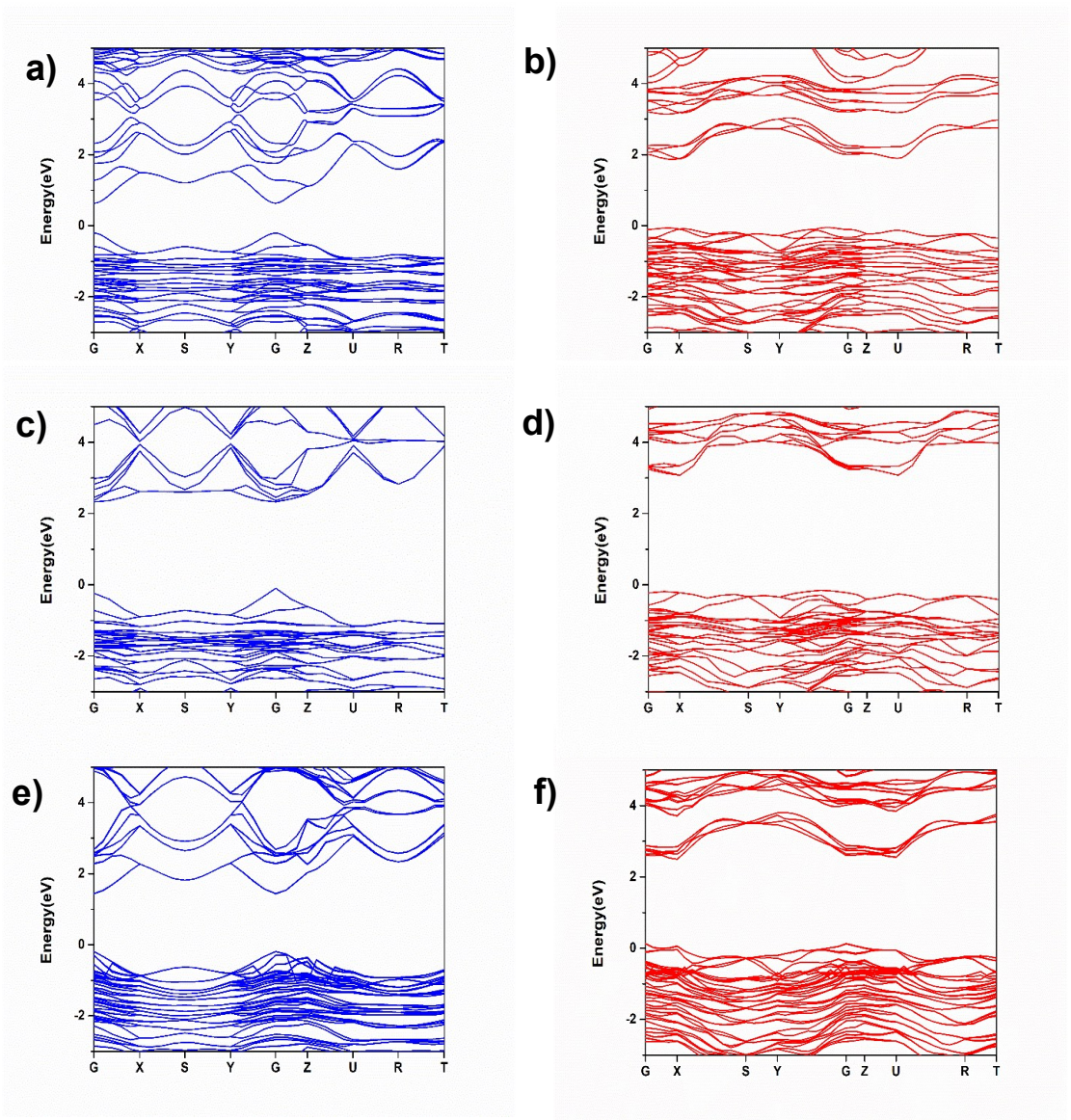

Fig. S2 Electronic band structures of γ-$CsPbI_3$ (a,c and e) and δ-$CsPbI_3$ (b,d and f) calculated using PBE+SOC (top), HSE06 (middle) and HSE06+SOC (bottom).

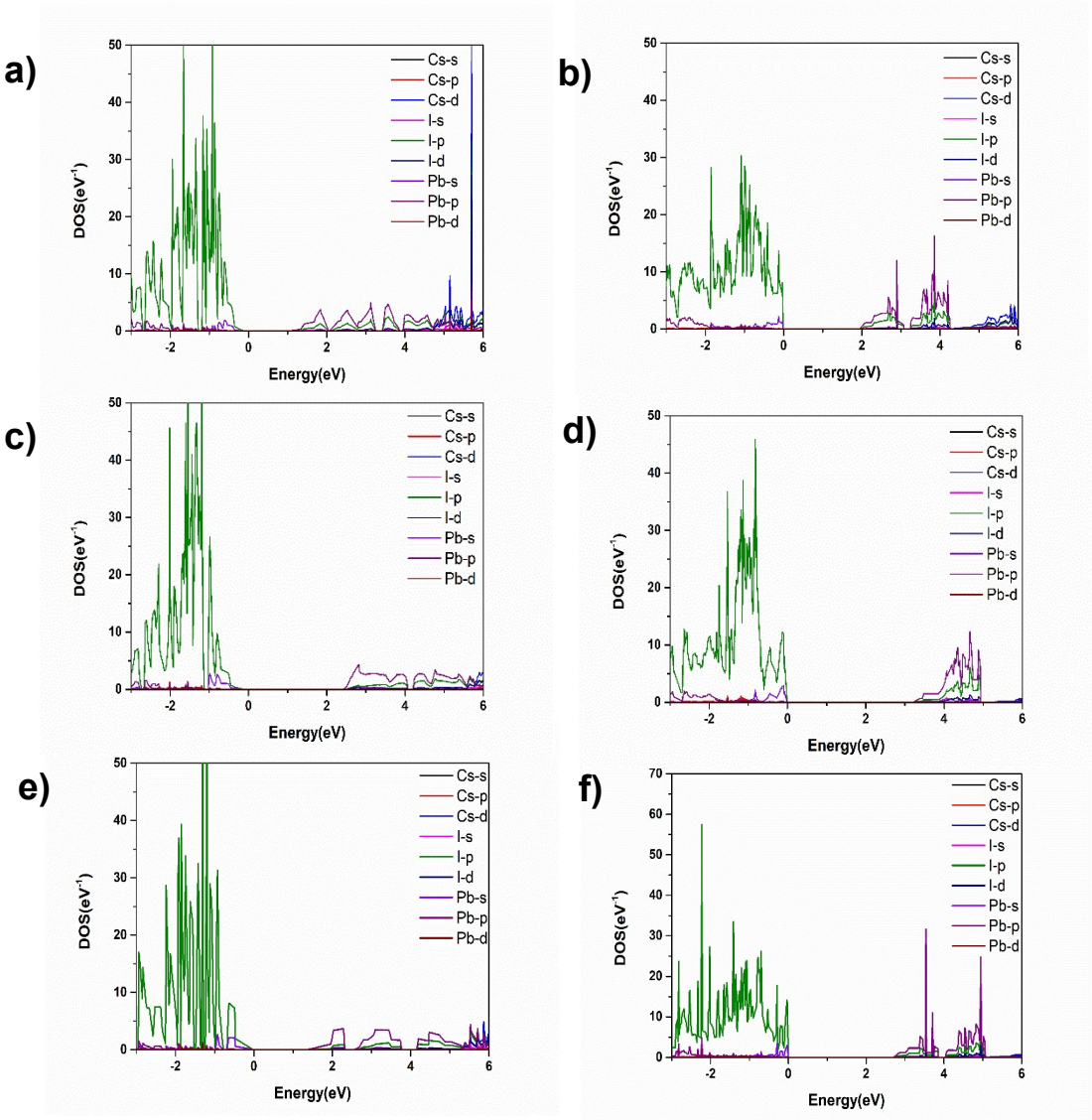

Fig. S3 DOS of γ-$CsPbI_3$ (a,c and e) and δ-$CsPbI_3$ (b,d and f) calculated using PBE+SOC (top), HSE06 (middle) and HSE06+SOC (bottom).).

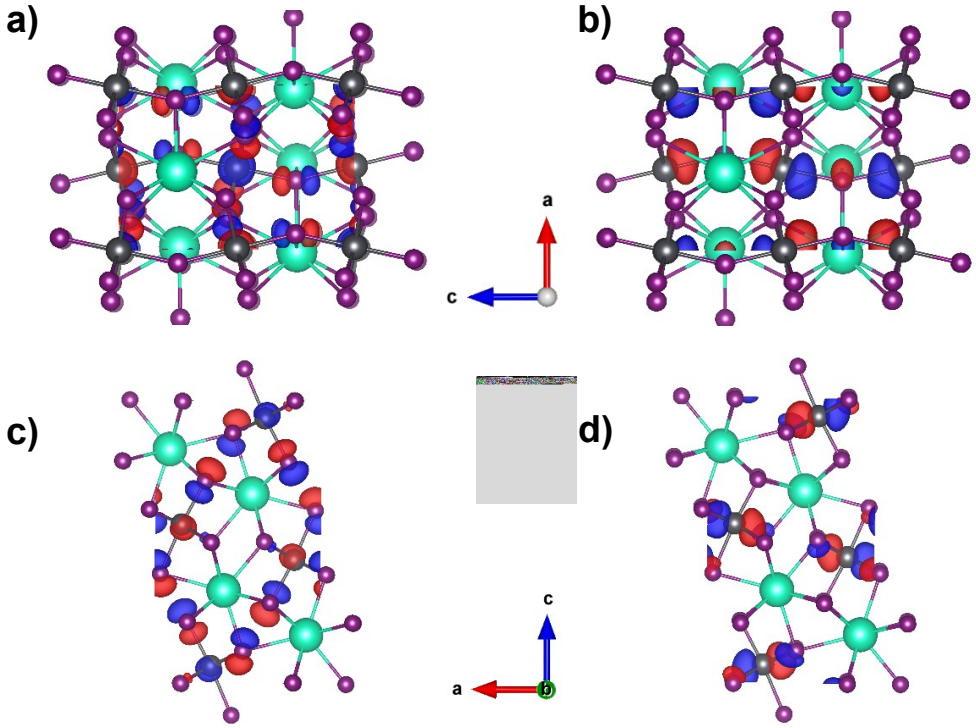

Fig. S4 The charge density distribution of the conduction band minimum (CBM) (a and c) and Valence band maximum (VBM) (b and d) orbitals of γ-$CsPbI_3$(top) and δ-$CsPbI_3$(bottom).

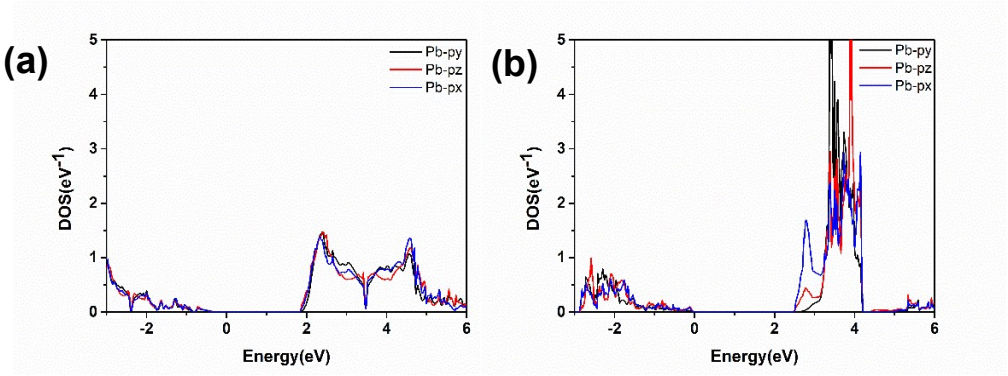

Fig. S5 Calculated partial DOS for Pb of γ-$CsPbI_3$ (a) and δ-$CsPbI_3$ (b).

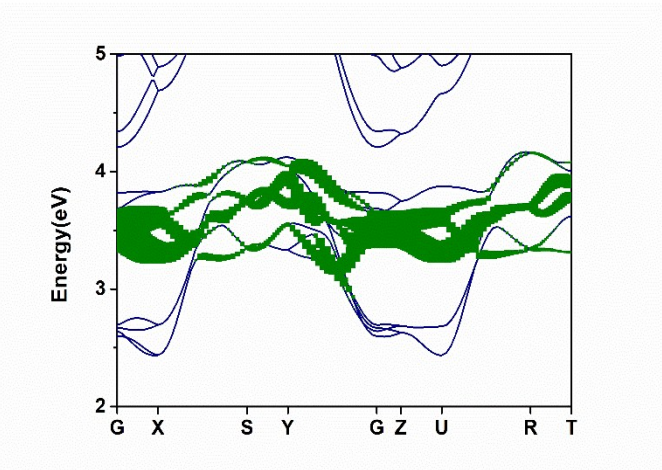

Fig. S6 Pb 6py orbitals of δ-$CsPbI_3$ projections on conduction band. Blue line: the conduction band of δ-$CsPbI_3$; Green line: the weight of Pb 6py orbitals in conduction band.

The main input and output files associated with this article on the site: https://github.com/Lizhigang1/CsPbI3/find/master?q=

References

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