materials

Supplementary Materials: Structural, Electronic, and Optical Properties of $CsPb(Br_{1-x}Cl_x)_3$ Perovskite: First-Principles Study with PBE–GGA and mBJ–GGA Methods

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Table S1. $CsPbBr_3$.

Lattice Parameters								
a		b	c	alpha	beta	gamma		
5.87400		5.87400	23.49600	90.0000	90.0000	90.0000		
Unit-cell volume = 810.703101 Å^3								
Structure Parameters								
		x	y	z	Occ.	B	Site	Sym.
1	Cs Cs1	0.00000	0.00000	0.00000	1.000	1.000	1a	1
2	Cs Cs2	0.00000	0.00000	0.25000	1.000	1.000	1a	1
3	Cs Cs3	0.00000	0.00000	0.50000	1.000	1.000	1a	1
4	Cs Cs4	0.00000	0.00000	0.75000	1.000	1.000	1a	1
5	Pb Pb1	0.50000	0.50000	0.12500	1.000	1.000	1a	1
6	Pb Pb2	0.50000	0.50000	0.37500	1.000	1.000	1a	1
7	Pb Pb3	0.50000	0.50000	0.62500	1.000	1.000	1a	1
8	Pb Pb4	0.50000	0.50000	0.87500	1.000	1.000	1a	1
9	Br Br1	0.50000	0.50000	1.00000	1.000	1.000	1a	1
10	Br Br2	0.00000	0.50000	0.12500	1.000	1.000	1a	1
11	Br Br3	0.50000	0.00000	0.12500	1.000	1.000	1a	1
12	Br Br4	0.50000	0.50000	0.25000	1.000	1.000	1a	1
13	Br Br5	0.00000	0.50000	0.37500	1.000	1.000	1a	1
14	Br Br6	0.50000	0.00000	0.37500	1.000	1.000	1a	1
15	Br Br7	0.50000	0.50000	0.50000	1.000	1.000	1a	1
16	Br Br8	0.00000	0.50000	0.62500	1.000	1.000	1a	1
17	Br Br9	0.50000	0.00000	0.62500	1.000	1.000	1a	1
18	Br Br10	0.50000	0.50000	0.75000	1.000	1.000	1a	1
19	Br Br11	0.00000	0.50000	0.87500	1.000	1.000	1a	1
20	Br Br12	0.50000	0.0000	0.87500	1.000	1.000	1a	1

Lattice type: P; Space group name: P 1; Space group number: 1; Setting number:1.

Table S2. $CsPbBr_{2.75}C_{l0.25}$.

Lattice Parameters							
a	**b**	**c**	**alpha**	**beta**	**gamma**		
5. 80100	5.80100	23.42026	90.0000	90.0000	90.0000		
Unit-cell volume = 807.008322 Å^3							
Structure Parameters							
		x	**y**	**z**	**Occ.**	**B**	**Site**	**Sym.**
1	Cs Cs1	0.00000	0.00000	0.00000	1.000	1.000	1a	1
2	Cs Cs2	0.00000	0.00000	0.25000	1.000	1.000	1a	1
3	Cs Cs3	0.00000	0.00000	0.50000	1.000	1.000	1a	1
4	Cs Cs4	0.00000	0.00000	0.75000	1.000	1.000	1a	1
5	Pb Pb1	0.50000	0.50000	0.12144	1.000	1.000	1a	1
6	Pb Pb2	0.50000	0.50000	0.37437	1.000	1.000	1a	1
7	Pb Pb3	0.50000	0.50000	0.62563	1.000	1.000	1a	1
8	Pb Pb4	0.50000	0.50000	0.87856	1.000	1.000	1a	1
9	Cl Cl1	0.50000	0.50000	1.00000	1.000	1.000	1a	1
10	Br Br1	0.00000	0.50000	0.12488	1.000	1.000	1a	1
11	Br Br2	0.50000	0.00000	0.12486	1.000	1.000	1a	1
12	Br Br3	0.50000	0.50000	0.24829	1.000	1.000	1a	1
13	Cl Cl2	0.00000	0.50000	0.37504	1.000	1.000	1a	1
14	Br Br4	0.50000	0.00000	0.37507	1.000	1.000	1a	1
15	Br Br5	0.50000	0.50000	0.50000	1.000	1.000	1a	1
16	Br Br6	0.00000	0.50000	0.62493	1.000	1.000	1a	1
17	Cl Cl3	0.50000	0.00000	0.62496	1.000	1.000	1a	1
18	Br Br7	0.50000	0.50000	0.75171	1.000	1.000	1a	1
19	Br Br8	0.00000	0.50000	0.87514	1.000	1.000	1a	1
20	Br Br9	0.50000	0.00000	0.87512	1.000	1.000	1a	1

Lattice type: P; Space group name: P 1; Space group number: 1; Setting number:1.

Table S3. $CsPbBr_2Cl$

Lattice Parameters							
a	**b**	**c**	**alpha**	**beta**	**gamma**		
5.78433	5.78433	23.13731	90.0000	90.0000	90.0000		
Unit-cell volume = 774.138727 Å^3							
Structure Parameters							
		x	y	z	Occ	B	Site	Sym.
1	Cs Cs1	0.00000	0.00000	0.00000	1.000	1.000	1a	1
2	Cs Cs2	0.00000	0.00000	0.25000	1.000	1.000	1a	1
3	Cs Cs3	0.00000	0.00000	0.50000	1.000	1.000	1a	1
4	Cs Cs4	0.00000	0.00000	0.75000	1.000	1.000	1a	1
5	Pb Pb1	0.50000	0.50000	0.12500	1.000	1.000	1a	1
6	Pb Pb2	0.50000	0.50000	0.37500	1.000	1.000	1a	1
7	Pb Pb3	0.50000	0.50000	0.62500	1.000	1.000	1a	1
8	Pb Pb4	0.50000	0.50000	0.87500	1.000	1.000	1a	1
9	Br Br1	0.50000	0.50000	0.00000	1.000	1.000	1a	1
10	Br Br2	0.00000	0.50000	0.12500	1.000	1.000	1a	1
11	Cl Cl1	0.50000	0.00000	0.12500	1.000	1.000	1a	1
12	Br Br3	0.50000	0.50000	0.25000	1.000	1.000	1a	1
13	Br Br4	0.00000	0.50000	0.37500	1.000	1.000	1a	1
14	Cl Cl2	0.50000	0.00000	0.37500	1.000	1.000	1a	1
15	Br Br5	0.50000	0.50000	0.50000	1.000	1.000	1a	1

16	Br Br6	0.00000	0.50000	0.62500	1.000	1.000	1a	1
17	Cl Cl3	0.50000	0.00000	0.62500	1.000	1.000	1a	1
18	Br Br7	0.50000	0.50000	0.75000	1.000	1.000	1a	1
19	Br Br8	0.00000	0.50000	0.87500	1.000	1.000	1a	1
20	Cl Cl4	0.50000	0.00000	0.87500	1.000	1.000	1a	1

Lattice type: P; Space group name: P 1; Space group number: 1; Setting number:1.

Table S4. $CsPbBr_{1.5}Cl_{1.5}$

Lattice Parameters					
a	**b**	**c**	**alpha**	**beta**	**gamma**
5.73950	5.73950	22.95799	90.0000	90.0000	90.0000
Unit-cell volume = 756.278366 Å^3					

Structure Parameters								
		x	**y**	**z**	**Occ**	**B**	**Site**	**Sym.**
1	Cs Cs1	0.00000	0.00000	0.00000	1.000	1.000	1a	1
2	Cs Cs2	0.00000	0.00000	0.25000	1.000	1.000	1a	1
3	Cs Cs3	0.00000	0.00000	0.50000	1.000	1.000	1a	1
4	Cs Cs4	0.00000	0.00000	0.75000	1.000	1.000	1a	1
5	Pb Pb1	0.50000	0.50000	0.12500	1.000	1.000	1a	1
6	Pb Pb2	0.50000	0.50000	0.37500	1.000	1.000	1a	1
7	Pb Pb3	0.50000	0.50000	0.62500	1.000	1.000	1a	1
8	Pb b4	0.50000	0.50000	0.87500	1.000	1.000	1a	1
9	Cl Cl1	0.50000	0.50000	1.00000	1.000	1.000	1a	1
10	Br Br1	0.00000	0.50000	0.12490	1.000	1.000	1a	1
11	Cl Cl2	0.50000	0.00000	0.12495	1.000	1.000	1a	1
12	Br Br2	0.50000	0.50000	0.25000	1.000	1.000	1a	1
13	Cl Cl3	0.00000	0.50000	0.37505	1.000	1.000	1a	1
14	Br Br3	0.50000	0.00000	0.37510	1.000	1.000	1a	1
15	Cl Cl4	0.50000	0.50000	0.50000	1.000	1.000	1a	1
16	Br Br4	0.00000	0.50000	0.62490	1.000	1.000	1a	1
17	Cl Cl5	0.50000	0.00000	0.62495	1.000	1.000	1a	1
18	Br Br5	0.50000	0.50000	0.75000	1.000	1.000	1a	1
19	Cl Cl6	0.00000	0.50000	0.87505	1.000	1.000	1a	1
20	Br Br6	0.50000	0.00000	0.87510	1.000	1.000	1a	1

Lattice type: P; Space group name: P 1; Space group number: 1; Setting number:1.

Table S5. $CsPbBrCl_2$.

Lattice Parameters					
a	**b**	**c**	**alpha**	**beta**	**gamma**
5.69466	5.69466	22.77865	90.0000	90.0000	90.0000
Unit-cell volume = 738.691816 Å^3					

Structure Parameters								
		x	**y**	**z**	**Occ.**	**B**	**Site**	**Sym.**
1	Cs Cs1	0.00000	0.00000	0.00000	1.000	1.000	1a	1
2	Cs Cs2	0.00000	0.00000	0.25000	1.000	1.000	1a	1
3	Cs Cs3	0.00000	0.00000	0.50000	1.000	1.000	1a	1
4	Cs Cs4	0.00000	0.00000	0.75000	1.000	1.000	1a	1
5	Pb Pb1	0.50000	0.50000	0.12500	1.000	1.000	1a	1

6	Pb Pb2	0.50000	0.50000	0.37500	1.000	1.000	1a	1
7	Pb Pb3	0.50000	0.50000	0.62500	1.000	1.000	1a	1
8	Pb Pb4	0.50000	0.50000	0.87500	1.000	1.000	1a	1
9	Cl Cl1	0.50000	0.50000	1.00000	1.000	1.000	1a	1
10	Cl Cl2	0.00000	0.50000	0.12500	1.000	1.000	1a	1
11	Br Br1	0.50000	0.00000	0.12500	1.000	1.000	1a	1
12	Cl Cl3	0.50000	0.50000	0.25000	1.000	1.000	1a	1
13	Cl Cl4	0.00000	0.50000	0.37500	1.000	1.000	1a	1
14	Br Br2	0.50000	0.00000	0.37500	1.000	1.000	1a	1
15	Cl Cl5	0.50000	0.50000	0.50000	1.000	1.000	1a	1
16	Cl Cl6	0.00000	0.50000	0.62500	1.000	1.000	1a	1
17	Br Br3	0.50000	0.00000	0.62500	1.000	1.000	1a	1
18	Cl Cl7	0.50000	0.50000	0.75000	1.000	1.000	1a	1
19	Cl Cl8	0.00000	0.50000	0.87500	1.000	1.000	1a	1
20	Br Br4	0.50000	0.00000	0.87500	1.000	1.000	1a	1

Lattice type: P; Space group name: P 1; Space group number: 1; Setting number:1.

Table S6. $CsPbBr_{0.25}Cl_{2.75}$.

Lattice Parameters					
a	**b**	**c**	**alpha**	**beta**	**gamma**
5.67225	5.67225	22.68899	90.0000	90.0000	90.0000
Unit-cell volume = 730.004601 Å^3					

Structure Parameters								
		x	**y**	**z**	**Occ.**	**B**	**Site**	**Sym.**
1	Cs Cs1	0.00000	0.00000	0.00000	1.000	1.000	1a	1
2	Cs Cs2	0.00000	0.00000	0.25000	1.000	1.000	1a	1
3	Cs Cs3	0.00000	0.00000	0.50000	1.000	1.000	1a	1
4	Cs Cs4	0.00000	0.00000	0.75000	1.000	1.000	1a	1
5	Pb Pb1	0.50000	0.50000	0.12848	1.000	1.000	1a	1
6	Pb Pb2	0.50000	0.50000	0.37562	1.000	1.000	1a	1
7	Pb Pb3	0.50000	0.50000	0.62438	1.000	1.000	1a	1
8	Pb Pb4	0.50000	0.50000	0.87153	1.000	1.000	1a	1
9	Br Br1	0.50000	0.50000	1.00000	1.000	1.000	1a	1
10	Cl Cl1	0.00000	0.50000	0.12521	1.000	1.000	1a	1
11	Cl Cl2	0.50000	0.00000	0.12523	1.000	1.000	1a	1
12	Cl Cl3	0.50000	0.50000	0.25166	1.000	1.000	1a	1
13	Br Br2	0.00000	0.50000	0.37492	1.000	1.000	1a	1
14	Cl Cl4	0.50000	0.00000	0.37493	1.000	1.000	1a	1
15	Cl Cl5	0.50000	0.50000	0.50000	1.000	1.000	1a	1
16	Cl Cl6	0.00000	0.50000	0.62507	1.000	1.000	1a	1
17	Br Br3	0.50000	0.00000	0.62508	1.000	1.000	1a	1
18	Cl Cl7	0.50000	0.50000	0.74834	1.000	1.000	1a	1
19	Cl Cl8	0.00000	0.50000	0.87477	1.000	1.000	1a	1
20	Cl Cl9	0.50000	0.00000	0.87479	1.000	1.000	1a	1

Lattice type: P; Space group name: P 1; Space group number: 1; Setting number:1.

Table S7. $CsPbCl_3$.

Lattice Parameters					
a	**b**	**c**	**alpha**	**beta**	**gamma**
5.60500	5.60500	22.41999	90.0000	90.0000	90.0000
Unit-cell volume = 704.346569 Å^3					

Structure Parameters								
		x	y	z	Occ.	B	Site	Sym.
1	Cs Cs1	0.00000	0.00000	0.00000	1.000	1.000	1a	1
2	Cs Cs2	0.00000	0.00000	0.25000	1.000	1.000	1a	1
3	Cs Cs3	0.00000	0.00000	0.50000	1.000	1.000	1a	1
4	Cs Cs4	0.00000	0.00000	0.75000	1.000	1.000	1a	1
5	Pb Pb1	0.50000	0.50000	0.12500	1.000	1.000	1a	1
6	Pb Pb2	0.50000	0.50000	0.37500	1.000	1.000	1a	1
7	Pb Pb3	0.50000	0.50000	0.62500	1.000	1.000	1a	1
8	Pb Pb4	0.50000	0.50000	0.87500	1.000	1.000	1a	1
9	Cl Cl1	0.50000	0.50000	1.00000	1.000	1.000	1a	1
10	Cl Cl2	0.00000	0.50000	0.12500	1.000	1.000	1a	1
11	Cl Cl3	0.50000	0.00000	0.12500	1.000	1.000	1a	1
12	Cl Cl4	0.50000	0.50000	0.25000	1.000	1.000	1a	1
13	Cl Cl5	0.00000	0.50000	0.37500	1.000	1.000	1a	1
14	Cl Cl6	0.50000	0.00000	0.37500	1.000	1.000	1a	1
15	Cl Cl7	0.50000	0.50000	0.50000	1.000	1.000	1a	1
16	Cl Cl8	0.00000	0.50000	0.62500	1.000	1.000	1a	1
17	Cl Cl9	0.50000	0.00000	0.62500	1.000	1.000	1a	1
18	Cl Cl10	0.50000	0.50000	0.75000	1.000	1.000	1a	1
19	Cl Cl11	0.00000	0.50000	0.87500	1.000	1.000	1a	1
20	Cl Cl12	0.50000	0.00000	0.87500	1.000	1.000	1a	1

Lattice type: P; Space group name: P 1; Space group number: 1; Setting number:1.

Table S8. Effective mass of electron (m_e^*) and hole (m_h^*), reduced mass (μ_r), bohr diameter (a_0), dielectric constant (ε), and exciton binding energy (E_b) values calculated by PBE–GGA, mBJ– GGA, and mBJ-GGA + SOC potentials.

Perovskites	m_e^*	m_h^*	μ_r	a_0 (nm)	$\varepsilon(0)$	E_b (meV)
$CsPbBr_3$	$0.215^{PBE–GGA}$ $0.283^{mBJ–GGA}$ $0.049^{mBJ + SOC}$ 0.22 [1] 0.2 [2] 0.15 [3] 0.149 [4] 0.26 [5] 0.15 [6]	$0.043^{PBE–GGA}$ $0.053^{mBJ–GGA}$ $0.045^{mBJ + SOC}$ 0.14 [1,3] 0.12 [2,5] 0.143 [4] 0.23 [5] 0.10 [5] 0.14 [6]	$0.036^{PBE–GGA}$ $0.045^{mBJ–GGA}$ $0.023^{mBJ + SOC}$	$12.5^{PBE–GGA}$ $8.1^{mBJ–GGA}$ 5.5 [5] 4.2 [5] 7 [3] $5.8^{our\ paper}$	$4.69^{PBE–GGA}$ $3.82^{mBJ–GGA}$ 4.631 [7] 4.96 [3]	$22^{PBE–GGA}$ $42^{mBJ–GGA}$ $58^{our\ paper}$ 70 [5] 106 [5] 40 [3] 35 [8] 40 [9]
$CsPbBr_{2.75}Cl_{0.25}$	$0.133^{PBE–GGA}$ $0.125^{mbj–GGA}$ $0.061^{mBJ + SOC}$	$0.047^{PBE–GGA}$ $0.058^{mBJ–GGA}$ $0.054^{mBJ + SOC}$	$0.035^{PBE–GGA}$ $0.039^{mBJ–GGA}$ $0.029^{mBJ + SOC}$	$11.8^{PBE–GGA}$ $8.8^{mBJ–GGA}$	$4.34^{PBE–GGA}$ $3.59^{mBJ–GGA}$	$25^{PBE–GGA}$ $41^{mBJ–GGA}$
$CsPbBr_2Cl$	$0.119^{PBE–GGA}$ $0.346^{mBJ–GGA}$ $0.067^{mBJ + SOC}$	$0.058^{PBE–GGA}$ $0.073^{mBJ–GGA}$ $0.063^{mBJ + SOC}$	$0.027^{PBE–GGA}$ $0.060^{mBJ–GGA}$ $0.032^{mBJ + SOC}$	$14.9^{PBE–GGA}$ $5.7^{mBJ–GGA}$	$4.23^{PBE–GGA}$ $3.57^{mBJ–GGA}$	$21^{PBE–GGA}$ $46^{mBJ–GGA}$
$CsPbBr_{1.5}Cl_{1.5}$	$0.197^{PBE–GGA}$ $0.255^{mBJ–GGA}$ $0.064^{mBJ + SOC}$	$0.046^{PBE–GGA}$ $0.057^{mBJ–GGA}$ $0.055^{mBJ + SOC}$	$0.037^{PBE–GGA}$ $0.047^{mBJ–GGA}$ $0.029^{mBJ + SOC}$	$10.6^{PBE–GGA}$ $7.2^{mBJ–GGA}$	$4.12^{PBE–GGA}$ $3.56^{mBJ–GGA}$	$30^{PBE–GGA}$ $50^{mBJ–GGA}$
$CsPbBrCl_2$	$0.202^{PBE–GGA}$ $0.255^{mBJ–GGA}$ $0.054^{mBJ + SOC}$	$0.037^{PBE–GGA}$ $0.045^{mBJ–GGA}$ $0.045^{mBJ + SOC}$	$0.031^{PBE–GGA}$ $0.038^{mBJ–GGA}$ $0.025^{mBJ + SOC}$	$12.6^{PBE–GGA}$ $8.9^{mBJ–GGA}$	$4.10^{PBE–GGA}$ $3.55^{mBJ–GGA}$	$25^{PBE–GGA}$ $41^{mBJ–GGA}$
$CsPbBr_{0.25}Cl_{2.75}$	$0.197^{PBE–GGA}$ $0.178^{mBJ–GGA}$ $0.067^{mBJ + SOC}$	$0.046^{PBE–GGA}$ $0.057^{mBJ–GGA}$ $0.054^{mBJ + SOC}$	$0.037^{PBE–GGA}$ $0.043^{mBJ–GGA}$ $0.030^{mBJ + SOC}$	$10.0^{PBE–GGA}$ $7.6^{mBJ–GGA}$	$3.89^{PBE–GGA}$ $3.4^{mBJ–GGA}$	$33^{PBE–GGA}$ $50^{mBJ–GGA}$

$CsPbCl_3$	$0.237^{PBE-GGA}$ $0.312^{mBJ-GGA}$ $0.073^{mBJ+SOC}$ 0.28 [1] 0.218 [4] 0.23 [5] 0.20 [3]	$0.053^{PBE-GGA}$ $0.067^{mBJ-GGA}$ $0.061^{mBJ+SOC}$ 0.18 [1] 0.189 [4] 0.10 [5] 0.17 [3]	$0.043^{PBE-GGA}$ $0.055^{mBJ-GGA}$ $0.033^{mBJ+SOC}$	$8.6^{PBE-GGA}$ $5.6^{mBJ-GGA}$ 4.1 [5] 5.5 [5] 5 [3]	$3.87^{PBE-GGA}$ $3.23^{mBJ-GGA}$ 4.1 [7] 2.723 [5] 3.09 [5] 4.07 [3]	$39^{PBE-GGA}$ $72^{mBJ-GGA}$ 130 [5] 85 [5] 75 [3]

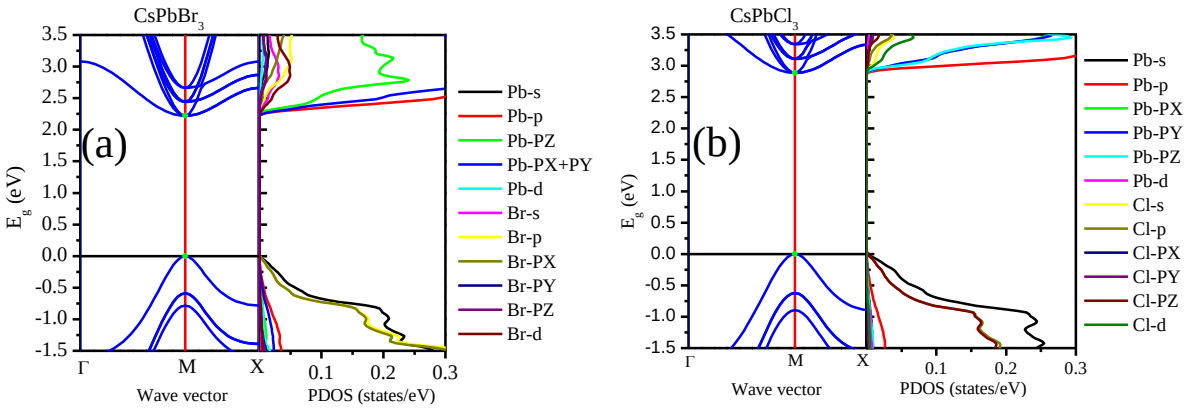

Figure S1. Band structures and PDOS of (**a**) $CsPbBr_3$ and (**b**) $CsPbCl_3$ obtained using the mBJ–GGA potential.

References

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