

Supporting Information

High throughput screening of promising inorganic halide double perovskites via first-principles calculations

Zhengyang Gao^{a,b,c}, Guangyang Mao^{a,b,c}, Shengyi Chen^{a,b,c}, Yang Bai^{a,b,c}, Peng Gao^{a,b,c},
Chongchong Wu^h, Ian D. Gates^h, Weijie Yang^{*a,b,c}, Xunlei Ding^{*d,e}, Jianxi Yao^{*f,g}

^a Department of Power Engineering, North China Electric Power University, Baoding 071003, Hebei, China.

^b Hebei Key Laboratory of Low Carbon and High Efficiency Power Generation Technology, North China Electric Power University, Baoding 071003, Hebei, China.

^c Baoding Key Laboratory of Low Carbon and High Efficiency Power Generation Technology, North China Electric Power University, Baoding 071003, Hebei, China.

^d School of Mathematics and Physics, North China Electric Power University, Beijing 102206, China.

^e Institute of Clusters and Low Dimensional Nanomaterials, School of Mathematics and Physics, North China Electric Power University, Beijing, People's Republic of China

^f State Key Laboratory of Alternate Electrical Power System With Renewable Energy Sources, North China Electric Power University, Beijing 102206, China.

^g Beijing Key Laboratory of Energy Safety and Clean Utilization, North China Electric Power University, Beijing 102206, China.

^h Department of Chemical and Petroleum Engineering, University of Calgary, T2N 1N4, Calgary, Alberta, Canada.

* Corresponding Authors:

Weijie Yang (yangwj@ncepu.edu.cn)

Xunlei Ding (dingxl@ncepu.edu.cn)

Jianxi Yao (jianxiyao@ncepu.edu.cn)

Table of contents

Table S1. Ionic radius.

Table S2. Ligand field stabilization energy of B site

Figure S1. Test of K-point.

Figure S2 . The energy of $\text{Cs}_2\text{FeZnBr}_6$ arranged in FeBr_6 (red) + ZnBr_6 (green) patterns with different symmetry.

Table S3. Goldschmidt tolerance factor t and octahedral factor μ of inorganic double perovskites.

Table S4. Goldschmidt tolerance factor range of inorganic double perovskites

Table S5. Double perovskite with minimum tolerance factor in unstable region

Table S6. Double perovskite with maximum tolerance factor in unstable region

Table S7. New tolerance factors τ of the 14 predicted all-inorganic double perovskite materials.

Table S8. The band gaps for PBE functional.

Table S9. The band gaps for HSE functional.

Figure S3. HSE calculated band structures for (a) $\text{Cs}_2\text{PbSnI}_6$, (b) $\text{Cs}_2\text{PbGeI}_6$ (c) $\text{Cs}_2\text{MnPtF}_6$, (d) $\text{Cs}_2\text{PbSnBr}_6$, (e) $\text{Cs}_2\text{PbGeBr}_6$, and (f) $\text{Cs}_2\text{SnGeCl}_6$.

Figure S4. HSE calculated projected density of states (PDOS) for (a) $\text{Cs}_2\text{PbSnI}_6$, (b) $\text{Cs}_2\text{PbGeI}_6$ (c) $\text{Cs}_2\text{MnPtF}_6$, (d) $\text{Cs}_2\text{PbSnBr}_6$, (e) $\text{Cs}_2\text{PbGeBr}_6$, and (f) $\text{Cs}_2\text{SnGeCl}_6$.

Table S10. Band gaps of the 14 predicted all-inorganic double perovskite materials.

Figure S5. The X-ray diffraction evolution of cubic structure with the temperature of 800 K for $\text{Cs}_2\text{PbSnI}_6$, $\text{Cs}_2\text{PbGeI}_6$, $\text{Cs}_2\text{PbSnBr}_6$, $\text{Cs}_2\text{PbGeBr}_6$, $\text{Cs}_2\text{SnGeCl}_6$, $\text{Cs}_2\text{MnPtF}_6$.

Figure S6. Calculated optical properties for $\text{Cs}_2\text{CdTeF}_6$, $\text{Cs}_2\text{MgMnI}_6$, $\text{Cs}_2\text{PbSnCl}_6$, $\text{Cs}_2\text{CdBeBr}_6$, $\text{Cs}_2\text{ZnTeF}_6$, $\text{Cs}_2\text{PbGeCl}_6$, $\text{Cs}_2\text{CaZnI}_6$, $\text{Cs}_2\text{FeTeF}_6$. Absorption coefficient: (a) and (c). Joint density of states (JDOS): (b) and (d).

Table S1. Ionic radius

Symbol	Ionic radius (pm)	Valence	Atomic number
Cs	167	+1	55
F	133	-1	9
Cl	181	-1	17
Br	196	-1	35
I	220	-1	53
Pb	119	+2	82
Sn	122	+2	50
Ge	73	+2	32
Be	45	+2	4
Mg	72	+2	12
Ca	100	+2	20
Sr	118	+2	38
Ba	135	+2	56
Mn	80	+2	25
Fe	78	+2	26
Co	74.5	+2	27
Ni	69	+2	28
Cu	73	+2	29
Zn	74	+2	30
Pd	86	+2	46
Ir	90	+2	77
Pt	80	+2	78
Te	100	+2	52
Cd	95	+2	48

Table S2. Ligand field stabilization energy of B site

Ion	<i>d</i> orbital electron number	LFSE
Pb ²⁺	10	0
Sn ²⁺	10	0
Ge ²⁺	10	0
Be ²⁺	0	0
Mg ²⁺	0	0
Ca ²⁺	0	0
Sr ²⁺	10	0
Ba ²⁺	10	0
Mn ²⁺	5	0
Fe ²⁺	6	0.4
Co ²⁺	7	0.8
Ni ²⁺	8	1.2
Cu ²⁺	9	0.6
Zn ²⁺	10	0
Pd ²⁺	8	1.2
Ir ²⁺	7	0.8
Pt ²⁺	8	1.2
Te ²⁺	10	0
Cd ²⁺	10	0

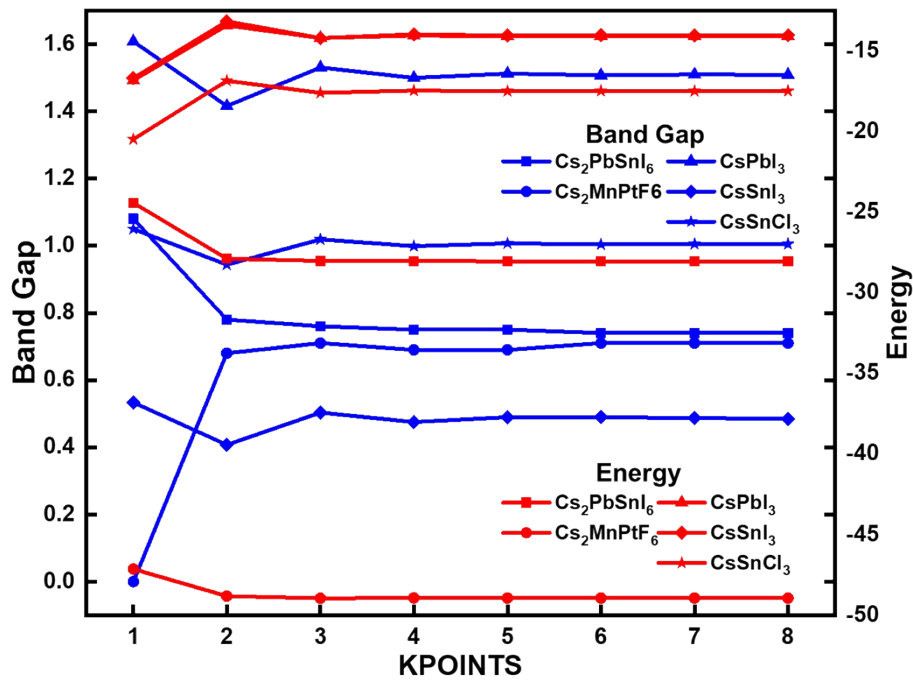


Figure S1. Test of K-point

Considering the band gap value and the convergence curve of energy comprehensively, we choose the K-point of $6 \times 6 \times 6$.

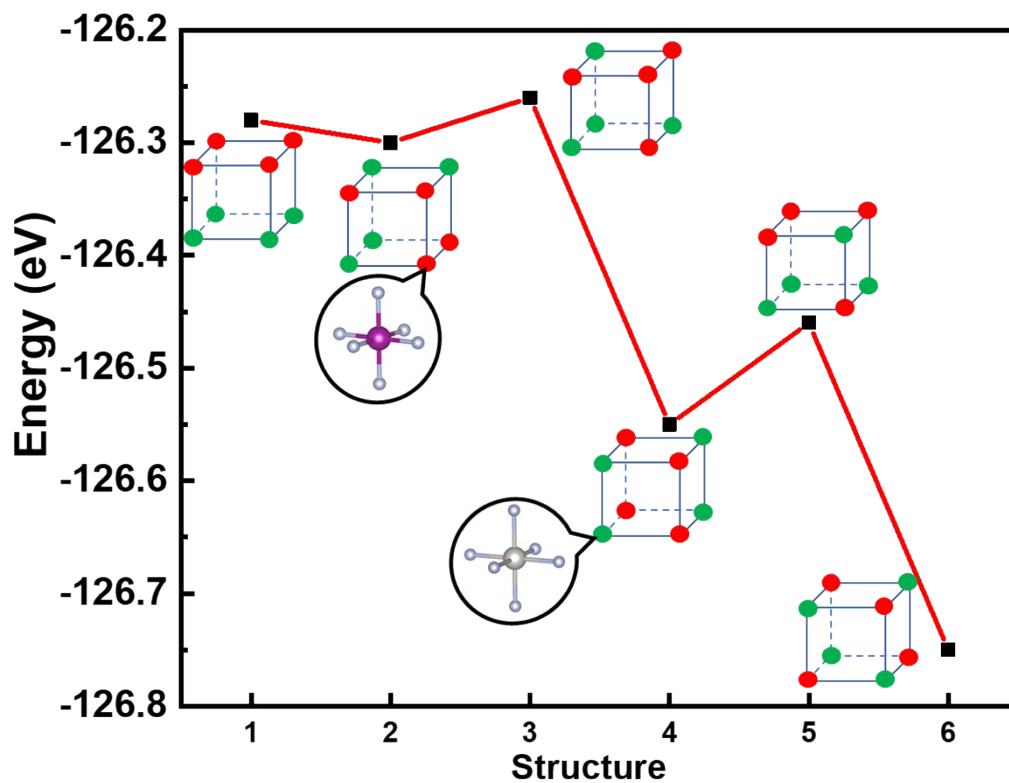


Figure S2 . The energy of $\text{Cs}_2\text{FeZnBr}_6$ arranged in FeBr_6 (red) + ZnBr_6 (green) patterns with different symmetry.

Table S3. Goldschmidt tolerance factor t and octahedral factor u of inorganic double perovskites

Material	t	u	Material	t	u	Material	t	u
Cs ₂ PbSnI ₆	0.816	0.525	Cs ₂ SnCaF ₆	0.888	0.797	Cs ₂ GeNiI ₆	0.940	0.323
Cs ₂ PbSnF ₆	0.854	0.868	Cs ₂ SnSrI ₆	0.817	0.523	Cs ₂ GeNiF ₆	1.040	0.534
Cs ₂ PbGeI ₆	0.866	0.436	Cs ₂ SnSrF ₆	0.855	0.865	Cs ₂ GeCuI ₆	0.934	0.332
Cs ₂ PbGeF ₆	0.926	0.722	Cs ₂ SnBaI ₆	0.797	0.561	Cs ₂ GeCuF ₆	1.030	0.549
Cs ₂ PbBeI ₆	0.906	0.373	Cs ₂ SnMnI ₆	0.884	0.407	Cs ₂ GeZnI ₆	0.932	0.334
Cs ₂ PbBeF ₆	0.987	0.617	Cs ₂ SnMnF ₆	0.953	0.673	Cs ₂ GeZnF ₆	1.027	0.553
Cs ₂ PbMgI ₆	0.867	0.434	Cs ₂ SnFeI ₆	0.869	0.432	Cs ₂ GePdI ₆	0.914	0.361
Cs ₂ PbMgF ₆	0.928	0.718	Cs ₂ SnFeF ₆	0.930	0.714	Cs ₂ GePdF ₆	0.998	0.598
Cs ₂ PbCaI ₆	0.831	0.498	Cs ₂ SnCoI ₆	0.874	0.424	Cs ₂ GeIrI ₆	0.908	0.370
Cs ₂ PbCaF ₆	0.875	0.823	Cs ₂ SnCoF ₆	0.938	0.701	Cs ₂ GeIrF ₆	0.989	0.613
Cs ₂ PbSrI ₆	0.808	0.539	Cs ₂ SnNiI ₆	0.881	0.411	Cs ₂ GePtI ₆	0.914	0.361
Cs ₂ PbSrF ₆	0.843	0.891	Cs ₂ SnNiF ₆	0.949	0.680	Cs ₂ GePtF ₆	0.998	0.598
Cs ₂ PbBaI ₆	0.789	0.577	Cs ₂ SnCuI ₆	0.876	0.42	Cs ₂ GeTeI ₆	0.893	0.393
Cs ₂ PbMnI ₆	0.874	0.423	Cs ₂ SnCuF ₆	0.941	0.695	Cs ₂ GeTeF ₆	0.966	0.650
Cs ₂ PbMnF ₆	0.939	0.699	Cs ₂ SnZnI ₆	0.874	0.423	Cs ₂ BeMgI ₆	0.983	0.266
Cs ₂ PbFeI ₆	0.859	0.448	Cs ₂ SnZnF ₆	0.939	0.699	Cs ₂ BeMgF ₆	1.108	0.440
Cs ₂ PbFeF ₆	0.916	0.741	Cs ₂ SnPdI ₆	0.858	0.450	Cs ₂ BeCaI ₆	0.936	0.330
Cs ₂ PbCoI ₆	0.864	0.44	Cs ₂ SnPdF ₆	0.914	0.744	Cs ₂ BeCaF ₆	1.032	0.545
Cs ₂ PbCoF ₆	0.923	0.727	Cs ₂ SnIrI ₆	0.852	0.459	Cs ₂ BeSrI ₆	0.908	0.370
Cs ₂ PbNiI ₆	0.871	0.427	Cs ₂ SnIrF ₆	0.907	0.759	Cs ₂ BeSrF ₆	0.989	0.613
Cs ₂ PbNiF ₆	0.935	0.707	Cs ₂ SnPtI ₆	0.858	0.450	Cs ₂ BeBaI ₆	0.883	0.409
Cs ₂ PbCuI ₆	0.866	0.436	Cs ₂ SnPtF ₆	0.914	0.744	Cs ₂ BeBaF ₆	0.951	0.677
Cs ₂ PbCuF ₆	0.926	0.722	Cs ₂ SnTeI ₆	0.839	0.482	Cs ₂ BeMnI ₆	0.991	0.255
Cs ₂ PbZnI ₆	0.865	0.439	Cs ₂ SnTeF ₆	0.888	0.797	Cs ₂ BeMnF ₆	1.122	0.421
Cs ₂ PbZnF ₆	0.924	0.726	Cs ₂ GeBeI ₆	0.981	0.268	Cs ₂ BeFeI ₆	0.972	0.280
Cs ₂ PbPdI ₆	0.849	0.466	Cs ₂ GeBeF ₆	1.105	0.444	Cs ₂ BeFeF ₆	1.091	0.462
Cs ₂ PbPdF ₆	0.901	0.771	Cs ₂ GeMgI ₆	0.936	0.330	Cs ₂ BeCoI ₆	0.978	0.272
Cs ₂ PbIrI ₆	0.843	0.475	Cs ₂ GeMgF ₆	1.032	0.545	Cs ₂ BeCoF ₆	1.101	0.449
Cs ₂ PbIrF ₆	0.893	0.786	Cs ₂ GeCaI ₆	0.893	0.393	Cs ₂ BeNiI ₆	0.988	0.259
Cs ₂ PbPtI ₆	0.849	0.466	Cs ₂ GeCaF ₆	0.966	0.650	Cs ₂ BeNiF ₆	1.116	0.429
Cs ₂ PbPtF ₆	0.901	0.771	Cs ₂ GeSrI ₆	0.867	0.434	Cs ₂ BeCuI ₆	0.981	0.268
Cs ₂ PbTeI ₆	0.831	0.498	Cs ₂ GeSrF ₆	0.928	0.718	Cs ₂ BeCuF ₆	1.105	0.444
Cs ₂ PbTeF ₆	0.875	0.823	Cs ₂ GeBaI ₆	0.845	0.473	Cs ₂ BeZnI ₆	0.979	0.270
Cs ₂ SnGeI ₆	0.876	0.42	Cs ₂ GeBaF ₆	0.895	0.782	Cs ₂ BeZnF ₆	1.102	0.447
Cs ₂ SnGeF ₆	0.941	0.695	Cs ₂ GeMnI ₆	0.944	0.318	Cs ₂ BePdI ₆	0.958	0.298
Cs ₂ SnBeI ₆	0.917	0.357	Cs ₂ GeMnF ₆	1.045	0.526	Cs ₂ BePdF ₆	1.069	0.492
Cs ₂ SnBeF ₆	1.003	0.590	Cs ₂ GeFeI ₆	0.926	0.343	Cs ₂ BeIrI ₆	0.952	0.307
Cs ₂ SnMgI ₆	0.877	0.418	Cs ₂ GeFeF ₆	1.017	0.568	Cs ₂ BeIrF ₆	1.058	0.508
Cs ₂ SnMgF ₆	0.943	0.692	Cs ₂ GeCoI ₆	0.932	0.335	Cs ₂ BePtI ₆	0.958	0.298
Cs ₂ SnCaI ₆	0.839	0.482	Cs ₂ GeCoF ₆	1.026	0.555	Cs ₂ BePtF ₆	1.069	0.492

Material	t	u	Material	t	u	Material	t	u
Cs ₂ BeTeI ₆	0.936	0.33	Cs ₂ CaCuI ₆	0.893	0.393	Cs ₂ BaNiF ₆	0.903	0.767
Cs ₂ BeTeF ₆	1.032	0.545	Cs ₂ CaCuF ₆	0.966	0.650	Cs ₂ BaCuI ₆	0.845	0.473
Cs ₂ MgCaI ₆	0.894	0.391	Cs ₂ CaZnI ₆	0.891	0.395	Cs ₂ BaCuF ₆	0.895	0.782
Cs ₂ MgCaF ₆	0.969	0.647	Cs ₂ CaZnF ₆	0.964	0.654	Cs ₂ BaZnI ₆	0.843	0.475
Cs ₂ MgSrI ₆	0.869	0.432	Cs ₂ CaPdI ₆	0.874	0.423	Cs ₂ BaZnF ₆	0.893	0.786
Cs ₂ MgSrF ₆	0.930	0.714	Cs ₂ CaPdF ₆	0.939	0.699	Cs ₂ BaPdI ₆	0.828	0.502
Cs ₂ MgBaI ₆	0.846	0.470	Cs ₂ CaIrI ₆	0.869	0.432	Cs ₂ BaPdF ₆	0.871	0.831
Cs ₂ MgBaF ₆	0.897	0.778	Cs ₂ CaIrF ₆	0.930	0.714	Cs ₂ BaIrI ₆	0.823	0.511
Cs ₂ MgMnI ₆	0.945	0.316	Cs ₂ CaPtI ₆	0.874	0.423	Cs ₂ BaIrF ₆	0.864	0.846
Cs ₂ MgMnF ₆	1.048	0.523	Cs ₂ CaPtF ₆	0.939	0.699	Cs ₂ BaPtI ₆	0.828	0.502
Cs ₂ MgFeI ₆	0.928	0.341	Cs ₂ CaTeI ₆	0.855	0.455	Cs ₂ BaPtF ₆	0.871	0.831
Cs ₂ MgFeF ₆	1.020	0.564	Cs ₂ CaTeF ₆	0.910	0.752	Cs ₂ BaTeI ₆	0.811	0.534
Cs ₂ MgCoI ₆	0.933	0.333	Cs ₂ SrBaI ₆	0.790	0.575	Cs ₂ BaTeF ₆	0.847	0.883
Cs ₂ MgCoF ₆	1.029	0.551	Cs ₂ SrMnI ₆	0.876	0.420	Cs ₂ MnFeI ₆	0.936	0.330
Cs ₂ MgNiI ₆	0.942	0.320	Cs ₂ SrMnF ₆	0.941	0.695	Cs ₂ MnFeF ₆	1.032	0.545
Cs ₂ MgNiF ₆	1.042	0.530	Cs ₂ SrFeI ₆	0.861	0.445	Cs ₂ MnCoI ₆	0.941	0.322
Cs ₂ MgCuI ₆	0.936	0.330	Cs ₂ SrFeF ₆	0.918	0.737	Cs ₂ MnCoF ₆	1.041	0.532
Cs ₂ MgCuF ₆	1.032	0.545	Cs ₂ SrCoI ₆	0.865	0.438	Cs ₂ MnNiI ₆	0.95	0.309
Cs ₂ MgZnI ₆	0.934	0.332	Cs ₂ SrCoF ₆	0.925	0.724	Cs ₂ MnNiF ₆	1.055	0.511
Cs ₂ MgZnF ₆	1.030	0.549	Cs ₂ SrNiI ₆	0.873	0.425	Cs ₂ MnCuI ₆	0.944	0.318
Cs ₂ MgPdI ₆	0.915	0.359	Cs ₂ SrNiF ₆	0.937	0.703	Cs ₂ MnCuF ₆	1.045	0.526
Cs ₂ MgPdF ₆	1.001	0.594	Cs ₂ SrCuI ₆	0.867	0.434	Cs ₂ MnZnI ₆	0.942	0.320
Cs ₂ MgIrI ₆	0.909	0.368	Cs ₂ SrCuF ₆	0.928	0.718	Cs ₂ MnZnF ₆	1.042	0.530
Cs ₂ MgIrF ₆	0.991	0.609	Cs ₂ SrZnI ₆	0.866	0.436	Cs ₂ MnPdI ₆	0.923	0.348
Cs ₂ MgPtI ₆	0.915	0.359	Cs ₂ SrZnF ₆	0.926	0.722	Cs ₂ MnPdF ₆	1.013	0.575
Cs ₂ MgPtF ₆	1.001	0.594	Cs ₂ SrPdI ₆	0.850	0.464	Cs ₂ MnIrI ₆	0.917	0.357
Cs ₂ MgTeI ₆	0.894	0.391	Cs ₂ SrPdF ₆	0.903	0.767	Cs ₂ MnIrF ₆	1.003	0.590
Cs ₂ MgTeF ₆	0.969	0.647	Cs ₂ SrIrI ₆	0.845	0.473	Cs ₂ MnPtI ₆	0.923	0.348
Cs ₂ CaSrI ₆	0.832	0.495	Cs ₂ SrIrF ₆	0.895	0.782	Cs ₂ MnPtF ₆	1.013	0.575
Cs ₂ CaSrF ₆	0.877	0.820	Cs ₂ SrPtI ₆	0.850	0.464	Cs ₂ MnTeI ₆	0.902	0.380
Cs ₂ CaBaI ₆	0.811	0.534	Cs ₂ SrPtF ₆	0.903	0.767	Cs ₂ MnTeF ₆	0.980	0.628
Cs ₂ CaBaF ₆	0.847	0.883	Cs ₂ SrTeI ₆	0.832	0.495	Cs ₂ FeCoI ₆	0.924	0.347
Cs ₂ CaMnI ₆	0.902	0.380	Cs ₂ SrTeF ₆	0.877	0.82	Cs ₂ FeCoF ₆	1.014	0.573
Cs ₂ CaMnF ₆	0.980	0.628	Cs ₂ BaMnI ₆	0.852	0.459	Cs ₂ FeNiI ₆	0.932	0.334
Cs ₂ CaFeI ₆	0.886	0.405	Cs ₂ BaMnF ₆	0.907	0.759	Cs ₂ FeNiF ₆	1.027	0.553
Cs ₂ CaFeF ₆	0.956	0.669	Cs ₂ BaFeI ₆	0.838	0.484	Cs ₂ FeCuI ₆	0.926	0.343
Cs ₂ CaCoI ₆	0.891	0.397	Cs ₂ BaFeF ₆	0.886	0.801	Cs ₂ FeCuF ₆	1.017	0.568
Cs ₂ CaCoF ₆	0.963	0.656	Cs ₂ BaCoI ₆	0.843	0.476	Cs ₂ FeZnI ₆	0.924	0.345
Cs ₂ CaNiI ₆	0.899	0.384	Cs ₂ BaCoF ₆	0.892	0.788	Cs ₂ FeZnF ₆	1.015	0.571
Cs ₂ CaNiF ₆	0.975	0.635	Cs ₂ BaNiI ₆	0.850	0.464	Cs ₂ FePdI ₆	0.906	0.373

Material	t	u	Material	t	u	Material	t	u
Cs ₂ FePdF ₆	0.987	0.617	Cs ₂ CuPtF ₆	0.998	0.598	Cs ₂ CdMnF ₆	0.991	0.609
Cs ₂ FeIrI ₆	0.900	0.382	Cs ₂ CuTeI ₆	0.893	0.393	Cs ₂ CdFeI ₆	0.893	0.393
Cs ₂ FeIrF ₆	0.978	0.632	Cs ₂ CuTeF ₆	0.966	0.650	Cs ₂ CdFeF ₆	0.966	0.650
Cs ₂ FePtI ₆	0.906	0.373	Cs ₂ ZnPdI ₆	0.912	0.364	Cs ₂ CdCoI ₆	0.898	0.385
Cs ₂ FePtF ₆	0.987	0.617	Cs ₂ ZnPdF ₆	0.996	0.602	Cs ₂ CdCoF ₆	0.974	0.637
Cs ₂ FeTeI ₆	0.886	0.405	Cs ₂ ZnIrI ₆	0.906	0.373	Cs ₂ CdNiI ₆	0.906	0.373
Cs ₂ FeTeF ₆	0.956	0.669	Cs ₂ ZnIrF ₆	0.987	0.617	Cs ₂ CdNiF ₆	0.987	0.617
Cs ₂ CoNiI ₆	0.938	0.326	Cs ₂ ZnPtI ₆	0.912	0.364	Cs ₂ CdCuI ₆	0.900	0.382
Cs ₂ CoNiF ₆	1.036	0.539	Cs ₂ ZnPtF ₆	0.996	0.602	Cs ₂ CdCuF ₆	0.978	0.632
Cs ₂ CoCuI ₆	0.932	0.335	Cs ₂ ZnTeI ₆	0.891	0.395	Cs ₂ CdZnI ₆	0.899	0.384
Cs ₂ CoCuF ₆	1.026	0.555	Cs ₂ ZnTeF ₆	0.964	0.654	Cs ₂ CdZnF ₆	0.975	0.635
Cs ₂ CoZnI ₆	0.930	0.338	Cs ₂ PdIrI ₆	0.888	0.400	Cs ₂ CdPdI ₆	0.881	0.411
Cs ₂ CoZnF ₆	1.024	0.558	Cs ₂ PdIrF ₆	0.960	0.662	Cs ₂ CdPdF ₆	0.949	0.680
Cs ₂ CoPdI ₆	0.911	0.365	Cs ₂ PdPtI ₆	0.894	0.391	Cs ₂ CdIrI ₆	0.876	0.420
Cs ₂ CoPdF ₆	0.995	0.603	Cs ₂ PdPtF ₆	0.969	0.647	Cs ₂ CdIrF ₆	0.941	0.695
Cs ₂ CoIrI ₆	0.905	0.374	Cs ₂ PdTeI ₆	0.874	0.423	Cs ₂ CdPtI ₆	0.881	0.411
Cs ₂ CoIrF ₆	0.986	0.618	Cs ₂ PdTeF ₆	0.939	0.699	Cs ₂ CdPtF ₆	0.949	0.680
Cs ₂ CoPtI ₆	0.911	0.365	Cs ₂ IrPtI ₆	0.888	0.4000	Cs ₂ CdTeI ₆	0.862	0.443
Cs ₂ CoPtF ₆	0.995	0.603	Cs ₂ IrPtF ₆	0.960	0.662	Cs ₂ CdTeF ₆	0.920	0.733
Cs ₂ CoTeI ₆	0.891	0.397	Cs ₂ IrTeI ₆	0.869	0.432	Cs ₂ PbSnBr ₆	0.824	0.589
Cs ₂ CoTeF ₆	0.963	0.656	Cs ₂ IrTeF ₆	0.930	0.714	Cs ₂ PbSnCl ₆	0.830	0.638
Cs ₂ NiCuI ₆	0.940	0.323	Cs ₂ PtTeI ₆	0.874	0.423	Cs ₂ PbGeBr ₆	0.879	0.490
Cs ₂ NiCuF ₆	1.040	0.534	Cs ₂ PtTeF ₆	0.939	0.699	Cs ₂ PbGeCl ₆	0.888	0.530
Cs ₂ NiZnI ₆	0.939	0.325	Cs ₂ CdPbI ₆	0.837	0.486	Cs ₂ PbBeBr ₆	0.923	0.418
Cs ₂ NiZnF ₆	1.037	0.538	Cs ₂ CdPbF ₆	0.884	0.805	Cs ₂ PbBeCl ₆	0.936	0.453
Cs ₂ NiPdI ₆	0.920	0.352	Cs ₂ CdSnI ₆	0.846	0.470	Cs ₂ PbMgBr ₆	0.881	0.487
Cs ₂ NiPdF ₆	1.008	0.583	Cs ₂ CdSnF ₆	0.897	0.778	Cs ₂ PbMgCl ₆	0.890	0.528
Cs ₂ NiIrI ₆	0.914	0.361	Cs ₂ CdGeI ₆	0.900	0.382	Cs ₂ PbCaBr ₆	0.840	0.559
Cs ₂ NiIrF ₆	0.998	0.598	Cs ₂ CdGeF ₆	0.978	0.632	Cs ₂ PbCaCl ₆	0.847	0.605
Cs ₂ NiPtI ₆	0.920	0.352	Cs ₂ CdBeI ₆	0.944	0.318	Cs ₂ PbSrBr ₆	0.816	0.605
Cs ₂ NiPtF ₆	1.008	0.583	Cs ₂ CdBeF ₆	1.045	0.526	Cs ₂ PbSrCl ₆	0.822	0.655
Cs ₂ NiTeI ₆	0.899	0.384	Cs ₂ CdMgI ₆	0.902	0.380	Cs ₂ PbBaBr ₆	0.795	0.648
Cs ₂ NiTeF ₆	0.975	0.635	Cs ₂ CdMgF ₆	0.980	0.628	Cs ₂ PbBaCl ₆	0.799	0.702
Cs ₂ CuZnI ₆	0.932	0.334	Cs ₂ CdCaI ₆	0.862	0.443	Cs ₂ PbMnBr ₆	0.888	0.474
Cs ₂ CuZnF ₆	1.027	0.553	Cs ₂ CdCaF ₆	0.920	0.733	Cs ₂ PbMnCl ₆	0.898	0.514
Cs ₂ CuPdI ₆	0.914	0.361	Cs ₂ CdSrI ₆	0.838	0.484	Cs ₂ PbFeBr ₆	0.872	0.503
Cs ₂ CuPdF ₆	0.998	0.598	Cs ₂ CdSrF ₆	0.886	0.801	Cs ₂ PbFeCl ₆	0.880	0.544
Cs ₂ CuIrI ₆	0.908	0.370	Cs ₂ CdBaI ₆	0.817	0.523	Cs ₂ PbCoBr ₆	0.877	0.494
Cs ₂ CuIrF ₆	0.989	0.613	Cs ₂ CdBaF ₆	0.855	0.865	Cs ₂ PbCoCl ₆	0.886	0.535
Cs ₂ CuPtI ₆	0.914	0.361	Cs ₂ CdMnI ₆	0.909	0.368	Cs ₂ PbNiBr ₆	0.885	0.480

Material	t	u	Material	t	u	Material	t	u
Cs ₂ PbNiCl ₆	0.895	0.519	Cs ₂ SnIrCl ₆	0.873	0.558	Cs ₂ BeSrCl ₆	0.937	0.450
Cs ₂ PbCuBr ₆	0.879	0.490	Cs ₂ SnPtBr ₆	0.870	0.505	Cs ₂ BeBaBr ₆	0.897	0.459
Cs ₂ PbCuCl ₆	0.888	0.530	Cs ₂ SnPtCl ₆	0.879	0.547	Cs ₂ BeBaCl ₆	0.908	0.497
Cs ₂ PbZnBr ₆	0.878	0.492	Cs ₂ SnTeBr ₆	0.850	0.541	Cs ₂ BeMnBr ₆	1.019	0.286
Cs ₂ PbZnCl ₆	0.887	0.533	Cs ₂ SnTeCl ₆	0.857	0.586	Cs ₂ BeMnCl ₆	1.038	0.309
Cs ₂ PbPdBr ₆	0.860	0.523	Cs ₂ GeBeBr ₆	1.007	0.301	Cs ₂ BeFeBr ₆	0.997	0.314
Cs ₂ PbPdCl ₆	0.868	0.566	Cs ₂ GeBeCl ₆	1.025	0.326	Cs ₂ BeFeCl ₆	1.015	0.340
Cs ₂ PbIrBr ₆	0.854	0.533	Cs ₂ GeMgBr ₆	0.956	0.370	Cs ₂ BeCoBr ₆	1.004	0.305
Cs ₂ PbIrCl ₆	0.862	0.577	Cs ₂ GeMgCl ₆	0.971	0.401	Cs ₂ BeCoCl ₆	1.022	0.330
Cs ₂ PbPtBr ₆	0.860	0.523	Cs ₂ GeCaBr ₆	0.909	0.441	Cs ₂ BeNiBr ₆	1.015	0.291
Cs ₂ PbPtCl ₆	0.868	0.566	Cs ₂ GeCaCl ₆	0.920	0.478	Cs ₂ BeNiCl ₆	1.034	0.315
Cs ₂ PbTeBr ₆	0.840	0.559	Cs ₂ GeSrBr ₆	0.881	0.487	Cs ₂ BeCuBr ₆	1.007	0.301
Cs ₂ PbTeCl ₆	0.847	0.605	Cs ₂ GeSrCl ₆	0.890	0.528	Cs ₂ BeCuCl ₆	1.025	0.326
Cs ₂ SnGeBr ₆	0.890	0.472	Cs ₂ GeBaBr ₆	0.856	0.531	Cs ₂ BeZnBr ₆	1.005	0.304
Cs ₂ SnGeCl ₆	0.900	0.511	Cs ₂ GeBaCl ₆	0.863	0.575	Cs ₂ BeZnCl ₆	1.023	0.329
Cs ₂ SnBeBr ₆	0.935	0.401	Cs ₂ GeMnBr ₆	0.965	0.357	Cs ₂ BePdBr ₆	0.982	0.334
Cs ₂ SnBeCl ₆	0.948	0.434	Cs ₂ GeMnCl ₆	0.980	0.387	Cs ₂ BePdCl ₆	0.998	0.362
Cs ₂ SnMgBr ₆	0.891	0.469	Cs ₂ GeFeBr ₆	0.945	0.385	Cs ₂ BeIrBr ₆	0.974	0.344
Cs ₂ SnMgCl ₆	0.901	0.508	Cs ₂ GeFeCl ₆	0.959	0.417	Cs ₂ BeIrCl ₆	0.990	0.373
Cs ₂ SnCaBr ₆	0.850	0.541	Cs ₂ GeCoBr ₆	0.952	0.376	Cs ₂ BePtBr ₆	0.982	0.334
Cs ₂ SnCaCl ₆	0.857	0.586	Cs ₂ GeCoCl ₆	0.966	0.407	Cs ₂ BePtCl ₆	0.998	0.362
Cs ₂ SnSrBr ₆	0.825	0.587	Cs ₂ GeNiBr ₆	0.961	0.362	Cs ₂ BeTeBr ₆	0.956	0.370
Cs ₂ SnSrCl ₆	0.831	0.635	Cs ₂ GeNiCl ₆	0.976	0.392	Cs ₂ BeTeCl ₆	0.971	0.401
Cs ₂ SnBaBr ₆	0.803	0.630	Cs ₂ GeCuBr ₆	0.954	0.372	Cs ₂ MgCaBr ₆	0.910	0.439
Cs ₂ SnBaCl ₆	0.808	0.682	Cs ₂ GeCuCl ₆	0.969	0.403	Cs ₂ MgCaCl ₆	0.922	0.475
Cs ₂ SnMnBr ₆	0.899	0.457	Cs ₂ GeZnBr ₆	0.952	0.375	Cs ₂ MgSrBr ₆	0.882	0.485
Cs ₂ SnMnCl ₆	0.910	0.494	Cs ₂ GeZnCl ₆	0.967	0.406	Cs ₂ MgSrCl ₆	0.892	0.525
Cs ₂ SnFeBr ₆	0.882	0.485	Cs ₂ GePdBr ₆	0.932	0.406	Cs ₂ MgBaBr ₆	0.857	0.528
Cs ₂ SnFeCl ₆	0.892	0.525	Cs ₂ GePdCl ₆	0.945	0.439	Cs ₂ MgBaCl ₆	0.865	0.572
Cs ₂ SnCoBr ₆	0.887	0.476	Cs ₂ GeIrBr ₆	0.925	0.416	Cs ₂ MgMnBr ₆	0.967	0.355
Cs ₂ SnCoCl ₆	0.897	0.515	Cs ₂ GeIrCl ₆	0.937	0.45	Cs ₂ MgMnCl ₆	0.982	0.384
Cs ₂ SnNiBr ₆	0.896	0.462	Cs ₂ GePtBr ₆	0.932	0.406	Cs ₂ MgFeBr ₆	0.947	0.383
Cs ₂ SnNiCl ₆	0.906	0.500	Cs ₂ GePtCl ₆	0.945	0.439	Cs ₂ MgFeCl ₆	0.961	0.414
Cs ₂ SnCuBr ₆	0.89	0.472	Cs ₂ GeTeBr ₆	0.909	0.441	Cs ₂ MgCoBr ₆	0.953	0.374
Cs ₂ SnCuCl ₆	0.900	0.511	Cs ₂ GeTeCl ₆	0.92	0.478	Cs ₂ MgCoCl ₆	0.968	0.405
Cs ₂ SnZnBr ₆	0.888	0.474	Cs ₂ BeMgBr ₆	1.009	0.298	Cs ₂ MgNiBr ₆	0.963	0.360
Cs ₂ SnZnCl ₆	0.898	0.514	Cs ₂ BeMgCl ₆	1.027	0.323	Cs ₂ MgNiCl ₆	0.978	0.390
Cs ₂ SnPdBr ₆	0.870	0.505	Cs ₂ BeCaBr ₆	0.956	0.370	Cs ₂ MgCuBr ₆	0.956	0.370
Cs ₂ SnPdCl ₆	0.879	0.547	Cs ₂ BeCaCl ₆	0.971	0.401	Cs ₂ MgCuCl ₆	0.971	0.401
Cs ₂ SnIrBr ₆	0.864	0.515	Cs ₂ BeSrBr ₆	0.925	0.416	Cs ₂ MgZnBr ₆	0.954	0.372

Material	t	u	Material	t	u	Material	t	u
Cs ₂ MgZnCl ₆	0.969	0.403	Cs ₂ SrCoCl ₆	0.888	0.532	Cs ₂ MnNiCl ₆	0.988	0.376
Cs ₂ MgPdBr ₆	0.933	0.403	Cs ₂ SrNiBr ₆	0.887	0.477	Cs ₂ MnCuBr ₆	0.965	0.357
Cs ₂ MgPdCl ₆	0.946	0.436	Cs ₂ SrNiCl ₆	0.896	0.517	Cs ₂ MnCuCl ₆	0.980	0.387
Cs ₂ MgIrBr ₆	0.927	0.413	Cs ₂ SrCuBr ₆	0.881	0.487	Cs ₂ MnZnBr ₆	0.963	0.360
Cs ₂ MgIrCl ₆	0.939	0.448	Cs ₂ SrCuCl ₆	0.890	0.528	Cs ₂ MnZnCl ₆	0.978	0.390
Cs ₂ MgPtBr ₆	0.933	0.403	Cs ₂ SrZnBr ₆	0.879	0.490	Cs ₂ MnPdBr ₆	0.942	0.390
Cs ₂ MgPtCl ₆	0.946	0.436	Cs ₂ SrZnCl ₆	0.888	0.530	Cs ₂ MnPdCl ₆	0.956	0.423
Cs ₂ MgTeBr ₆	0.910	0.439	Cs ₂ SrPdBr ₆	0.861	0.520	Cs ₂ MnIrBr ₆	0.935	0.401
Cs ₂ MgTeCl ₆	0.922	0.475	Cs ₂ SrPdCl ₆	0.870	0.564	Cs ₂ MnIrCl ₆	0.948	0.434
Cs ₂ CaSrBr ₆	0.842	0.556	Cs ₂ SrIrBr ₆	0.856	0.531	Cs ₂ MnPtBr ₆	0.942	0.390
Cs ₂ CaSrCl ₆	0.849	0.602	Cs ₂ SrIrCl ₆	0.863	0.575	Cs ₂ MnPtCl ₆	0.956	0.423
Cs ₂ CaBaBr ₆	0.819	0.599	Cs ₂ SrPtBr ₆	0.861	0.520	Cs ₂ MnTeBr ₆	0.918	0.426
Cs ₂ CaBaCl ₆	0.824	0.649	Cs ₂ SrPtCl ₆	0.870	0.564	Cs ₂ MnTeCl ₆	0.930	0.461
Cs ₂ CaMnBr ₆	0.918	0.426	Cs ₂ SrTeBr ₆	0.842	0.556	Cs ₂ FeCoBr ₆	0.943	0.389
Cs ₂ CaMnCl ₆	0.930	0.461	Cs ₂ SrTeCl ₆	0.849	0.602	Cs ₂ FeCoCl ₆	0.957	0.421
Cs ₂ CaFeBr ₆	0.901	0.454	Cs ₂ BaMnBr ₆	0.864	0.515	Cs ₂ FeNiBr ₆	0.952	0.375
Cs ₂ CaFeCl ₆	0.911	0.492	Cs ₂ BaMnCl ₆	0.873	0.558	Cs ₂ FeNiCl ₆	0.967	0.406
Cs ₂ CaCoBr ₆	0.906	0.445	Cs ₂ BaFeBr ₆	0.849	0.543	Cs ₂ FeCuBr ₆	0.945	0.385
Cs ₂ CaCoCl ₆	0.917	0.482	Cs ₂ BaFeCl ₆	0.856	0.588	Cs ₂ FeCuCl ₆	0.959	0.417
Cs ₂ CaNiBr ₆	0.915	0.431	Cs ₂ BaCoBr ₆	0.853	0.534	Cs ₂ FeZnBr ₆	0.944	0.388
Cs ₂ CaNiCl ₆	0.927	0.467	Cs ₂ BaCoCl ₆	0.861	0.579	Cs ₂ FeZnCl ₆	0.957	0.420
Cs ₂ CaCuBr ₆	0.909	0.441	Cs ₂ BaNiBr ₆	0.861	0.520	Cs ₂ FePdBr ₆	0.923	0.418
Cs ₂ CaCuCl ₆	0.920	0.478	Cs ₂ BaNiCl ₆	0.870	0.564	Cs ₂ FePdCl ₆	0.936	0.453
Cs ₂ CaZnBr ₆	0.907	0.444	Cs ₂ BaCuBr ₆	0.856	0.531	Cs ₂ FeIrBr ₆	0.917	0.429
Cs ₂ CaZnCl ₆	0.918	0.481	Cs ₂ BaCuCl ₆	0.863	0.575	Cs ₂ FeIrCl ₆	0.929	0.464
Cs ₂ CaPdBr ₆	0.888	0.474	Cs ₂ BaZnBr ₆	0.854	0.533	Cs ₂ FePtBr ₆	0.923	0.418
Cs ₂ CaPdCl ₆	0.898	0.514	Cs ₂ BaZnCl ₆	0.862	0.577	Cs ₂ FePtCl ₆	0.936	0.453
Cs ₂ CaIrBr ₆	0.882	0.485	Cs ₂ BaPdBr ₆	0.837	0.564	Cs ₂ FeTeBr ₆	0.901	0.454
Cs ₂ CaIrCl ₆	0.892	0.525	Cs ₂ BaPdCl ₆	0.844	0.610	Cs ₂ FeTeCl ₆	0.911	0.492
Cs ₂ CaPtBr ₆	0.888	0.474	Cs ₂ BaIrBr ₆	0.832	0.574	Cs ₂ CoNiBr ₆	0.959	0.366
Cs ₂ CaPtCl ₆	0.898	0.514	Cs ₂ BaIrCl ₆	0.838	0.622	Cs ₂ CoNiCl ₆	0.974	0.396
Cs ₂ CaTeBr ₆	0.867	0.510	Cs ₂ BaPtBr ₆	0.837	0.564	Cs ₂ CoCuBr ₆	0.952	0.376
Cs ₂ CaTeCl ₆	0.876	0.552	Cs ₂ BaPtCl ₆	0.844	0.610	Cs ₂ CoCuCl ₆	0.966	0.407
Cs ₂ SrBaBr ₆	0.796	0.645	Cs ₂ BaTeBr ₆	0.819	0.599	Cs ₂ CoZnBr ₆	0.95	0.379
Cs ₂ SrBaCl ₆	0.800	0.699	Cs ₂ BaTeCl ₆	0.824	0.649	Cs ₂ CoZnCl ₆	0.964	0.410
Cs ₂ SrMnBr ₆	0.890	0.472	Cs ₂ MnFeBr ₆	0.956	0.370	Cs ₂ CoPdBr ₆	0.929	0.409
Cs ₂ SrMnCl ₆	0.900	0.511	Cs ₂ MnFeCl ₆	0.971	0.401	Cs ₂ CoPdCl ₆	0.942	0.443
Cs ₂ SrFeBr ₆	0.873	0.500	Cs ₂ MnCoBr ₆	0.962	0.361	Cs ₂ CoIrBr ₆	0.922	0.420
Cs ₂ SrFeCl ₆	0.882	0.541	Cs ₂ MnCoCl ₆	0.977	0.391	Cs ₂ CoIrCl ₆	0.935	0.454
Cs ₂ SrCoBr ₆	0.878	0.491	Cs ₂ MnNiBr ₆	0.972	0.347	Cs ₂ CoPtBr ₆	0.929	0.409

Material	t	u	Material	t	u	Material	t	u
Cs ₂ CoPtCl ₆	0.942	0.443	Cs ₂ IrPtCl ₆	0.915	0.486	Cs ₂ CdTeCl ₆	0.884	0.539
Cs ₂ CoTeBr ₆	0.906	0.445	Cs ₂ IrTeBr ₆	0.882	0.485	⁶ CsPbI ₃	0.807	0.541
Cs ₂ CoTeCl ₆	0.917	0.482	Cs ₂ IrTeCl ₆	0.892	0.525	CsSnF ₃	0.866	0.842
Cs ₂ NiCuBr ₆	0.961	0.362	Cs ₂ PtTeBr ₆	0.888	0.474	CsSnI ₃	0.824	0.509
Cs ₂ NiCuCl ₆	0.976	0.392	Cs ₂ PtTeCl ₆	0.898	0.514	CsGeF ₃	1.03	0.549
Cs ₂ NiZnBr ₆	0.960	0.365	Cs ₂ CdPbBr ₆	0.847	0.546	CsGeI ₃	0.934	0.332
Cs ₂ NiZnCl ₆	0.975	0.395	Cs ₂ CdPbCl ₆	0.854	0.591	CsBeF ₃	1.192	0.338
Cs ₂ NiPdBr ₆	0.939	0.395	Cs ₂ CdSnBr ₆	0.857	0.528	CsBeI ₃	1.033	0.205
Cs ₂ NiPdCl ₆	0.952	0.428	Cs ₂ CdSnCl ₆	0.865	0.572	CsMgF ₃	1.035	0.541
Cs ₂ NiIrBr ₆	0.932	0.406	Cs ₂ CdGeBr ₆	0.917	0.429	CsMgI ₃	0.937	0.327
Cs ₂ NiIrCl ₆	0.945	0.439	Cs ₂ CdGeCl ₆	0.929	0.464	CsCaF ₃	0.910	0.752
Cs ₂ NiPtBr ₆	0.939	0.395	Cs ₂ CdBeBr ₆	0.965	0.357	CsCaI ₃	0.855	0.455
Cs ₂ NiPtCl ₆	0.952	0.428	Cs ₂ CdBeCl ₆	0.980	0.387	CsSrF ₃	0.845	0.887
Cs ₂ NiTeBr ₆	0.915	0.431	Cs ₂ CdMgBr ₆	0.918	0.426	CsSrI ₃	0.810	0.536
Cs ₂ NiTeCl ₆	0.927	0.467	Cs ₂ CdMgCl ₆	0.930	0.461	CsBaF ₃	0.792	1.015
Cs ₂ CuZnBr ₆	0.952	0.375	Cs ₂ CdCaBr ₆	0.875	0.497	CsBaI ₃	0.771	0.614
Cs ₂ CuZnCl ₆	0.967	0.406	Cs ₂ CdCaCl ₆	0.884	0.539	CsMnF ₃	1.061	0.504
Cs ₂ CuPdBr ₆	0.932	0.406	Cs ₂ CdSrBr ₆	0.849	0.543	CsMnI ₃	0.953	0.305
Cs ₂ CuPdCl ₆	0.945	0.439	Cs ₂ CdSrCl ₆	0.856	0.588	CsSnF ₃	0.866	0.842
Cs ₂ CuIrBr ₆	0.925	0.416	Cs ₂ CdBaBr ₆	0.825	0.587	CsSnI ₃	0.824	0.509
Cs ₂ CuIrCl ₆	0.937	0.45	Cs ₂ CdBaCl ₆	0.831	0.635	CsCoF ₃	1.022	0.560
Cs ₂ CuPtBr ₆	0.932	0.406	Cs ₂ CdMnBr ₆	0.927	0.413	CsCoI ₃	0.929	0.339
Cs ₂ CuPtCl ₆	0.945	0.439	Cs ₂ CdMnCl ₆	0.939	0.448	CsNiF ₃	1.050	0.519
Cs ₂ CuTeBr ₆	0.909	0.441	Cs ₂ CdFeBr ₆	0.909	0.441	CsNiI ₃	0.947	0.314
Cs ₂ CuTeCl ₆	0.920	0.478	Cs ₂ CdFeCl ₆	0.920	0.478	CsCuF ₃	1.030	0.549
Cs ₂ ZnPdBr ₆	0.930	0.408	Cs ₂ CdCoBr ₆	0.914	0.432	CsCuI ₃	0.934	0.332
Cs ₂ ZnPdCl ₆	0.943	0.442	Cs ₂ CdCoCl ₆	0.926	0.468	CsZnF ₃	1.025	0.556
Cs ₂ ZnIrBr ₆	0.923	0.418	Cs ₂ CdNiBr ₆	0.923	0.418	CsZnI ₃	0.931	0.336
Cs ₂ ZnIrCl ₆	0.936	0.453	Cs ₂ CdNiCl ₆	0.936	0.453	CsPdF ₃	0.969	0.647
Cs ₂ ZnPtBr ₆	0.930	0.408	Cs ₂ CdCuBr ₆	0.917	0.429	CsPdI ₃	0.894	0.391
Cs ₂ ZnPtCl ₆	0.943	0.442	Cs ₂ CdCuCl ₆	0.929	0.464	CsIrF ₃	0.951	0.677
Cs ₂ ZnTeBr ₆	0.907	0.444	Cs ₂ CdZnBr ₆	0.915	0.431	CsIrI ₃	0.883	0.409
Cs ₂ ZnTeCl ₆	0.918	0.481	Cs ₂ CdZnCl ₆	0.927	0.467	CsPtF ₃	0.969	0.647
Cs ₂ PdIrBr ₆	0.904	0.449	Cs ₂ CdPdBr ₆	0.896	0.462	CsPtI ₃	0.894	0.391
Cs ₂ PdIrCl ₆	0.915	0.486	Cs ₂ CdPdCl ₆	0.906	0.500	CsTeF ₃	0.910	0.752
Cs ₂ PdPtBr ₆	0.910	0.439	Cs ₂ CdIrBr ₆	0.890	0.472	CsTeI ₃	0.855	0.455
Cs ₂ PdPtCl ₆	0.922	0.475	Cs ₂ CdIrCl ₆	0.900	0.511	CsPbCl ₃	0.820	0.657
Cs ₂ PdTeBr ₆	0.888	0.474	Cs ₂ CdPtBr ₆	0.896	0.462	CsPbBr ₃	0.815	0.607
Cs ₂ PdTeCl ₆	0.898	0.514	Cs ₂ CdPtCl ₆	0.906	0.500	CsSnCl ₃	0.840	0.619
Cs ₂ IrPtBr ₆	0.904	0.449	Cs ₂ CdTeBr ₆	0.875	0.497	CsSnBr ₃	0.833	0.571

Material	t	u	Material	t	u
CsGeCl ₃	0.969	0.403	CsCuCl ₃	0.969	0.403
CsGeBr ₃	0.954	0.372	CsCuBr ₃	0.954	0.372
CsBeCl ₃	1.089	0.249	CsZnCl ₃	0.965	0.409
CsBeBr ₃	1.065	0.230	CsZnBr ₃	0.951	0.378
CsMgCl ₃	0.973	0.398	CsPdCl ₃	0.922	0.475
CsMgBr ₃	0.958	0.367	CsPdBr ₃	0.910	0.439
CsCaCl ₃	0.876	0.552	CsIrCl ₃	0.908	0.497
CsCaBr ₃	0.867	0.510	CsIrBr ₃	0.897	0.459
CsSrCl ₃	0.823	0.652	CsPtCl ₃	0.922	0.475
CsSrBr ₃	0.817	0.602	CsPtBr ₃	0.910	0.439
CsBaCl ₃	0.779	0.746	CsTeCl ₃	0.876	0.552
CsBaBr ₃	0.775	0.689	CsTeBr ₃	0.867	0.510
CsMnCl ₃	0.992	0.370			
CsMnBr ₃	0.976	0.342			
CsSnCl ₃	0.84	0.619			
CsSnBr ₃	0.833	0.571			
CsCoCl ₃	0.963	0.412			
CsCoBr ₃	0.949	0.380			
CsNiCl ₃	0.984	0.381			
CsNiBr ₃	0.969	0.352			
CsGeCl ₃	0.969	0.403			
CsGeBr ₃	0.954	0.372			
CsBeCl ₃	1.089	0.249			
CsBeBr ₃	1.065	0.230			
CsMgCl ₃	0.973	0.398			
CsMgBr ₃	0.958	0.367			
CsCaCl ₃	0.876	0.552			
CsCaBr ₃	0.867	0.510			
CsSrCl ₃	0.823	0.652			
CsSrBr ₃	0.817	0.602			
CsBaCl ₃	0.779	0.746			
CsBaBr ₃	0.775	0.689			
CsMnCl ₃	0.992	0.370			
CsMnBr ₃	0.976	0.342			
CsSnCl ₃	0.840	0.619			
CsSnBr ₃	0.833	0.571			
CsCoCl ₃	0.963	0.412			
CsCoBr ₃	0.949	0.380			
CsNiCl ₃	0.984	0.381			
CsNiBr ₃	0.969	0.352			

Table S4. Goldschmidt tolerance factor range of inorganic double perovskites

Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}
Cs ₂ PbSnF ₆	0.842	0.866	Cs ₂ PbMnBr ₆	0.815	0.976	Cs ₂ SnPtF ₆	0.866	0.969
Cs ₂ PbGeF ₆	0.842	1.030	Cs ₂ PbFeBr ₆	0.815	0.937	Cs ₂ SnTeF ₆	0.866	0.910
Cs ₂ PbBeF ₆	0.842	1.192	Cs ₂ PbCoBr ₆	0.815	0.949	Cs ₂ SnGeCl ₆	0.840	0.969
Cs ₂ PbMgF ₆	0.842	1.035	Cs ₂ PbNiBr ₆	0.815	0.969	Cs ₂ SnBeCl ₆	0.84	1.089
Cs ₂ PbCaF ₆	0.842	0.910	Cs ₂ PbCuBr ₆	0.815	0.954	Cs ₂ SnMgCl ₆	0.840	0.973
Cs ₂ PbSrF ₆	0.842	0.845	Cs ₂ PbZnBr ₆	0.815	0.951	Cs ₂ SnCaCl ₆	0.840	0.876
Cs ₂ PbMnF ₆	0.842	1.061	Cs ₂ PbPdBr ₆	0.815	0.910	Cs ₂ SnSrCl ₆	0.840	0.823
Cs ₂ PbFeF ₆	0.842	1.005	Cs ₂ PbIrBr ₆	0.815	0.897	Cs ₂ SnBaCl ₆	0.840	0.779
Cs ₂ PbCoF ₆	0.842	1.022	Cs ₂ PbPtBr ₆	0.815	0.910	Cs ₂ SnMnCl ₆	0.840	0.992
Cs ₂ PbNiF ₆	0.842	1.050	Cs ₂ PbTeBr ₆	0.815	0.867	Cs ₂ SnFeCl ₆	0.840	0.950
Cs ₂ PbCuF ₆	0.842	1.030	Cs ₂ PbSnI ₆	0.807	0.824	Cs ₂ SnCoCl ₆	0.840	0.963
Cs ₂ PbZnF ₆	0.842	1.025	Cs ₂ PbGeI ₆	0.807	0.934	Cs ₂ SnNiCl ₆	0.840	0.984
Cs ₂ PbPdF ₆	0.842	0.969	Cs ₂ PbBeI ₆	0.807	1.033	Cs ₂ SnCuCl ₆	0.840	0.969
Cs ₂ PbIrF ₆	0.842	0.951	Cs ₂ PbMgI ₆	0.807	0.937	Cs ₂ SnZnCl ₆	0.840	0.965
Cs ₂ PbPtF ₆	0.842	0.969	Cs ₂ PbCaI ₆	0.807	0.855	Cs ₂ SnPdCl ₆	0.840	0.922
Cs ₂ PbTeF ₆	0.842	0.910	Cs ₂ PbSrI ₆	0.807	0.810	Cs ₂ SnIrCl ₆	0.840	0.908
Cs ₂ PbSnCl ₆	0.820	0.840	Cs ₂ PbBaI ₆	0.807	0.771	Cs ₂ SnPtCl ₆	0.840	0.922
Cs ₂ PbGeCl ₆	0.820	0.969	Cs ₂ PbMnI ₆	0.807	0.953	Cs ₂ SnTeCl ₆	0.840	0.876
Cs ₂ PbBeCl ₆	0.820	1.089	Cs ₂ PbFeI ₆	0.807	0.918	Cs ₂ SnGeBr ₆	0.833	0.954
Cs ₂ PbMgCl ₆	0.820	0.973	Cs ₂ PbCoI ₆	0.807	0.929	Cs ₂ SnBeBr ₆	0.833	1.065
Cs ₂ PbCaCl ₆	0.820	0.876	Cs ₂ PbNiI ₆	0.807	0.947	Cs ₂ SnMgBr ₆	0.833	0.958
Cs ₂ PbSrCl ₆	0.820	0.823	Cs ₂ PbCuI ₆	0.807	0.934	Cs ₂ SnCaBr ₆	0.833	0.867
Cs ₂ PbBaCl ₆	0.820	0.779	Cs ₂ PbZnI ₆	0.807	0.931	Cs ₂ SnSrBr ₆	0.833	0.817
Cs ₂ PbMnCl ₆	0.820	0.992	Cs ₂ PbPdI ₆	0.807	0.894	Cs ₂ SnBaBr ₆	0.833	0.775
Cs ₂ PbFeCl ₆	0.820	0.950	Cs ₂ PbIrI ₆	0.807	0.883	Cs ₂ SnMnBr ₆	0.833	0.976
Cs ₂ PbCoCl ₆	0.820	0.963	Cs ₂ PbPtI ₆	0.807	0.894	Cs ₂ SnFeBr ₆	0.833	0.937
Cs ₂ PbNiCl ₆	0.820	0.984	Cs ₂ PbTeI ₆	0.807	0.855	Cs ₂ SnCoBr ₆	0.833	0.949
Cs ₂ PbCuCl ₆	0.820	0.969	Cs ₂ SnGeF ₆	0.866	1.030	Cs ₂ SnNiBr ₆	0.833	0.969
Cs ₂ PbZnCl ₆	0.820	0.965	Cs ₂ SnBeF ₆	0.866	1.192	Cs ₂ SnCuBr ₆	0.833	0.954
Cs ₂ PbPdCl ₆	0.820	0.922	Cs ₂ SnMgF ₆	0.866	1.035	Cs ₂ SnZnBr ₆	0.833	0.951
Cs ₂ PbIrCl ₆	0.820	0.908	Cs ₂ SnCaF ₆	0.866	0.910	Cs ₂ SnPdBr ₆	0.833	0.910
Cs ₂ PbPtCl ₆	0.820	0.922	Cs ₂ SnSrF ₆	0.866	0.845	Cs ₂ SnIrBr ₆	0.833	0.897
Cs ₂ PbTeCl ₆	0.820	0.876	Cs ₂ SnMnF ₆	0.866	1.061	Cs ₂ SnPtBr ₆	0.833	0.910
Cs ₂ PbSnBr ₆	0.815	0.833	Cs ₂ SnFeF ₆	0.866	1.005	Cs ₂ SnTeBr ₆	0.833	0.867
Cs ₂ PbGeBr ₆	0.815	0.954	Cs ₂ SnCoF ₆	0.866	1.022	Cs ₂ SnGeI ₆	0.824	0.934
Cs ₂ PbBeBr ₆	0.815	1.065	Cs ₂ SnNiF ₆	0.866	1.050	Cs ₂ SnBeI ₆	0.824	1.033
Cs ₂ PbMgBr ₆	0.815	0.958	Cs ₂ SnCuF ₆	0.866	1.030	Cs ₂ SnMgI ₆	0.824	0.937
Cs ₂ PbCaBr ₆	0.815	0.867	Cs ₂ SnZnF ₆	0.866	1.025	Cs ₂ SnCaI ₆	0.824	0.855
Cs ₂ PbSrBr ₆	0.815	0.817	Cs ₂ SnPdF ₆	0.866	0.969	Cs ₂ SnSrI ₆	0.824	0.810
Cs ₂ PbBaBr ₆	0.815	0.775	Cs ₂ SnIrF ₆	0.866	0.951	Cs ₂ SnBaI ₆	0.824	0.771

Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}
Cs ₂ SnMnI ₆	0.824	0.953	Cs ₂ GeBeBr ₆	0.954	1.065	Cs ₂ BePdF ₆	0.969	1.192
Cs ₂ SnFeI ₆	0.824	0.918	Cs ₂ GeMgBr ₆	0.954	0.958	Cs ₂ BeIrF ₆	0.951	1.192
Cs ₂ SnCoI ₆	0.824	0.929	Cs ₂ GeCaBr ₆	0.954	0.867	Cs ₂ BePtF ₆	0.969	1.192
Cs ₂ SnNiI ₆	0.824	0.947	Cs ₂ GeSrBr ₆	0.954	0.817	Cs ₂ BeTeF ₆	0.910	1.192
Cs ₂ SnCuI ₆	0.824	0.934	Cs ₂ GeBaBr ₆	0.954	0.775	Cs ₂ BeMgCl ₆	0.973	1.089
Cs ₂ SnZnI ₆	0.824	0.931	Cs ₂ GeMnBr ₆	0.954	0.976	Cs ₂ BeCaCl ₆	0.876	1.089
Cs ₂ SnPdI ₆	0.824	0.894	Cs ₂ GeFeBr ₆	0.954	0.937	Cs ₂ BeSrCl ₆	0.823	1.089
Cs ₂ SnIrI ₆	0.824	0.883	Cs ₂ GeCoBr ₆	0.954	0.949	Cs ₂ BeBaCl ₆	0.779	1.089
Cs ₂ SnPtI ₆	0.824	0.894	Cs ₂ GeNiBr ₆	0.954	0.969	Cs ₂ BeMnCl ₆	0.992	1.089
Cs ₂ SnTeI ₆	0.824	0.855	Cs ₂ GeCuBr ₆	0.954	0.954	Cs ₂ BeFeCl ₆	0.950	1.089
Cs ₂ GeBeF ₆	1.030	1.192	Cs ₂ GeZnBr ₆	0.954	0.951	Cs ₂ BeCoCl ₆	0.963	1.089
Cs ₂ GeMgF ₆	1.030	1.035	Cs ₂ GePdBr ₆	0.954	0.910	Cs ₂ BeNiCl ₆	0.984	1.089
Cs ₂ GeCaF ₆	1.030	0.910	Cs ₂ GeIrBr ₆	0.954	0.897	Cs ₂ BeCuCl ₆	0.969	1.089
Cs ₂ GeSrF ₆	1.030	0.845	Cs ₂ GePtBr ₆	0.954	0.910	Cs ₂ BeZnCl ₆	0.965	1.089
Cs ₂ GeBaF ₆	1.030	0.792	Cs ₂ GeTeBr ₆	0.954	0.867	Cs ₂ BePdCl ₆	0.922	1.089
Cs ₂ GeMnF ₆	1.030	1.061	Cs ₂ GeBeI ₆	0.934	1.033	Cs ₂ BeIrCl ₆	0.908	1.089
Cs ₂ GeFeF ₆	1.030	1.005	Cs ₂ GeMgI ₆	0.934	0.937	Cs ₂ BePtCl ₆	0.922	1.089
Cs ₂ GeCoF ₆	1.030	1.022	Cs ₂ GeCaI ₆	0.934	0.855	Cs ₂ BeTeCl ₆	0.876	1.089
Cs ₂ GeNiF ₆	1.030	1.050	Cs ₂ GeSrI ₆	0.934	0.810	Cs ₂ BeMgBr ₆	0.958	1.065
Cs ₂ GeCuF ₆	1.030	1.030	Cs ₂ GeBaI ₆	0.934	0.771	Cs ₂ BeCaBr ₆	0.867	1.065
Cs ₂ GeZnF ₆	1.030	1.025	Cs ₂ GeMnI ₆	0.934	0.953	Cs ₂ BeSrBr ₆	0.817	1.065
Cs ₂ GePdF ₆	1.030	0.969	Cs ₂ GeFeI ₆	0.934	0.918	Cs ₂ BeBaBr ₆	0.775	1.065
Cs ₂ GeIrF ₆	1.030	0.951	Cs ₂ GeCoI ₆	0.934	0.929	Cs ₂ BeMnBr ₆	0.976	1.065
Cs ₂ GePtF ₆	1.030	0.969	Cs ₂ GeNiI ₆	0.934	0.947	Cs ₂ BeFeBr ₆	0.937	1.065
Cs ₂ GeTeF ₆	1.030	0.910	Cs ₂ GeCuI ₆	0.934	0.934	Cs ₂ BeCoBr ₆	0.949	1.065
Cs ₂ GeBeCl ₆	0.969	1.089	Cs ₂ GeZnI ₆	0.934	0.931	Cs ₂ BeNiBr ₆	0.969	1.065
Cs ₂ GeMgCl ₆	0.969	0.973	Cs ₂ GePdI ₆	0.934	0.894	Cs ₂ BeCuBr ₆	0.954	1.065
Cs ₂ GeCaCl ₆	0.969	0.876	Cs ₂ GeIrI ₆	0.934	0.883	Cs ₂ BeZnBr ₆	0.951	1.065
Cs ₂ GeSrCl ₆	0.969	0.823	Cs ₂ GePtI ₆	0.934	0.894	Cs ₂ BePdBr ₆	0.910	1.065
Cs ₂ GeBaCl ₆	0.969	0.779	Cs ₂ GeTeI ₆	0.934	0.855	Cs ₂ BeIrBr ₆	0.897	1.065
Cs ₂ GeMnCl ₆	0.969	0.992	Cs ₂ BeMgF ₆	1.035	1.192	Cs ₂ BePtBr ₆	0.910	1.065
Cs ₂ GeFeCl ₆	0.969	0.950	Cs ₂ BeCaF ₆	0.910	1.192	Cs ₂ BeTeBr ₆	0.867	1.065
Cs ₂ GeCoCl ₆	0.969	0.963	Cs ₂ BeSrF ₆	0.845	1.192	Cs ₂ BeMgI ₆	0.937	1.033
Cs ₂ GeNiCl ₆	0.969	0.984	Cs ₂ BeBaF ₆	0.792	1.192	Cs ₂ BeCaI ₆	0.855	1.033
Cs ₂ GeCuCl ₆	0.969	0.969	Cs ₂ BeMnF ₆	1.061	1.192	Cs ₂ BeSrI ₆	0.810	1.033
Cs ₂ GeZnCl ₆	0.969	0.965	Cs ₂ BeFeF ₆	1.005	1.192	Cs ₂ BeBaI ₆	0.771	1.033
Cs ₂ GePdCl ₆	0.969	0.922	Cs ₂ BeCoF ₆	1.022	1.192	Cs ₂ BeMnI ₆	0.953	1.033
Cs ₂ GeIrCl ₆	0.969	0.908	Cs ₂ BeNiF ₆	1.050	1.192	Cs ₂ BeFeI ₆	0.918	1.033
Cs ₂ GePtCl ₆	0.969	0.922	Cs ₂ BeCuF ₆	1.030	1.192	Cs ₂ BeCoI ₆	0.929	1.033
Cs ₂ GeTeCl ₆	0.969	0.876	Cs ₂ BeZnF ₆	1.025	1.192	Cs ₂ BeNiI ₆	0.947	1.033

Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}
Cs ₂ BeCuI ₆	0.934	1.033	Cs ₂ MgZnBr ₆	0.951	0.958	Cs ₂ CaPtCl ₆	0.876	0.922
Cs ₂ BeZnI ₆	0.931	1.033	Cs ₂ MgPdBr ₆	0.91	0.958	Cs ₂ CaTeCl ₆	0.876	0.876
Cs ₂ BePdI ₆	0.894	1.033	Cs ₂ MgIrBr ₆	0.897	0.958	Cs ₂ CaSrBr ₆	0.817	0.867
Cs ₂ BeIrI ₆	0.883	1.033	Cs ₂ MgPtBr ₆	0.91	0.958	Cs ₂ CaBaBr ₆	0.775	0.867
Cs ₂ BePtI ₆	0.894	1.033	Cs ₂ MgTeBr ₆	0.867	0.958	Cs ₂ CaMnBr ₆	0.867	0.976
Cs ₂ BeTeI ₆	0.855	1.033	Cs ₂ MgCaI ₆	0.855	0.937	Cs ₂ CaFeBr ₆	0.867	0.937
Cs ₂ MgCaF ₆	0.910	1.035	Cs ₂ MgSrI ₆	0.81	0.937	Cs ₂ CaCoBr ₆	0.867	0.949
Cs ₂ MgSrF ₆	0.845	1.035	Cs ₂ MgBaI ₆	0.771	0.937	Cs ₂ CaNiBr ₆	0.867	0.969
Cs ₂ MgBaF ₆	0.792	1.035	Cs ₂ MgMnI ₆	0.953	0.937	Cs ₂ CaCuBr ₆	0.867	0.954
Cs ₂ MgMnF ₆	1.061	1.035	Cs ₂ MgFeI ₆	0.918	0.937	Cs ₂ CaZnBr ₆	0.867	0.951
Cs ₂ MgFeF ₆	1.005	1.035	Cs ₂ MgCoI ₆	0.929	0.937	Cs ₂ CaPdBr ₆	0.867	0.910
Cs ₂ MgCoF ₆	1.022	1.035	Cs ₂ MgNiI ₆	0.947	0.937	Cs ₂ CaIrBr ₆	0.867	0.897
Cs ₂ MgNiF ₆	1.050	1.035	Cs ₂ MgCuI ₆	0.934	0.937	Cs ₂ CaPtBr ₆	0.867	0.910
Cs ₂ MgCuF ₆	1.030	1.035	Cs ₂ MgZnI ₆	0.931	0.937	Cs ₂ CaTeBr ₆	0.867	0.867
Cs ₂ MgZnF ₆	1.025	1.035	Cs ₂ MgPdI ₆	0.894	0.937	Cs ₂ CaSrI ₆	0.810	0.855
Cs ₂ MgPdF ₆	0.969	1.035	Cs ₂ MgIrI ₆	0.883	0.937	Cs ₂ CaBaI ₆	0.771	0.855
Cs ₂ MgIrF ₆	0.951	1.035	Cs ₂ MgPtI ₆	0.894	0.937	Cs ₂ CaMnI ₆	0.855	0.953
Cs ₂ MgPtF ₆	0.969	1.035	Cs ₂ MgTeI ₆	0.855	0.937	Cs ₂ CaFeI ₆	0.855	0.918
Cs ₂ MgTeF ₆	0.910	1.035	Cs ₂ CaSrF ₆	0.845	0.910	Cs ₂ CaCoI ₆	0.855	0.929
Cs ₂ MgCaCl ₆	0.876	0.973	Cs ₂ CaBaF ₆	0.792	0.910	Cs ₂ CaNiI ₆	0.855	0.947
Cs ₂ MgSrCl ₆	0.823	0.973	Cs ₂ CaMnF ₆	0.910	1.061	Cs ₂ CaCuI ₆	0.855	0.934
Cs ₂ MgBaCl ₆	0.779	0.973	Cs ₂ CaFeF ₆	0.910	1.005	Cs ₂ CaZnI ₆	0.855	0.931
Cs ₂ MgMnCl ₆	0.992	0.973	Cs ₂ CaCoF ₆	0.910	1.022	Cs ₂ CaPdI ₆	0.855	0.894
Cs ₂ MgFeCl ₆	0.950	0.973	Cs ₂ CaNiF ₆	0.910	1.050	Cs ₂ CaIrI ₆	0.855	0.883
Cs ₂ MgCoCl ₆	0.963	0.973	Cs ₂ CaCuF ₆	0.910	1.030	Cs ₂ CaPtI ₆	0.855	0.894
Cs ₂ MgNiCl ₆	0.984	0.973	Cs ₂ CaZnF ₆	0.910	1.025	Cs ₂ CaTeI ₆	0.855	0.855
Cs ₂ MgCuCl ₆	0.969	0.973	Cs ₂ CaPdF ₆	0.910	0.969	Cs ₂ SrMnF ₆	0.845	1.061
Cs ₂ MgZnCl ₆	0.965	0.973	Cs ₂ CaIrF ₆	0.910	0.951	Cs ₂ SrFeF ₆	0.845	1.005
Cs ₂ MgPdCl ₆	0.922	0.973	Cs ₂ CaPtF ₆	0.910	0.969	Cs ₂ SrCoF ₆	0.845	1.022
Cs ₂ MgIrCl ₆	0.908	0.973	Cs ₂ CaTeF ₆	0.910	0.910	Cs ₂ SrNiF ₆	0.845	1.050
Cs ₂ MgPtCl ₆	0.922	0.973	Cs ₂ CaSrCl ₆	0.823	0.876	Cs ₂ SrCuF ₆	0.845	1.030
Cs ₂ MgTeCl ₆	0.876	0.973	Cs ₂ CaBaCl ₆	0.779	0.876	Cs ₂ SrZnF ₆	0.845	1.025
Cs ₂ MgCaBr ₆	0.867	0.958	Cs ₂ CaMnCl ₆	0.876	0.992	Cs ₂ SrPdF ₆	0.845	0.969
Cs ₂ MgSrBr ₆	0.817	0.958	Cs ₂ CaFeCl ₆	0.876	0.950	Cs ₂ SrIrF ₆	0.845	0.951
Cs ₂ MgBaBr ₆	0.775	0.958	Cs ₂ CaCoCl ₆	0.876	0.963	Cs ₂ SrPtF ₆	0.845	0.969
Cs ₂ MgMnBr ₆	0.976	0.958	Cs ₂ CaNiCl ₆	0.876	0.984	Cs ₂ SrTeF ₆	0.845	0.910
Cs ₂ MgFeBr ₆	0.937	0.958	Cs ₂ CaCuCl ₆	0.876	0.969	Cs ₂ SrBaCl ₆	0.779	0.823
Cs ₂ MgCoBr ₆	0.949	0.958	Cs ₂ CaZnCl ₆	0.876	0.965	Cs ₂ SrMnCl ₆	0.823	0.992
Cs ₂ MgNiBr ₆	0.969	0.958	Cs ₂ CaPdCl ₆	0.876	0.922	Cs ₂ SrFeCl ₆	0.823	0.950
Cs ₂ MgCuBr ₆	0.954	0.958	Cs ₂ CaIrCl ₆	0.876	0.908	Cs ₂ SrCoCl ₆	0.823	0.963

Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}
Cs ₂ SrNiCl ₆	0.823	0.984	Cs ₂ BaFeCl ₆	0.779	0.95	Cs ₂ MnNiCl ₆	0.984	0.992
Cs ₂ SrCuCl ₆	0.823	0.969	Cs ₂ BaCoCl ₆	0.779	0.963	Cs ₂ MnCuCl ₆	0.969	0.992
Cs ₂ SrZnCl ₆	0.823	0.965	Cs ₂ BaNiCl ₆	0.779	0.984	Cs ₂ MnZnCl ₆	0.965	0.992
Cs ₂ SrPdCl ₆	0.823	0.922	Cs ₂ BaCuCl ₆	0.779	0.969	Cs ₂ MnPdCl ₆	0.922	0.992
Cs ₂ SrIrCl ₆	0.823	0.908	Cs ₂ BaZnCl ₆	0.779	0.965	Cs ₂ MnIrCl ₆	0.908	0.992
Cs ₂ SrPtCl ₆	0.823	0.922	Cs ₂ BaPdCl ₆	0.779	0.922	Cs ₂ MnPtCl ₆	0.922	0.992
Cs ₂ SrTeCl ₆	0.823	0.876	Cs ₂ BaIrCl ₆	0.779	0.908	Cs ₂ MnTeCl ₆	0.876	0.992
Cs ₂ SrBaBr ₆	0.775	0.817	Cs ₂ BaPtCl ₆	0.779	0.922	Cs ₂ MnFeBr ₆	0.937	0.976
Cs ₂ SrMnBr ₆	0.817	0.976	Cs ₂ BaTeCl ₆	0.779	0.876	Cs ₂ MnCoBr ₆	0.949	0.976
Cs ₂ SrFeBr ₆	0.817	0.937	Cs ₂ BaMnBr ₆	0.775	0.976	Cs ₂ MnNiBr ₆	0.969	0.976
Cs ₂ SrCoBr ₆	0.817	0.949	Cs ₂ BaFeBr ₆	0.775	0.937	Cs ₂ MnCuBr ₆	0.954	0.976
Cs ₂ SrNiBr ₆	0.817	0.969	Cs ₂ BaCoBr ₆	0.775	0.949	Cs ₂ MnZnBr ₆	0.951	0.976
Cs ₂ SrCuBr ₆	0.817	0.954	Cs ₂ BaNiBr ₆	0.775	0.969	Cs ₂ MnPdBr ₆	0.910	0.976
Cs ₂ SrZnBr ₆	0.817	0.951	Cs ₂ BaCuBr ₆	0.775	0.954	Cs ₂ MnIrBr ₆	0.897	0.976
Cs ₂ SrPdBr ₆	0.817	0.910	Cs ₂ BaZnBr ₆	0.775	0.951	Cs ₂ MnPtBr ₆	0.910	0.976
Cs ₂ SrIrBr ₆	0.817	0.897	Cs ₂ BaPdBr ₆	0.775	0.910	Cs ₂ MnTeBr ₆	0.867	0.976
Cs ₂ SrPtBr ₆	0.817	0.910	Cs ₂ BaIrBr ₆	0.775	0.897	Cs ₂ MnFeI ₆	0.918	0.953
Cs ₂ SrTeBr ₆	0.817	0.867	Cs ₂ BaPtBr ₆	0.775	0.910	Cs ₂ MnCoI ₆	0.929	0.953
Cs ₂ SrBaI ₆	0.771	0.810	Cs ₂ BaTeBr ₆	0.775	0.867	Cs ₂ MnNiI ₆	0.947	0.953
Cs ₂ SrMnI ₆	0.810	0.953	Cs ₂ BaMnI ₆	0.771	0.953	Cs ₂ MnCuI ₆	0.934	0.953
Cs ₂ SrFeI ₆	0.810	0.918	Cs ₂ BaFeI ₆	0.771	0.918	Cs ₂ MnZnI ₆	0.931	0.953
Cs ₂ SrCoI ₆	0.810	0.929	Cs ₂ BaCoI ₆	0.771	0.929	Cs ₂ MnPdI ₆	0.894	0.953
Cs ₂ SrNiI ₆	0.810	0.947	Cs ₂ BaNiI ₆	0.771	0.947	Cs ₂ MnIrI ₆	0.883	0.953
Cs ₂ SrCuI ₆	0.810	0.934	Cs ₂ BaCuI ₆	0.771	0.934	Cs ₂ MnPtI ₆	0.894	0.953
Cs ₂ SrZnI ₆	0.810	0.931	Cs ₂ BaZnI ₆	0.771	0.931	Cs ₂ MnTeI ₆	0.855	0.953
Cs ₂ SrPdI ₆	0.810	0.894	Cs ₂ BaPdI ₆	0.771	0.894	Cs ₂ FeCoF ₆	1.022	1.005
Cs ₂ SrIrI ₆	0.810	0.883	Cs ₂ BaIrI ₆	0.771	0.883	Cs ₂ FeNiF ₆	1.050	1.005
Cs ₂ SrPtI ₆	0.810	0.894	Cs ₂ BaPtI ₆	0.771	0.894	Cs ₂ FeCuF ₆	1.030	1.005
Cs ₂ SrTeI ₆	0.81	0.855	Cs ₂ BaTeI ₆	0.771	0.855	Cs ₂ FeZnF ₆	1.025	1.005
Cs ₂ BaMnF ₆	0.792	1.061	Cs ₂ MnFeF ₆	1.005	1.061	Cs ₂ FePdF ₆	0.969	1.005
Cs ₂ BaFeF ₆	0.792	1.005	Cs ₂ MnCoF ₆	1.022	1.061	Cs ₂ FeIrF ₆	0.951	1.005
Cs ₂ BaCoF ₆	0.792	1.022	Cs ₂ MnNiF ₆	1.050	1.061	Cs ₂ FePtF ₆	0.969	1.005
Cs ₂ BaNiF ₆	0.792	1.050	Cs ₂ MnCuF ₆	1.030	1.061	Cs ₂ FeTeF ₆	0.910	1.005
Cs ₂ BaCuF ₆	0.792	1.030	Cs ₂ MnZnF ₆	1.025	1.061	Cs ₂ FeCoCl ₆	0.950	0.963
Cs ₂ BaZnF ₆	0.792	1.025	Cs ₂ MnPdF ₆	0.969	1.061	Cs ₂ FeNiCl ₆	0.950	0.984
Cs ₂ BaPdF ₆	0.792	0.969	Cs ₂ MnIrF ₆	0.951	1.061	Cs ₂ FeCuCl ₆	0.950	0.969
Cs ₂ BaIrF ₆	0.792	0.951	Cs ₂ MnPtF ₆	0.969	1.061	Cs ₂ FeZnCl ₆	0.950	0.965
Cs ₂ BaPtF ₆	0.792	0.969	Cs ₂ MnTeF ₆	0.910	1.061	Cs ₂ FePdCl ₆	0.922	0.950
Cs ₂ BaTeF ₆	0.792	0.910	Cs ₂ MnFeCl ₆	0.950	0.992	Cs ₂ FeIrCl ₆	0.908	0.950
Cs ₂ BaMnCl ₆	0.779	0.992	Cs ₂ MnCoCl ₆	0.963	0.992	Cs ₂ FePtCl ₆	0.922	0.950

Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}
Cs ₂ FeTeCl ₆	0.876	0.950	Cs ₂ CoZnI ₆	0.929	0.931	Cs ₂ CuPdBr ₆	0.910	0.954
Cs ₂ FeCoBr ₆	0.937	0.949	Cs ₂ CoPdI ₆	0.894	0.929	Cs ₂ CuIrBr ₆	0.897	0.954
Cs ₂ FeNiBr ₆	0.937	0.969	Cs ₂ CoIrI ₆	0.883	0.929	Cs ₂ CuPtBr ₆	0.910	0.954
Cs ₂ FeCuBr ₆	0.937	0.954	Cs ₂ CoPtI ₆	0.894	0.929	Cs ₂ CuTeBr ₆	0.867	0.954
Cs ₂ FeZnBr ₆	0.937	0.951	Cs ₂ CoTeI ₆	0.855	0.929	Cs ₂ CuZnI ₆	0.931	0.934
Cs ₂ FePdBr ₆	0.910	0.937	Cs ₂ NiCuF ₆	1.030	1.050	Cs ₂ CuPdI ₆	0.894	0.934
Cs ₂ FeIrBr ₆	0.897	0.937	Cs ₂ NiZnF ₆	1.025	1.050	Cs ₂ CuIrI ₆	0.883	0.934
Cs ₂ FePtBr ₆	0.910	0.937	Cs ₂ NiPdF ₆	0.969	1.050	Cs ₂ CuPtI ₆	0.894	0.934
Cs ₂ FeTeBr ₆	0.867	0.937	Cs ₂ NiIrF ₆	0.951	1.050	Cs ₂ CuTeI ₆	0.855	0.934
Cs ₂ FeCoI ₆	0.918	0.929	Cs ₂ NiPtF ₆	0.969	1.050	Cs ₂ ZnPdF ₆	0.969	1.025
Cs ₂ FeNiI ₆	0.918	0.947	Cs ₂ NiTeF ₆	0.910	1.050	Cs ₂ ZnIrF ₆	0.951	1.025
Cs ₂ FeCuI ₆	0.918	0.934	Cs ₂ NiCuCl ₆	0.969	0.984	Cs ₂ ZnPtF ₆	0.969	1.025
Cs ₂ FeZnI ₆	0.918	0.931	Cs ₂ NiZnCl ₆	0.965	0.984	Cs ₂ ZnTeF ₆	0.910	1.025
Cs ₂ FePdI ₆	0.894	0.918	Cs ₂ NiPdCl ₆	0.922	0.984	Cs ₂ ZnPdCl ₆	0.922	0.965
Cs ₂ FeIrI ₆	0.883	0.918	Cs ₂ NiIrCl ₆	0.908	0.984	Cs ₂ ZnIrCl ₆	0.908	0.965
Cs ₂ FePtI ₆	0.894	0.918	Cs ₂ NiPtCl ₆	0.922	0.984	Cs ₂ ZnPtCl ₆	0.922	0.965
Cs ₂ FeTeI ₆	0.855	0.918	Cs ₂ NiTeCl ₆	0.876	0.984	Cs ₂ ZnTeCl ₆	0.876	0.965
Cs ₂ CoNiF ₆	1.022	1.050	Cs ₂ NiCuBr ₆	0.954	0.969	Cs ₂ ZnPdBr ₆	0.910	0.951
Cs ₂ CoCuF ₆	1.022	1.030	Cs ₂ NiZnBr ₆	0.951	0.969	Cs ₂ ZnIrBr ₆	0.897	0.951
Cs ₂ CoZnF ₆	1.022	1.025	Cs ₂ NiPdBr ₆	0.910	0.969	Cs ₂ ZnPtBr ₆	0.910	0.951
Cs ₂ CoPdF ₆	0.969	1.022	Cs ₂ NiIrBr ₆	0.897	0.969	Cs ₂ ZnTeBr ₆	0.867	0.951
Cs ₂ CoIrF ₆	0.951	1.022	Cs ₂ NiPtBr ₆	0.910	0.969	Cs ₂ ZnPdI ₆	0.894	0.931
Cs ₂ CoPtF ₆	0.969	1.022	Cs ₂ NiTeBr ₆	0.867	0.969	Cs ₂ ZnIrI ₆	0.883	0.931
Cs ₂ CoTeF ₆	0.910	1.022	Cs ₂ NiCuI ₆	0.934	0.947	Cs ₂ ZnPtI ₆	0.894	0.931
Cs ₂ CoNiCl ₆	0.963	0.984	Cs ₂ NiZnI ₆	0.931	0.947	Cs ₂ ZnTeI ₆	0.855	0.931
Cs ₂ CoCuCl ₆	0.963	0.969	Cs ₂ NiPdI ₆	0.894	0.947	Cs ₂ PdIrF ₆	0.951	0.969
Cs ₂ CoZnCl ₆	0.963	0.965	Cs ₂ NiIrI ₆	0.883	0.947	Cs ₂ PdPtF ₆	0.969	0.969
Cs ₂ CoPdCl ₆	0.922	0.963	Cs ₂ NiPtI ₆	0.894	0.947	Cs ₂ PdTeF ₆	0.910	0.969
Cs ₂ CoIrCl ₆	0.908	0.963	Cs ₂ NiTeI ₆	0.855	0.947	Cs ₂ PdIrCl ₆	0.908	0.922
Cs ₂ CoPtCl ₆	0.922	0.963	Cs ₂ CuZnF ₆	1.025	1.030	Cs ₂ PdPtCl ₆	0.922	0.922
Cs ₂ CoTeCl ₆	0.876	0.963	Cs ₂ CuPdF ₆	0.969	1.030	Cs ₂ PdTeCl ₆	0.876	0.922
Cs ₂ CoNiBr ₆	0.949	0.969	Cs ₂ CuIrF ₆	0.951	1.030	Cs ₂ PdIrBr ₆	0.897	0.910
Cs ₂ CoCuBr ₆	0.949	0.954	Cs ₂ CuPtF ₆	0.969	1.030	Cs ₂ PdPtBr ₆	0.910	0.910
Cs ₂ CoZnBr ₆	0.949	0.951	Cs ₂ CuTeF ₆	0.910	1.030	Cs ₂ PdTeBr ₆	0.867	0.910
Cs ₂ CoPdBr ₆	0.910	0.949	Cs ₂ CuZnCl ₆	0.965	0.969	Cs ₂ PdIrI ₆	0.883	0.894
Cs ₂ CoIrBr ₆	0.897	0.949	Cs ₂ CuPdCl ₆	0.922	0.969	Cs ₂ PdPtI ₆	0.894	0.894
Cs ₂ CoPtBr ₆	0.910	0.949	Cs ₂ CuIrCl ₆	0.908	0.969	Cs ₂ PdTeI ₆	0.855	0.894
Cs ₂ CoTeBr ₆	0.867	0.949	Cs ₂ CuPtCl ₆	0.922	0.969	Cs ₂ IrPtF ₆	0.969	0.951
Cs ₂ CoNiI ₆	0.929	0.947	Cs ₂ CuTeCl ₆	0.876	0.969	Cs ₂ IrTeF ₆	0.910	0.951
Cs ₂ CoCuI ₆	0.929	0.934	Cs ₂ CuZnBr ₆	0.951	0.954	Cs ₂ IrPtCl ₆	0.922	0.908

Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}
$\text{Cs}_2\text{IrTeCl}_6$	0.876	0.908	$\text{Cs}_2\text{CdZnCl}_6$	0.892	0.965	$\text{Cs}_2\text{CdTeI}_6$	0.855	0.869
$\text{Cs}_2\text{IrPtBr}_6$	0.897	0.910	$\text{Cs}_2\text{CdPdCl}_6$	0.892	0.922			
$\text{Cs}_2\text{IrTeBr}_6$	0.867	0.897	$\text{Cs}_2\text{CdIrCl}_6$	0.892	0.908			
$\text{Cs}_2\text{IrPtI}_6$	0.883	0.894	$\text{Cs}_2\text{CdPtCl}_6$	0.892	0.922			
$\text{Cs}_2\text{IrTeI}_6$	0.883	0.855	$\text{Cs}_2\text{CdTeCl}_6$	0.876	0.892			
$\text{Cs}_2\text{PtTeF}_6$	0.910	0.969	$\text{Cs}_2\text{CdPbBr}_6$	0.815	0.882			
$\text{Cs}_2\text{PtTeCl}_6$	0.876	0.922	$\text{Cs}_2\text{CdSnBr}_6$	0.833	0.882			
$\text{Cs}_2\text{PtTeBr}_6$	0.867	0.910	$\text{Cs}_2\text{CdGeBr}_6$	0.882	0.954			
$\text{Cs}_2\text{PtTeI}_6$	0.855	0.894	$\text{Cs}_2\text{CdBeBr}_6$	0.882	1.065			
$\text{Cs}_2\text{CdPbF}_6$	0.842	0.930	$\text{Cs}_2\text{CdMgBr}_6$	0.882	0.958			
$\text{Cs}_2\text{CdSnF}_6$	0.866	0.930	$\text{Cs}_2\text{CdCaBr}_6$	0.867	0.882			
$\text{Cs}_2\text{CdGeF}_6$	0.930	1.030	$\text{Cs}_2\text{CdSrBr}_6$	0.817	0.882			
$\text{Cs}_2\text{CdBeF}_6$	0.930	1.192	$\text{Cs}_2\text{CdBaBr}_6$	0.775	0.882			
$\text{Cs}_2\text{CdMgF}_6$	0.930	1.035	$\text{Cs}_2\text{CdMnBr}_6$	0.882	0.976			
$\text{Cs}_2\text{CdCaF}_6$	0.910	0.930	$\text{Cs}_2\text{CdFeBr}_6$	0.882	0.937			
$\text{Cs}_2\text{CdSrF}_6$	0.845	0.930	$\text{Cs}_2\text{CdCoBr}_6$	0.882	0.949			
$\text{Cs}_2\text{CdBaF}_6$	0.792	0.930	$\text{Cs}_2\text{CdNiBr}_6$	0.882	0.969			
$\text{Cs}_2\text{CdMnF}_6$	0.930	1.061	$\text{Cs}_2\text{CdCuBr}_6$	0.882	0.954			
$\text{Cs}_2\text{CdFeF}_6$	0.930	1.005	$\text{Cs}_2\text{CdZnBr}_6$	0.882	0.951			
$\text{Cs}_2\text{CdCoF}_6$	0.930	1.022	$\text{Cs}_2\text{CdPdBr}_6$	0.882	0.910			
$\text{Cs}_2\text{CdNiF}_6$	0.930	1.050	$\text{Cs}_2\text{CdIrBr}_6$	0.882	0.897			
$\text{Cs}_2\text{CdCuF}_6$	0.930	1.030	$\text{Cs}_2\text{CdPtBr}_6$	0.882	0.910			
$\text{Cs}_2\text{CdZnF}_6$	0.930	1.025	$\text{Cs}_2\text{CdTeBr}_6$	0.867	0.882			
$\text{Cs}_2\text{CdPdF}_6$	0.930	0.969	$\text{Cs}_2\text{CdPbI}_6$	0.807	0.869			
$\text{Cs}_2\text{CdIrF}_6$	0.930	0.951	$\text{Cs}_2\text{CdSnI}_6$	0.824	0.869			
$\text{Cs}_2\text{CdPtF}_6$	0.930	0.969	$\text{Cs}_2\text{CdGeI}_6$	0.869	0.934			
$\text{Cs}_2\text{CdTeF}_6$	0.910	0.930	$\text{Cs}_2\text{CdBeI}_6$	0.869	1.033			
$\text{Cs}_2\text{CdPbCl}_6$	0.820	0.892	$\text{Cs}_2\text{CdMgI}_6$	0.869	0.937			
$\text{Cs}_2\text{CdSnCl}_6$	0.840	0.892	$\text{Cs}_2\text{CdCaI}_6$	0.855	0.869			
$\text{Cs}_2\text{CdGeCl}_6$	0.892	0.969	$\text{Cs}_2\text{CdSrI}_6$	0.810	0.869			
$\text{Cs}_2\text{CdBeCl}_6$	0.892	1.089	$\text{Cs}_2\text{CdBaI}_6$	0.771	0.869			
$\text{Cs}_2\text{CdMgCl}_6$	0.892	0.973	$\text{Cs}_2\text{CdMnI}_6$	0.869	0.953			
$\text{Cs}_2\text{CdCaCl}_6$	0.876	0.892	$\text{Cs}_2\text{CdFeI}_6$	0.869	0.918			
$\text{Cs}_2\text{CdSrCl}_6$	0.823	0.892	$\text{Cs}_2\text{CdCoI}_6$	0.869	0.929			
$\text{Cs}_2\text{CdBaCl}_6$	0.779	0.892	$\text{Cs}_2\text{CdNiI}_6$	0.869	0.947			
$\text{Cs}_2\text{CdMnCl}_6$	0.892	0.992	$\text{Cs}_2\text{CdCuI}_6$	0.869	0.934			
$\text{Cs}_2\text{CdFeCl}_6$	0.892	0.950	$\text{Cs}_2\text{CdZnI}_6$	0.869	0.931			
$\text{Cs}_2\text{CdCoCl}_6$	0.892	0.963	$\text{Cs}_2\text{CdPdI}_6$	0.869	0.894			
$\text{Cs}_2\text{CdNiCl}_6$	0.892	0.984	$\text{Cs}_2\text{CdIrI}_6$	0.869	0.883			
$\text{Cs}_2\text{CdCuCl}_6$	0.892	0.969	$\text{Cs}_2\text{CdPtI}_6$	0.869	0.894			

Table S5. Double perovskite with minimum tolerance factor in unstable region

Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}	Material	t_{\min}	t_{\max}
Cs ₂ PbSnI ₆	0.807	0.824	Cs ₂ SrPdI ₆	0.810	0.894	Cs ₂ BaPdI ₆	0.771	0.894
Cs ₂ PbGeI ₆	0.807	0.934	Cs ₂ SrIrI ₆	0.810	0.883	Cs ₂ BaIrI ₆	0.771	0.883
Cs ₂ PbBeI ₆	0.807	1.033	Cs ₂ SrPtI ₆	0.810	0.894	Cs ₂ BaPtI ₆	0.771	0.894
Cs ₂ PbMgI ₆	0.807	0.937	Cs ₂ SrTeI ₆	0.810	0.855	Cs ₂ BaTeI ₆	0.771	0.855
Cs ₂ PbCaI ₆	0.807	0.855	Cs ₂ BaMnF ₆	0.792	1.061	Cs ₂ CdBaF ₆	0.792	0.930
Cs ₂ PbSrI ₆	0.807	0.810	Cs ₂ BaFeF ₆	0.792	1.005	Cs ₂ CdBaCl ₆	0.779	0.892
Cs ₂ PbBaI ₆	0.807	0.771	Cs ₂ BaCoF ₆	0.792	1.022	Cs ₂ CdBaBr ₆	0.775	0.882
Cs ₂ PbMnI ₆	0.807	0.953	Cs ₂ BaNiF ₆	0.792	1.050	Cs ₂ CdPbI ₆	0.807	0.869
Cs ₂ PbFeI ₆	0.807	0.918	Cs ₂ BaCuF ₆	0.792	1.030	Cs ₂ CdSrI ₆	0.810	0.869
Cs ₂ PbCoI ₆	0.807	0.929	Cs ₂ BaZnF ₆	0.792	1.025	Cs ₂ CdBaI ₆	0.771	0.869
Cs ₂ PbNiI ₆	0.807	0.947	Cs ₂ BaPdF ₆	0.792	0.969			
Cs ₂ PbCuI ₆	0.807	0.934	Cs ₂ BaIrF ₆	0.792	0.951			
Cs ₂ PbZnI ₆	0.807	0.931	Cs ₂ BaPtF ₆	0.792	0.969			
Cs ₂ PbPdI ₆	0.807	0.894	Cs ₂ BaTeF ₆	0.792	0.910			
Cs ₂ PbIrI ₆	0.807	0.883	Cs ₂ BaMnCl ₆	0.779	0.992			
Cs ₂ PbPtI ₆	0.807	0.894	Cs ₂ BaFeCl ₆	0.779	0.950			
Cs ₂ PbTeI ₆	0.807	0.855	Cs ₂ BaCoCl ₆	0.779	0.963			
Cs ₂ BeBaF ₆	0.792	1.192	Cs ₂ BaNiCl ₆	0.779	0.984			
Cs ₂ BeBaCl ₆	0.779	1.089	Cs ₂ BaCuCl ₆	0.779	0.969			
Cs ₂ BeSrI ₆	0.810	1.033	Cs ₂ BaZnCl ₆	0.779	0.965			
Cs ₂ BeBaI ₆	0.771	1.033	Cs ₂ BaPdCl ₆	0.779	0.922			
Cs ₂ MgBaF ₆	0.792	1.035	Cs ₂ BaIrCl ₆	0.779	0.908			
Cs ₂ MgBaCl ₆	0.779	0.973	Cs ₂ BaPtCl ₆	0.779	0.922			
Cs ₂ MgBaBr ₆	0.775	0.958	Cs ₂ BaTeCl ₆	0.779	0.876			
Cs ₂ MgSrI ₆	0.810	0.937	Cs ₂ BaMnBr ₆	0.775	0.976			
Cs ₂ MgBaI ₆	0.771	0.937	Cs ₂ BaFeBr ₆	0.775	0.937			
Cs ₂ CaBaF ₆	0.792	0.910	Cs ₂ BaCoBr ₆	0.775	0.949			
Cs ₂ CaBaCl ₆	0.779	0.876	Cs ₂ BaNiBr ₆	0.775	0.969			
Cs ₂ CaBaBr ₆	0.775	0.867	Cs ₂ BaCuBr ₆	0.775	0.954			
Cs ₂ CaSrI ₆	0.810	0.855	Cs ₂ BaZnBr ₆	0.775	0.951			
Cs ₂ CaBaI ₆	0.771	0.855	Cs ₂ BaPdBr ₆	0.775	0.910			
Cs ₂ SrBaCl ₆	0.779	0.823	Cs ₂ BaIrBr ₆	0.775	0.897			
Cs ₂ SrBaBr ₆	0.775	0.817	Cs ₂ BaPtBr ₆	0.775	0.910			
Cs ₂ SrBaI ₆	0.771	0.810	Cs ₂ BaTeBr ₆	0.775	0.867			
Cs ₂ SrMnI ₆	0.810	0.953	Cs ₂ BaMnI ₆	0.771	0.953			
Cs ₂ SrFeI ₆	0.810	0.918	Cs ₂ BaFeI ₆	0.771	0.918			
Cs ₂ SrCoI ₆	0.810	0.929	Cs ₂ BaCoI ₆	0.771	0.929			
Cs ₂ SrNiI ₆	0.810	0.947	Cs ₂ BaNiI ₆	0.771	0.947			
Cs ₂ SrCuI ₆	0.810	0.934	Cs ₂ BaCuI ₆	0.771	0.934			
Cs ₂ SrZnI ₆	0.810	0.931	Cs ₂ BaZnI ₆	0.771	0.931			

Table S6. Double perovskite with maximum tolerance factor in unstable region

Material	t_{\min}	t_{\max}
$\text{Cs}_2\text{PbBeF}_6$	0.842	1.192
$\text{Cs}_2\text{SnBeF}_6$	0.866	1.192
$\text{Cs}_2\text{GeBeF}_6$	1.030	1.192
$\text{Cs}_2\text{BeMgF}_6$	1.035	1.192
$\text{Cs}_2\text{BeCaF}_6$	0.910	1.192
$\text{Cs}_2\text{BeSrF}_6$	0.845	1.192
$\text{Cs}_2\text{BeBaF}_6$	0.792	1.192
$\text{Cs}_2\text{BeMnF}_6$	1.061	1.192
$\text{Cs}_2\text{BeFeF}_6$	1.005	1.192
$\text{Cs}_2\text{BeCoF}_6$	1.022	1.192
$\text{Cs}_2\text{BeNiF}_6$	1.050	1.192
$\text{Cs}_2\text{BeCuF}_6$	1.030	1.192
$\text{Cs}_2\text{BeZnF}_6$	1.025	1.192
$\text{Cs}_2\text{BePdF}_6$	0.969	1.192
$\text{Cs}_2\text{BeIrF}_6$	0.951	1.192
$\text{Cs}_2\text{BePtF}_6$	0.969	1.192
$\text{Cs}_2\text{BeTeF}_6$	0.910	1.192
$\text{Cs}_2\text{CdBeF}_6$	0.930	1.192

Table S7. New tolerance factors τ of the 14 predicted all-inorganic double perovskite materials

Material	new tolerance factors τ
$\text{Cs}_2\text{PbSnI}_6$	5.07
$\text{Cs}_2\text{PbGeI}_6$	4.43
$\text{Cs}_2\text{PbGeBr}_6$	4.18
$\text{Cs}_2\text{SnGeCl}_6$	4.04
$\text{Cs}_2\text{PbSnBr}_6$	4.87
$\text{Cs}_2\text{MnPtF}_6$	3.50
$\text{Cs}_2\text{CdTeF}_6$	3.55
$\text{Cs}_2\text{CdBeBr}_6$	4.54
$\text{Cs}_2\text{MgMnI}_6$	4.69
$\text{Cs}_2\text{PbSnCl}_6$	4.75
$\text{Cs}_2\text{FeTeF}_6$	3.48
$\text{Cs}_2\text{PbGeCl}_6$	4.03
$\text{Cs}_2\text{ZnTeF}_6$	3.47
$\text{Cs}_2\text{CaZnI}_6$	4.47

Table S8. The band gaps for PBE functional

Material	Gap	Material	Gap	Material	Gap	Material	Gap
Cs ₂ BaCuF ₆	0.00	Cs ₂ CaIrF ₆	0.00	Cs ₂ MgPtBr ₆	0.00	Cs ₂ FePtCl ₆	0.00
Cs ₂ BaIrF ₆	0.00	Cs ₂ SrTeI ₆	0.00	Cs ₂ IrPtCl ₆	0.00	Cs ₂ NiIrCl ₆	0.00
Cs ₂ FePdBr ₆	0.00	Cs ₂ BaFeI ₆	0.00	Cs ₂ PbCuF ₆	0.00	Cs ₂ SrCuF ₆	0.00
Cs ₂ NiCuBr ₆	0.00	Cs ₂ CdCoF ₆	0.00	Cs ₂ BeCuI ₆	0.00	Cs ₂ BaTeF ₆	0.00
Cs ₂ IrTeCl ₆	0.00	Cs ₂ PbCoCl ₆	0.00	Cs ₂ BaCoI ₆	0.00	Cs ₂ CoPtI ₆	0.00
Cs ₂ SnFeF ₆	0.00	Cs ₂ CoPtF ₆	0.00	Cs ₂ FeCuI ₆	0.00	Cs ₂ CaCoCl ₆	0.00
Cs ₂ SrFeI ₆	0.00	Cs ₂ NiTeI ₆	0.00	Cs ₂ SnFeCl ₆	0.00	Cs ₂ CaCuCl ₆	0.00
Cs ₂ BaPtI ₆	0.00	Cs ₂ IrPtI ₆	0.00	Cs ₂ CaFeBr ₆	0.00	Cs ₂ BaCoBr ₆	0.00
Cs ₂ CoNiF ₆	0.00	Cs ₂ FeCuBr ₆	0.00	Cs ₂ SrCoF ₆	0.00	Cs ₂ BaCuBr ₆	0.00
Cs ₂ CaIrBr ₆	0.00	Cs ₂ FeTeBr ₆	0.00	Cs ₂ CuPdF ₆	0.00	Cs ₂ CoZnCl ₆	0.00
Cs ₂ MnFeCl ₆	0.00	Cs ₂ CoPdCl ₆	0.00	Cs ₂ MgFeCl ₆	0.00	Cs ₂ NiCuCl ₆	0.00
Cs ₂ MnIrBr ₆	0.00	Cs ₂ MgFeI ₆	0.00	Cs ₂ BaFeBr ₆	0.00	Cs ₂ CuTeCl ₆	0.00
Cs ₂ PbFeF ₆	0.00	Cs ₂ MgNiI ₆	0.00	Cs ₂ MnCoCl ₆	0.00	Cs ₂ CdCuCl ₆	0.00
Cs ₂ MnFeI ₆	0.00	Cs ₂ MnCoI ₆	0.00	Cs ₂ MnNiBr ₆	0.00	Cs ₂ MgCuI ₆	0.00
Cs ₂ CoCuF ₆	0.00	Cs ₂ BeNiBr ₆	0.00	Cs ₂ FeNiBr ₆	0.00	Cs ₂ CoZnI ₆	0.00
Cs ₂ CoPdF ₆	0.00	Cs ₂ SrFeBr ₆	0.00	Cs ₂ CaCoI ₆	0.00	Cs ₂ CoZnF ₆	0.00
Cs ₂ CoTeF ₆	0.00	Cs ₂ BaCoCl ₆	0.00	Cs ₂ FeTeI ₆	0.00	Cs ₂ BeCoBr ₆	0.00
Cs ₂ NiIrI ₆	0.00	Cs ₂ CoZnBr ₆	0.00	Cs ₂ CoCuI ₆	0.00	Cs ₂ MgCuCl ₆	0.00
Cs ₂ CdFeF ₆	0.00	Cs ₂ CdFeBr ₆	0.00	Cs ₂ MgFeBr ₆	0.00	Cs ₂ CaCoBr ₆	0.00
Cs ₂ PbFeBr ₆	0.00	Cs ₂ GeCoF ₆	0.00	Cs ₂ MgPdBr ₆	0.00	Cs ₂ NiIrBr ₆	0.00
Cs ₂ BeFeBr ₆	0.00	Cs ₂ BeFeF ₆	0.00	Cs ₂ SrFeCl ₆	0.00	Cs ₂ ZnPtCl ₆	0.00
Cs ₂ FeZnBr ₆	0.00	Cs ₂ BeCoI ₆	0.00	Cs ₂ SrIrCl ₆	0.00	Cs ₂ GeCoI ₆	0.00
Cs ₂ NiTeCl ₆	0.00	Cs ₂ CaFeF ₆	0.00	Cs ₂ FeCoBr ₆	0.00	Cs ₂ PbFeCl ₆	0.00
Cs ₂ PbCoF ₆	0.00	Cs ₂ PbCoBr ₆	0.00	Cs ₂ FeNiCl ₆	0.00	Cs ₂ BaTeBr ₆	0.00
Cs ₂ GeFeF ₆	0.00	Cs ₂ PbTeCl ₆	0.00	Cs ₂ FeCuCl ₆	0.00	Cs ₂ CoIrBr ₆	0.00
Cs ₂ FeNiI ₆	0.00	Cs ₂ SnFeBr ₆	0.00	Cs ₂ MgCuF ₆	0.00	Cs ₂ GeFeI ₆	0.00
Cs ₂ BaFeCl ₆	0.00	Cs ₂ IrPtBr ₆	0.00	Cs ₂ MnCoF ₆	0.00	Cs ₂ GeCoBr ₆	0.00
Cs ₂ CdFeCl ₆	0.00	Cs ₂ SnCoF ₆	0.00	Cs ₂ GeFeBr ₆	0.00	Cs ₂ GeCoCl ₆	0.00
Cs ₂ CdCoCl ₆	0.00	Cs ₂ FePdCl ₆	0.00	Cs ₂ MnFeBr ₆	0.00	Cs ₂ BeIrCl ₆	0.00
Cs ₂ CaCoF ₆	0.00	Cs ₂ CoNiBr ₆	0.00	Cs ₂ SnCoI ₆	0.00	Cs ₂ CoCuBr ₆	0.00
Cs ₂ BaCoF ₆	0.00	Cs ₂ PbFeI ₆	0.00	Cs ₂ CaCuI ₆	0.00	Cs ₂ CoTeBr ₆	0.00
Cs ₂ FeZnF ₆	0.00	Cs ₂ CaTeI ₆	0.00	Cs ₂ BaFeF ₆	0.00	Cs ₂ ZnPdCl ₆	0.00
Cs ₂ CoIrI ₆	0.00	Cs ₂ BaCuI ₆	0.00	Cs ₂ FePtF ₆	0.00	Cs ₂ MgCoF ₆	0.00
Cs ₂ CdCoI ₆	0.00	Cs ₂ SnCoBr ₆	0.00	Cs ₂ GeFeCl ₆	0.00	Cs ₂ CaFeCl ₆	0.00
Cs ₂ BeFeCl ₆	0.00	Cs ₂ PdIrBr ₆	0.00	Cs ₂ CaIrCl ₆	0.00	Cs ₂ SrTeCl ₆	0.00
Cs ₂ CoPtCl ₆	0.00	Cs ₂ GePdF ₆	0.00	Cs ₂ BeFeI ₆	0.00	Cs ₂ FeTeCl ₆	0.00
Cs ₂ PbCoI ₆	0.00	Cs ₂ BeCoF ₆	0.00	Cs ₂ MnTeI ₆	0.00	Cs ₂ CoPtBr ₆	0.00
Cs ₂ SnFeI ₆	0.00	Cs ₂ PdIrF ₆	0.00	Cs ₂ IrPtF ₆	0.00	Cs ₂ SnTeF ₆	0.00
Cs ₂ MgFeF ₆	0.00	Cs ₂ SnCoCl ₆	0.00	Cs ₂ CdPtI ₆	0.00	Cs ₂ CaCuF ₆	0.00
Cs ₂ CaFeI ₆	0.00	Cs ₂ GePdCl ₆	0.00	Cs ₂ FeZnCl ₆	0.00	Cs ₂ FeIrF ₆	0.00

Material	Gap	Material	Gap	Material	Gap	Material	Gap
Cs ₂ CoNiCl ₆	0.00	Cs ₂ SrTeF ₆	0.00	Cs ₂ FePdF ₆	0.00	Cs ₂ BePdBr ₆	0.01
Cs ₂ PbTeF ₆	0.00	Cs ₂ CdCuF ₆	0.00	Cs ₂ PdPtF ₆	0.00	Cs ₂ NiTeF ₆	0.01
Cs ₂ SnNiI ₆	0.00	Cs ₂ MgPdCl ₆	0.00	Cs ₂ CdPtCl ₆	0.00	Cs ₂ BeZnI ₆	0.01
Cs ₂ SnTeI ₆	0.00	Cs ₂ SrCoBr ₆	0.00	Cs ₂ SnPtCl ₆	0.00	Cs ₂ ZnPdI ₆	0.01
Cs ₂ SrPdI ₆	0.00	Cs ₂ CaPtI ₆	0.00	Cs ₂ MgPtI ₆	0.00	Cs ₂ ZnPtI ₆	0.01
Cs ₂ PbPdBr ₆	0.00	Cs ₂ FeIrI ₆	0.00	Cs ₂ GeIrBr ₆	0.00	Cs ₂ CdPdCl ₆	0.01
Cs ₂ CoPdI ₆	0.00	Cs ₂ PbPdCl ₆	0.00	Cs ₂ CuPtCl ₆	0.00	Cs ₂ SnPtBr ₆	0.01
Cs ₂ SrCoCl ₆	0.00	Cs ₂ CoCuCl ₆	0.00	Cs ₂ MnCuF ₆	0.01	Cs ₂ CdNiI ₆	0.01
Cs ₂ CdIrCl ₆	0.00	Cs ₂ BaCuCl ₆	0.00	Cs ₂ NiZnCl ₆	0.01	Cs ₂ CdPbCl ₆	0.01
Cs ₂ BeNiI ₆	0.00	Cs ₂ MgIrF ₆	0.00	Cs ₂ PbNiI ₆	0.01	Cs ₂ MnNiI ₆	0.01
Cs ₂ CaTeF ₆	0.00	Cs ₂ SnPdCl ₆	0.00	Cs ₂ BeCuCl ₆	0.01	Cs ₂ CdIrBr ₆	0.01
Cs ₂ SrCoI ₆	0.00	Cs ₂ NiTeBr ₆	0.00	Cs ₂ CaTeCl ₆	0.01	Cs ₂ BePtI ₆	0.01
Cs ₂ SnPdBr ₆	0.00	Cs ₂ CdCoBr ₆	0.00	Cs ₂ SnIrCl ₆	0.01	Cs ₂ CdPtBr ₆	0.01
Cs ₂ BeCuBr ₆	0.00	Cs ₂ SrIrF ₆	0.00	Cs ₂ GeNiCl ₆	0.01	Cs ₂ FeIrBr ₆	0.01
Cs ₂ CuZnCl ₆	0.00	Cs ₂ CdPdI ₆	0.00	Cs ₂ BaIrBr ₆	0.01	Cs ₂ MgTeBr ₆	0.01
Cs ₂ CuPdBr ₆	0.00	Cs ₂ GeNiBr ₆	0.00	Cs ₂ PdTeBr ₆	0.01	Cs ₂ CuTeBr ₆	0.01
Cs ₂ CdNiBr ₆	0.00	Cs ₂ MgCuBr ₆	0.00	Cs ₂ CdTeCl ₆	0.01	Cs ₂ BePtBr ₆	0.01
Cs ₂ CdCuBr ₆	0.00	Cs ₂ BaTeCl ₆	0.00	Cs ₂ ZnPdBr ₆	0.01	Cs ₂ SnPtF ₆	0.01
Cs ₂ MgTeF ₆	0.00	Cs ₂ PdIrCl ₆	0.00	Cs ₂ CuZnF ₆	0.01	Cs ₂ CoTeI ₆	0.01
Cs ₂ MnPdI ₆	0.00	Cs ₂ CuTeI ₆	0.00	Cs ₂ GeTeF ₆	0.01	Cs ₂ BeTeCl ₆	0.01
Cs ₂ SnTeCl ₆	0.00	Cs ₂ GePtCl ₆	0.00	Cs ₂ GeTeCl ₆	0.01	Cs ₂ MgTeI ₆	0.01
Cs ₂ MgCoBr ₆	0.00	Cs ₂ PbTeI ₆	0.00	Cs ₂ MnIrF ₆	0.01	Cs ₂ MgPdI ₆	0.01
Cs ₂ SrCuCl ₆	0.00	Cs ₂ CaPdI ₆	0.00	Cs ₂ PbTeBr ₆	0.01	Cs ₂ CuPtF ₆	0.01
Cs ₂ MnTeBr ₆	0.00	Cs ₂ PbNiBr ₆	0.00	Cs ₂ MnCuCl ₆	0.01	Cs ₂ FePtBr ₆	0.01
Cs ₂ FeCoCl ₆	0.00	Cs ₂ NiZnI ₆	0.00	Cs ₂ BaTeI ₆	0.01	Cs ₂ GeTeI ₆	0.01
Cs ₂ GePtI ₆	0.00	Cs ₂ MgPtCl ₆	0.00	Cs ₂ CoNiI ₆	0.01	Cs ₂ NiZnBr ₆	0.01
Cs ₂ BeIrF ₆	0.00	Cs ₂ CaTeBr ₆	0.00	Cs ₂ NiIrF ₆	0.01	Cs ₂ MnZnI ₆	0.01
Cs ₂ CdCuI ₆	0.00	Cs ₂ NiCuI ₆	0.00	Cs ₂ SnNiBr ₆	0.01	Cs ₂ SnTeBr ₆	0.01
Cs ₂ GeTeBr ₆	0.00	Cs ₂ BeTeBr ₆	0.00	Cs ₂ NiPdCl ₆	0.01	Cs ₂ CuPdCl ₆	0.01
Cs ₂ CoTeCl ₆	0.00	Cs ₂ FePdI ₆	0.00	Cs ₂ CuZnI ₆	0.01	Cs ₂ BeTeI ₆	0.01
Cs ₂ CuZnBr ₆	0.00	Cs ₂ CuPdI ₆	0.00	Cs ₂ NiPtBr ₆	0.01	Cs ₂ CdTeI ₆	0.01
Cs ₂ CdTeBr ₆	0.00	Cs ₂ SrTeBr ₆	0.00	Cs ₂ PbPtI ₆	0.01	Cs ₂ ZnIrBr ₆	0.01
Cs ₂ BeCuF ₆	0.00	Cs ₂ PbIrCl ₆	0.00	Cs ₂ SrPtI ₆	0.01	Cs ₂ CdIrF ₆	0.01
Cs ₂ MgCoI ₆	0.00	Cs ₂ SrCuBr ₆	0.00	Cs ₂ SrCuI ₆	0.01	Cs ₂ PbIrI ₆	0.01
Cs ₂ BaPdI ₆	0.00	Cs ₂ MnIrCl ₆	0.00	Cs ₂ BePdCl ₆	0.01	Cs ₂ BePtCl ₆	0.01
Cs ₂ CaCuBr ₆	0.00	Cs ₂ NiPdBr ₆	0.00	Cs ₂ SnPdF ₆	0.01	Cs ₂ BaIrI ₆	0.01
Cs ₂ CoPdBr ₆	0.00	Cs ₂ BeTeF ₆	0.00	Cs ₂ BaIrCl ₆	0.01	Cs ₂ MnIrI ₆	0.01
Cs ₂ NiPtCl ₆	0.00	Cs ₂ SrIrBr ₆	0.00	Cs ₂ CdPdBr ₆	0.01	Cs ₂ PtTeCl ₆	0.01
Cs ₂ BeCoCl ₆	0.00	Cs ₂ MnTeCl ₆	0.00	Cs ₂ CuTeF ₆	0.01	Cs ₂ ZnTeBr ₆	0.01
Cs ₂ MgCoCl ₆	0.00	Cs ₂ FeIrCl ₆	0.00	Cs ₂ FeNiF ₆	0.01	Cs ₂ PbPtCl ₆	0.01

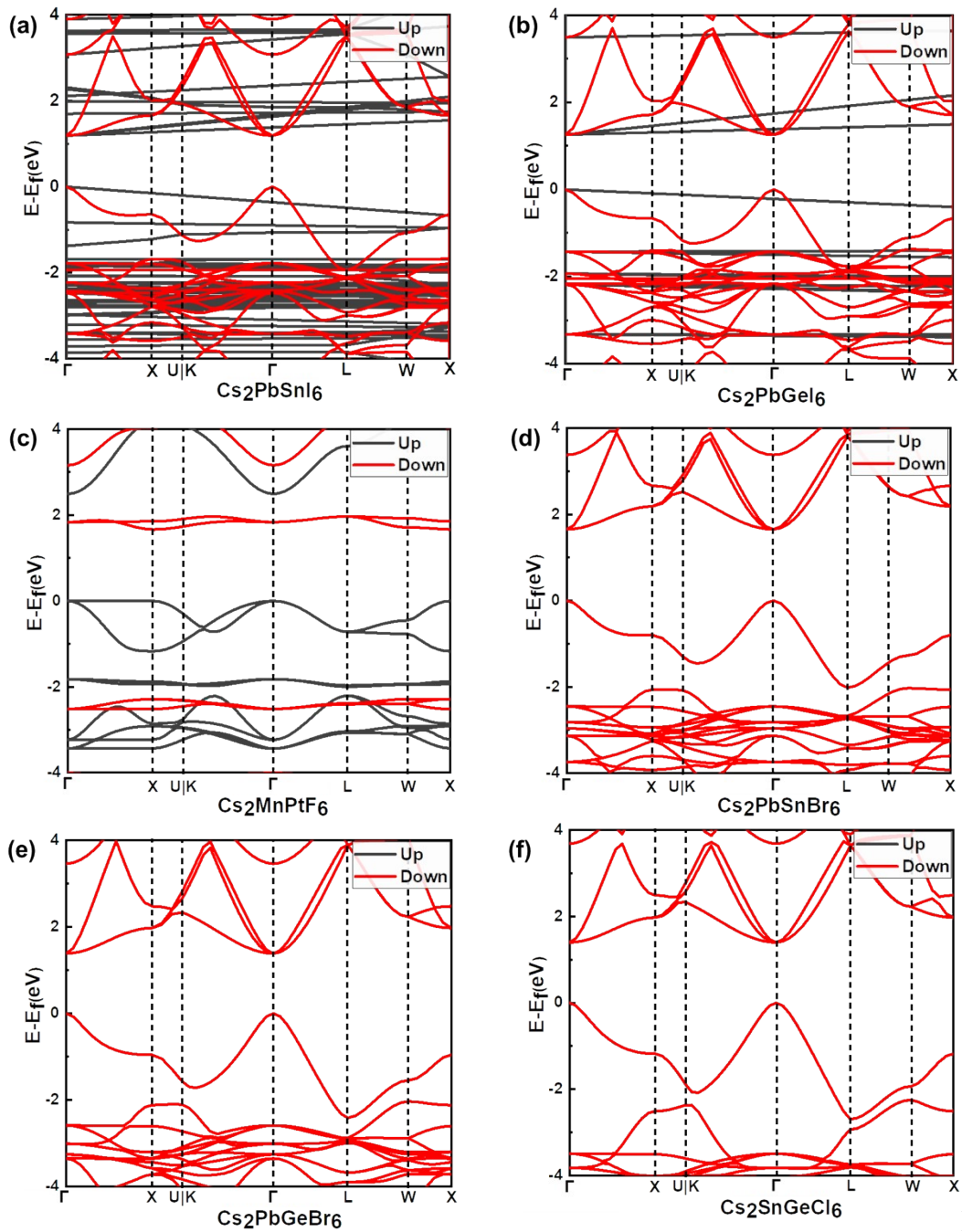
Material	Gap	Material	Gap	Material	Gap	Material	Gap
Cs ₂ MgTeCl ₆	0.01	Cs ₂ CdIrI ₆	0.02	Cs ₂ IrTeF ₆	0.12	Cs ₂ GeZnI ₆	0.52
Cs ₂ ZnPtBr ₆	0.01	Cs ₂ PdPtBr ₆	0.02	Cs ₂ SrPdBr ₆	0.13	Cs ₂ CdMnBr ₆	0.52
Cs ₂ SnPtI ₆	0.01	Cs ₂ GeNiI ₆	0.02	Cs ₂ FeCuF ₆	0.13	Cs ₂ BaPtCl ₆	0.53
Cs ₂ CuPtI ₆	0.01	Cs ₂ ZnTeCl ₆	0.02	Cs ₂ MnPdF ₆	0.15	Cs ₂ CdSnI ₆	0.54
Cs ₂ IrTeBr ₆	0.01	Cs ₂ NiPtI ₆	0.02	Cs ₂ CaPtBr ₆	0.15	Cs ₂ MnNiCl ₆	0.59
Cs ₂ PtTeBr ₆	0.01	Cs ₂ PdTeCl ₆	0.02	Cs ₂ PbNiCl ₆	0.17	Cs ₂ CdGeI ₆	0.60
Cs ₂ ZnTeI ₆	0.01	Cs ₂ SnIrI ₆	0.02	Cs ₂ BaPdBr ₆	0.18	Cs ₂ SnMnI ₆	0.61
Cs ₂ MnCuBr ₆	0.01	Cs ₂ GePtBr ₆	0.03	Cs ₂ SrPtBr ₆	0.18	Cs ₂ MgNiCl ₆	0.61
Cs ₂ MnPtCl ₆	0.01	Cs ₂ SnCuF ₆	0.03	Cs ₂ BeMnI ₆	0.23	Cs ₂ SnNiF ₆	0.65
Cs ₂ MnTeF ₆	0.01	Cs ₂ CaIrI ₆	0.03	Cs ₂ BaPtBr ₆	0.24	Cs ₂ BePdF ₆	0.66
Cs ₂ PbIrF ₆	0.01	Cs ₂ FeZnI ₆	0.03	Cs ₂ MgNiBr ₆	0.25	Cs ₂ CaNiBr ₆	0.66
Cs ₂ MnPdBr ₆	0.01	Cs ₂ GeIrCl ₆	0.03	Cs ₂ CaNiI ₆	0.25	Cs ₂ GeMnI ₆	0.69
Cs ₂ SnNiCl ₆	0.01	Cs ₂ PdPtI ₆	0.03	Cs ₂ PdTeF ₆	0.26	Cs ₂ SrNiBr ₆	0.71
Cs ₂ CuIrBr ₆	0.01	Cs ₂ PbCuCl ₆	0.03	Cs ₂ MnNiF ₆	0.28	Cs ₂ MnPtF ₆	0.72
Cs ₂ NiCuF ₆	0.01	Cs ₂ CdFeI ₆	0.03	Cs ₂ SrNiI ₆	0.30	Cs ₂ BaNiBr ₆	0.72
Cs ₂ MnPtI ₆	0.01	Cs ₂ MgIrBr ₆	0.03	Cs ₂ BeNiCl ₆	0.30	Cs ₂ PbSnI ₆	0.77
Cs ₂ PbCuI ₆	0.01	Cs ₂ SrIrI ₆	0.03	Cs ₂ PtTeF ₆	0.31	Cs ₂ GeNiF ₆	0.79
Cs ₂ SnIrF ₆	0.01	Cs ₂ CdNiCl ₆	0.03	Cs ₂ SnGeBr ₆	0.32	Cs ₂ CdBeBr ₆	0.79
Cs ₂ MnPtBr ₆	0.01	Cs ₂ SnCuBr ₆	0.03	Cs ₂ SnBaBr ₆	0.32	Cs ₂ FeTeF ₆	0.82
Cs ₂ CdMnI ₆	0.02	Cs ₂ SnIrBr ₆	0.03	Cs ₂ SnGeI ₆	0.36	Cs ₂ NiPtF ₆	0.83
Cs ₂ CuPtBr ₆	0.02	Cs ₂ GeCuBr ₆	0.04	Cs ₂ SrPdCl ₆	0.36	Cs ₂ PbGeI ₆	0.84
Cs ₂ PdTeI ₆	0.02	Cs ₂ MgIrI ₆	0.04	Cs ₂ CdPdF ₆	0.37	Cs ₂ PbGeBr ₆	0.86
Cs ₂ BeIrI ₆	0.02	Cs ₂ BeIrBr ₆	0.04	Cs ₂ BaNiI ₆	0.38	Cs ₂ SnGeCl ₆	0.86
Cs ₂ FePtI ₆	0.02	Cs ₂ FeCoF ₆	0.04	Cs ₂ CdMgI ₆	0.38	Cs ₂ BePtF ₆	0.87
Cs ₂ GeIrI ₆	0.02	Cs ₂ PbIrBr ₆	0.04	Cs ₂ CdPtF ₆	0.39	Cs ₂ GeBeI ₆	0.88
Cs ₂ MnCoBr ₆	0.02	Cs ₂ MgIrCl ₆	0.04	Cs ₂ SnZnI ₆	0.40	Cs ₂ BeNiF ₆	0.92
Cs ₂ GePdBr ₆	0.02	Cs ₂ ZnIrF ₆	0.05	Cs ₂ CdCaCl ₆	0.40	Cs ₂ MgPdF ₆	0.95
Cs ₂ GeIrF ₆	0.02	Cs ₂ GeCuI ₆	0.05	Cs ₂ CaPdCl ₆	0.40	Cs ₂ SnBeI ₆	0.95
Cs ₂ MnCuI ₆	0.02	Cs ₂ PdIrI ₆	0.05	Cs ₂ MnZnBr ₆	0.40	Cs ₂ PbZnI ₆	0.96
Cs ₂ ZnIrI ₆	0.02	Cs ₂ PbCuBr ₆	0.06	Cs ₂ CuIrCl ₆	0.43	Cs ₂ CdNiF ₆	0.97
Cs ₂ PbPtBr ₆	0.02	Cs ₂ SnCuI ₆	0.06	Cs ₂ NiPdF ₆	0.43	Cs ₂ NiZnF ₆	1.01
Cs ₂ GePdI ₆	0.02	Cs ₂ MgZnI ₆	0.06	Cs ₂ BaPdCl ₆	0.46	Cs ₂ MgMnI ₆	1.01
Cs ₂ GeCuF ₆	0.02	Cs ₂ ZnIrCl ₆	0.07	Cs ₂ PbPtF ₆	0.47	Cs ₂ CaNiCl ₆	1.02
Cs ₂ IrTeI ₆	0.02	Cs ₂ MnPdCl ₆	0.08	Cs ₂ CaPtCl ₆	0.48	Cs ₂ SrNiCl ₆	1.04
Cs ₂ PtTeI ₆	0.02	Cs ₂ CdBeI ₆	0.08	Cs ₂ BeMgI ₆	0.48	Cs ₂ CuIrF ₆	1.05
Cs ₂ PdPtCl ₆	0.02	Cs ₂ GePtF ₆	0.08	Cs ₂ BeZnBr ₆	0.49	Cs ₂ BaNiCl ₆	1.06
Cs ₂ NiPdI ₆	0.02	Cs ₂ SnCuCl ₆	0.08	Cs ₂ ZnPdF ₆	0.49	Cs ₂ BaPdF ₆	1.07
Cs ₂ CuIrI ₆	0.02	Cs ₂ CaPdBr ₆	0.08	Cs ₂ ZnPtF ₆	0.49	Cs ₂ SnZnBr ₆	1.09
Cs ₂ SnPdI ₆	0.02	Cs ₂ GeCuCl ₆	0.08	Cs ₂ CdZnBr ₆	0.49	Cs ₂ PbSnBr ₆	1.09
Cs ₂ BePdI ₆	0.02	Cs ₂ CdZnI ₆	0.10	Cs ₂ SrPtCl ₆	0.50	Cs ₂ PbMnI ₆	1.11

Material	Gap	Material	Gap	Material	Gap	Material	Gap
Cs ₂ PbNiF ₆	1.12	Cs ₂ SnBeBr ₆	1.73	Cs ₂ CaMnCl ₆	2.52	Cs ₂ SnZnF ₆	3.36
Cs ₂ MgPtF ₆	1.12	Cs ₂ GeBeBr ₆	1.75	Cs ₂ SnBeCl ₆	2.53	Cs ₂ CdZnF ₆	3.36
Cs ₂ GeZnBr ₆	1.13	Cs ₂ CdSnCl ₆	1.77	Cs ₂ GeBeCl ₆	2.55	Cs ₂ SnBaCl ₆	3.46
Cs ₂ CdSnBr ₆	1.14	Cs ₂ PbMnCl ₆	1.79	Cs ₂ GeCaI ₆	2.55	Cs ₂ BeSrBr ₆	3.49
Cs ₂ CdPbI ₆	1.14	Cs ₂ CdGeCl ₆	1.79	Cs ₂ SnSrI ₆	2.57	Cs ₂ GeZnF ₆	3.55
Cs ₂ SrPdF ₆	1.15	Cs ₂ SnZnCl ₆	1.80	Cs ₂ SnBaI ₆	2.58	Cs ₂ SnSrCl ₆	3.56
Cs ₂ CaPdF ₆	1.16	Cs ₂ SnGeF ₆	1.80	Cs ₂ SnCaI ₆	2.58	Cs ₂ SrBaI ₆	3.61
Cs ₂ CdGeBr ₆	1.19	Cs ₂ CdPbBr ₆	1.80	Cs ₂ CaZnBr ₆	2.59	Cs ₂ SnCaCl ₆	3.61
Cs ₂ CdMnCl ₆	1.19	Cs ₂ GeZnCl ₆	1.82	Cs ₂ MgZnCl ₆	2.62	Cs ₂ CdPbF ₆	3.65
Cs ₂ SnMnBr ₆	1.19	Cs ₂ CaMnI ₆	1.83	Cs ₂ BeBaI ₆	2.63	Cs ₂ PbBaBr ₆	3.65
Cs ₂ GeMnBr ₆	1.21	Cs ₂ MnFeF ₆	1.83	Cs ₂ GeSrI ₆	2.69	Cs ₂ CaBaI ₆	3.67
Cs ₂ MgNiF ₆	1.21	Cs ₂ BeMgBr ₆	1.83	Cs ₂ GeBaI ₆	2.74	Cs ₂ GeBaCl ₆	3.69
Cs ₂ MnZnCl ₆	1.22	Cs ₂ BaMnI ₆	1.83	Cs ₂ CdSnF ₆	2.75	Cs ₂ PbSrBr ₆	3.71
Cs ₂ BeMnBr ₆	1.24	Cs ₂ SrMnI ₆	1.85	Cs ₂ MgCaI ₆	2.76	Cs ₂ PbCaBr ₆	3.71
Cs ₂ BaPtF ₆	1.25	Cs ₂ CdSrI ₆	1.88	Cs ₂ CdMgCl ₆	2.78	Cs ₂ GeSrCl ₆	3.74
Cs ₂ SrPtF ₆	1.32	Cs ₂ BeCaI ₆	1.91	Cs ₂ CdCaBr ₆	2.79	Cs ₂ PbMgCl ₆	3.76
Cs ₂ CdTeF ₆	1.33	Cs ₂ CdBeCl ₆	1.96	Cs ₂ SrZnBr ₆	2.84	Cs ₂ GeCaCl ₆	3.77
Cs ₂ SnMnCl ₆	1.33	Cs ₂ PbMgI ₆	1.99	Cs ₂ SrMnF ₆	2.89	Cs ₂ CaSrI ₆	3.77
Cs ₂ CaPtF ₆	1.33	Cs ₂ BaZnI ₆	2.01	Cs ₂ PbCaI ₆	2.95	Cs ₂ BeBaBr ₆	3.83
Cs ₂ SrFeF ₆	1.35	Cs ₂ MgMnBr ₆	2.02	Cs ₂ PbMgBr ₆	2.96	Cs ₂ CdSrCl ₆	3.97
Cs ₂ PbBeI ₆	1.37	Cs ₂ PbSnF ₆	2.14	Cs ₂ CdGeF ₆	2.97	Cs ₂ BeZnF ₆	3.98
Cs ₂ CaZnI ₆	1.37	Cs ₂ BeSrI ₆	2.18	Cs ₂ CdSrBr ₆	3.00	Cs ₂ CaZnCl ₆	4.00
Cs ₂ CaNiF ₆	1.39	Cs ₂ BaMnBr ₆	2.20	Cs ₂ MgSrI ₆	3.02	Cs ₂ MgCaBr ₆	4.00
Cs ₂ CdMnF ₆	1.41	Cs ₂ BeMnCl ₆	2.23	Cs ₂ CaMnF ₆	3.02	Cs ₂ SnSrF ₆	4.01
Cs ₂ PbSnCl ₆	1.41	Cs ₂ SnMnF ₆	2.23	Cs ₂ SnMgCl ₆	3.03	Cs ₂ MgSrBr ₆	4.06
Cs ₂ MgZnBr ₆	1.42	Cs ₂ MnZnF ₆	2.24	Cs ₂ SnSrBr ₆	3.06	Cs ₂ PbZnF ₆	4.11
Cs ₂ GeMnCl ₆	1.46	Cs ₂ SnMgBr ₆	2.30	Cs ₂ SnCaBr ₆	3.08	Cs ₂ MgBaBr ₆	4.12
Cs ₂ CdMgBr ₆	1.46	Cs ₂ SrMnCl ₆	2.30	Cs ₂ GeMgCl ₆	3.09	Cs ₂ CdBeF ₆	4.13
Cs ₂ SrNiF ₆	1.46	Cs ₂ BaMnCl ₆	2.30	Cs ₂ PbSrI ₆	3.14	Cs ₂ GeBaF ₆	4.17
Cs ₂ GeMgI ₆	1.51	Cs ₂ CaMnBr ₆	2.31	Cs ₂ BeMnF ₆	3.17	Cs ₂ CaBaBr ₆	4.20
Cs ₂ BaNiF ₆	1.52	Cs ₂ PbGeF ₆	2.31	Cs ₂ PbBaI ₆	3.17	Cs ₂ SrBaBr ₆	4.20
Cs ₂ PbMnBr ₆	1.56	Cs ₂ SrMnBr ₆	2.33	Cs ₂ MgMnF ₆	3.19	Cs ₂ PbBaCl ₆	4.20
Cs ₂ SnMgI ₆	1.57	Cs ₂ GeMgBr ₆	2.35	Cs ₂ GeBaBr ₆	3.20	Cs ₂ CdBaCl ₆	4.23
Cs ₂ PbGeCl ₆	1.60	Cs ₂ PbMnF ₆	2.35	Cs ₂ GeCaBr ₆	3.21	Cs ₂ SnBeF ₆	4.25
Cs ₂ SrZnI ₆	1.64	Cs ₂ GeMnF ₆	2.37	Cs ₂ BaZnBr ₆	3.22	Cs ₂ SnCaF ₆	4.25
Cs ₂ CdZnCl ₆	1.65	Cs ₂ PbBeBr ₆	2.37	Cs ₂ PbBeCl ₆	3.22	Cs ₂ PbSrCl ₆	4.28
Cs ₂ ZnTeF ₆	1.68	Cs ₂ CdBaI ₆	2.42	Cs ₂ BeMgCl ₆	3.23	Cs ₂ CaSrBr ₆	4.28
Cs ₂ CdCaI ₆	1.68	Cs ₂ BaMnF ₆	2.43	Cs ₂ BeCaBr ₆	3.30	Cs ₂ PbCaCl ₆	4.32
Cs ₂ BeZnCl ₆	1.70	Cs ₂ MgMnCl ₆	2.45	Cs ₂ CdBaBr ₆	3.31	Cs ₂ SrZnCl ₆	4.38
Cs ₂ PbZnBr ₆	1.71	Cs ₂ PbZnCl ₆	2.46	Cs ₂ MgBaI ₆	3.33	Cs ₂ BaZnCl ₆	4.38

Material	Gap	Material	Gap	Material	Gap
Cs ₂ SnMgF ₆	4.44	CsSnCl ₃	0.80	CsNiCl ₃	0.01
Cs ₂ GeSrF ₆	4.53	CsSnBr ₃	0.56	CsNiBr ₃	0.01
Cs ₂ GeBeF ₆	4.55	CsSnI ₃	0.28	CsNiI ₃	0.07
Cs ₂ CdMgF ₆	4.68	CsGeF ₃	1.89	CsCuF ₃	0.01
Cs ₂ GeCaF ₆	4.76	CsGeCl ₃	0.91	CsCuCl ₃	0.03
Cs ₂ SrBaCl ₆	4.79	CsGeBr ₃	0.60	CsCuBr ₃	0.04
Cs ₂ CdBaF ₆	4.79	CsGeI ₃	0.44	CsCuI ₃	0.04
Cs ₂ PbSrF ₆	4.82	CsBeF ₃	5.43	CsZnF ₃	3.60
Cs ₂ GeMgF ₆	4.86	CsBeCl ₃	2.33	CsZnCl ₃	1.17
Cs ₂ BeCaCl ₆	4.86	CsBeBr ₃	0.88	CsZnBr ₃	0.18
Cs ₂ BeSrCl ₆	4.97	CsBeI ₃	0.06	CsZnI ₃	0.09
Cs ₂ MgBaCl ₆	4.97	CsMgF ₃	6.80	CsPdF ₃	0.04
Cs ₂ PbBeF ₆	5.01	CsMgCl ₃	3.87	CsPdCl ₃	0.01
Cs ₂ CaBaCl ₆	5.04	CsMgBr ₃	2.69	CsPdBr ₃	0.00
Cs ₂ CdSrF ₆	5.07	CsMgI ₃	1.19	CsPdI ₃	0.03
Cs ₂ BeBaCl ₆	5.07	CsCaF ₃	7.20	CsIrF ₃	0.01
Cs ₂ PbCaF ₆	5.08	CsCaCl ₃	5.43	CsIrCl ₃	0.01
Cs ₂ MgSrCl ₆	5.16	CsCaBr ₃	4.60	CsIrBr ₃	0.00
Cs ₂ BaZnF ₆	5.16	CsCaI ₃	3.70	CsIrI ₃	0.00
Cs ₂ CaSrCl ₆	5.22	CsSrF ₃	6.34	CsPtF ₃	0.01
Cs ₂ CdCaF ₆	5.29	CsSrCl ₃	5.16	CsPtCl ₃	0.03
Cs ₂ PbMgF ₆	5.30	CsSrBr ₃	4.27	CsPtBr ₃	0.01
Cs ₂ MgCaCl ₆	5.33	CsSrI ₃	3.64	CsPtI ₃	0.14
Cs ₂ MgZnF ₆	5.39	CsBaF ₃	5.20	CsTeF ₃	0.00
Cs ₂ SrZnF ₆	5.49	CsBaCl ₃	4.74	CsTeCl ₃	0.03
Cs ₂ CaZnF ₆	5.74	CsBaBr ₃	4.03	CsTeBr ₃	0.02
Cs ₂ BeMgF ₆	6.09	CsBaI ₃	3.57	CsTeI ₃	0.01
Cs ₂ CaBaF ₆	6.19	CsMnF ₃	2.06		
Cs ₂ CaSrF ₆	6.59	CsMnCl ₃	1.33		
Cs ₂ MgBaF ₆	6.72	CsMnBr ₃	0.93		
Cs ₂ BeBaF ₆	6.72	CsMnI ₃	0.14		
Cs ₂ MgSrF ₆	6.95	CsSnF ₃	0.02		
Cs ₂ BeSrF ₆	7.02	CsSnCl ₃	0.01		
Cs ₂ MgCaF ₆	7.04	CsSnBr ₃	0.00		
Cs ₂ BeCaF ₆	7.55	CsSnI ₃	0.00		
CsPbF ₃	2.76	CsCoF ₃	0.00		
CsPbCl ₃	1.98	CsCoCl ₃	0.01		
CsPbBr ₃	1.68	CsCoBr ₃	0.00		
CsPbI ₃	1.38	CsCoI ₃	0.02		
CsSnF ₃	1.62	CsNiF ₃	0.34		

Table S9. The band gaps for HSE functional

Material	Gap	Class	Material	Gap	Class
Cs ₂ PbSnI ₆	1.19	Direct	Cs ₂ BeMnBr ₆	2.66	Direct
Cs ₂ PbGeI ₆	1.26	Direct	Cs ₂ CdMgBr ₆	2.68	Direct
Cs ₂ GeBeI ₆	1.34	Indirect	Cs ₂ SnMnCl ₆	2.88	Indirect
Cs ₂ PbGeBr ₆	1.39	Direct	Cs ₂ PbMnBr ₆	2.89	Indirect
Cs ₂ SnGeCl ₆	1.40	Direct	Cs ₂ GeMnCl ₆	2.91	Indirect
Cs ₂ SnBeI ₆	1.43	Indirect	Cs ₂ CdMnCl ₆	3.03	Direct
Cs ₂ PbZnI ₆	1.65	Indirect	Cs ₂ SrZnI ₆	3.07	Direct
Cs ₂ PbSnBr ₆	1.65	Direct	Cs ₂ CdZnCl ₆	3.07	Direct
Cs ₂ MnPtF ₆	1.67	Direct	Cs ₂ BeZnCl ₆	3.08	Direct
Cs ₂ CdPbI ₆	1.83	Indirect	Cs ₂ MnZnCl ₆	3.09	Direct
Cs ₂ SnZnBr ₆	1.87	Indirect	Cs ₂ BePtF ₆	3.30	Direct
Cs ₂ CdTeF ₆	1.88	Direct	Cs ₂ NiPtF ₆	3.48	Indirect
Cs ₂ CdSnBr ₆	1.89	Indirect	Cs ₂ MgPtF ₆	3.63	Direct
Cs ₂ CdBeBr ₆	1.92	Direct	Cs ₂ BaPtF ₆	3.73	Indirect
Cs ₂ GeZnBr ₆	1.92	Indirect	Cs ₂ MgPdF ₆	3.81	Direct
Cs ₂ CdGeBr ₆	1.96	Indirect	Cs ₂ SrPtF ₆	3.83	Indirect
Cs ₂ MgMnI ₆	1.97	Direct	Cs ₂ CaPtF ₆	3.85	Indirect
Cs ₂ PbMnI ₆	2.04	Indirect	Cs ₂ CdMnF ₆	3.92	Indirect
Cs ₂ PbSnCl ₆	2.05	Direct	Cs ₂ BaPdF ₆	3.95	Indirect
Cs ₂ PbBeI ₆	2.06	Indirect	Cs ₂ CaPdF ₆	4.06	Indirect
Cs ₂ FeTeF ₆	2.15	Direct	Cs ₂ SrPdF ₆	4.07	Indirect
Cs ₂ SnMgI ₆	2.15	Indirect	Cs ₂ CaNiCl ₆	4.14	Indirect
Cs ₂ GeMgI ₆	2.20	Indirect	Cs ₂ GeNiF ₆	4.23	Indirect
Cs ₂ SnMnBr ₆	2.24	Indirect	Cs ₂ SrNiCl ₆	4.29	Indirect
Cs ₂ PbGeCl ₆	2.28	Direct	Cs ₂ BaNiCl ₆	4.34	Indirect
Cs ₂ ZnTeF ₆	2.31	Direct	Cs ₂ PbNiF ₆	4.96	Indirect
Cs ₂ CaZnI ₆	2.34	Direct	Cs ₂ SrFeF ₆	5.00	Direct
Cs ₂ SnBeBr ₆	2.40	Indirect	Cs ₂ BeNiF ₆	5.04	Indirect
Cs ₂ GeMnBr ₆	2.44	Indirect	Cs ₂ CdNiF ₆	5.49	Direct
Cs ₂ GeBeBr ₆	2.44	Indirect	Cs ₂ NiZnF ₆	5.61	Direct
Cs ₂ CuIrF ₆	2.59	Indirect	Cs ₂ MgNiF ₆	5.94	Direct
Cs ₂ PbZnBr ₆	2.63	Indirect	Cs ₂ CaNiF ₆	6.20	Direct
Cs ₂ MgZnBr ₆	2.65	Direct	Cs ₂ SrNiF ₆	6.28	Direct



Fig

Figure S3. HSE calculated band structures for (a) $\text{Cs}_2\text{PbSnI}_6$, (b) $\text{Cs}_2\text{PbGeI}_6$ (c) $\text{Cs}_2\text{MnPtF}_6$, (d) $\text{Cs}_2\text{PbSnBr}_6$, (e) $\text{Cs}_2\text{PbGeBr}_6$, and (f) $\text{Cs}_2\text{SnGeCl}_6$.

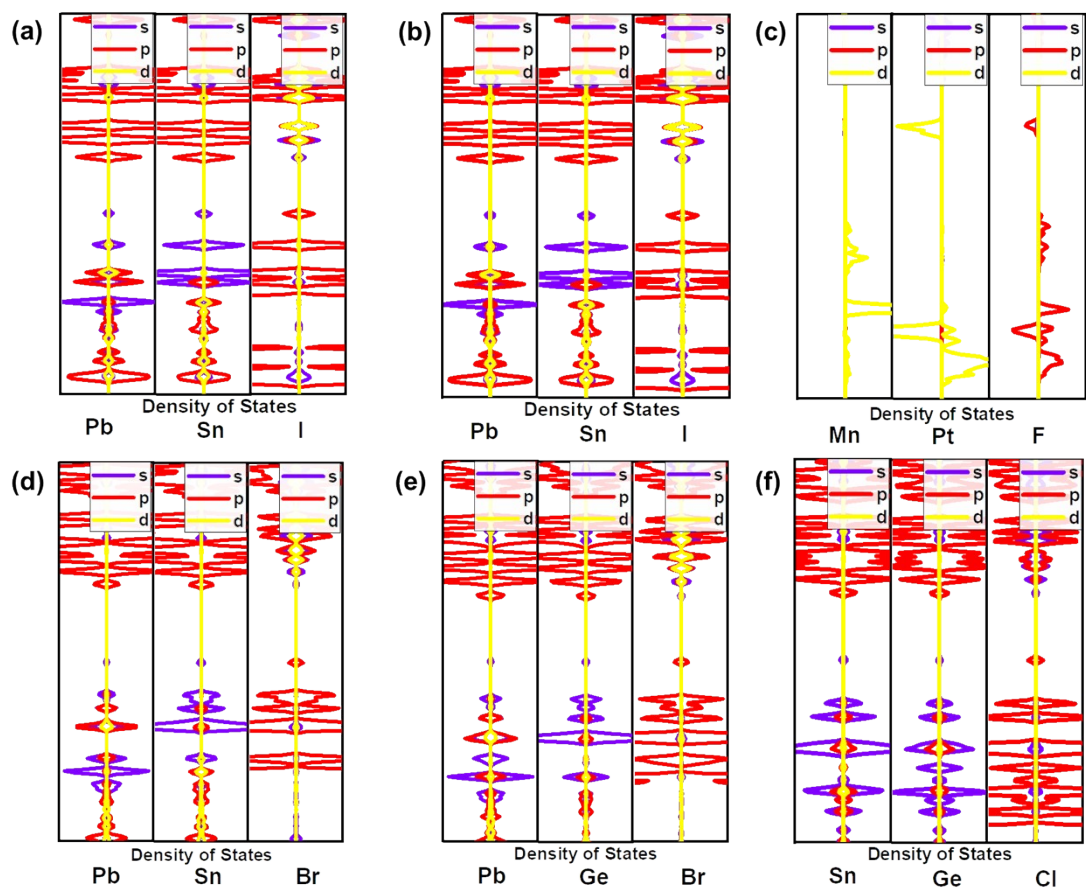


Figure S4. HSE calculated projected density of states (PDOS) for (a) $\text{Cs}_2\text{PbSnI}_6$, (b) $\text{Cs}_2\text{PbGeI}_6$ (c) $\text{Cs}_2\text{MnPtF}_6$, (d) $\text{Cs}_2\text{PbSnBr}_6$, (e) $\text{Cs}_2\text{PbGeBr}_6$, and (f) $\text{Cs}_2\text{SnGeCl}_6$.

Table S10. Band gaps of the 14 predicted all-inorganic double perovskite materials

Material	Predicted bandgap (PBE)	Predicted bandgap (HSE)	Predicted bandgap (HSE+SOC)
Cs ₂ PbSnI ₆	0.77	1.19	0.79
Cs ₂ PbGeI ₆	0.84	1.26	0.91
Cs ₂ PbGeBr ₆	0.86	1.38	1.19
Cs ₂ SnGeCl ₆	0.86	1.40	1.15
Cs ₂ PbSnBr ₆	1.09	1.65	0.89
Cs ₂ MnPtF ₆	0.72	1.67	1.14
Cs ₂ CdTeF ₆	1.33	1.88	1.48
Cs ₂ CdBeBr ₆	0.79	1.92	1.78
Cs ₂ MgMnI ₆	1.01	1.97	1.81
Cs ₂ PbSnCl ₆	1.41	2.05	1.30
Cs ₂ FeTeF ₆	0.82	2.15	2.02
Cs ₂ PbGeCl ₆	1.60	2.28	1.60
Cs ₂ ZnTeF ₆	1.68	2.31	1.93
Cs ₂ CaZnI ₆	1.37	2.34	2.11

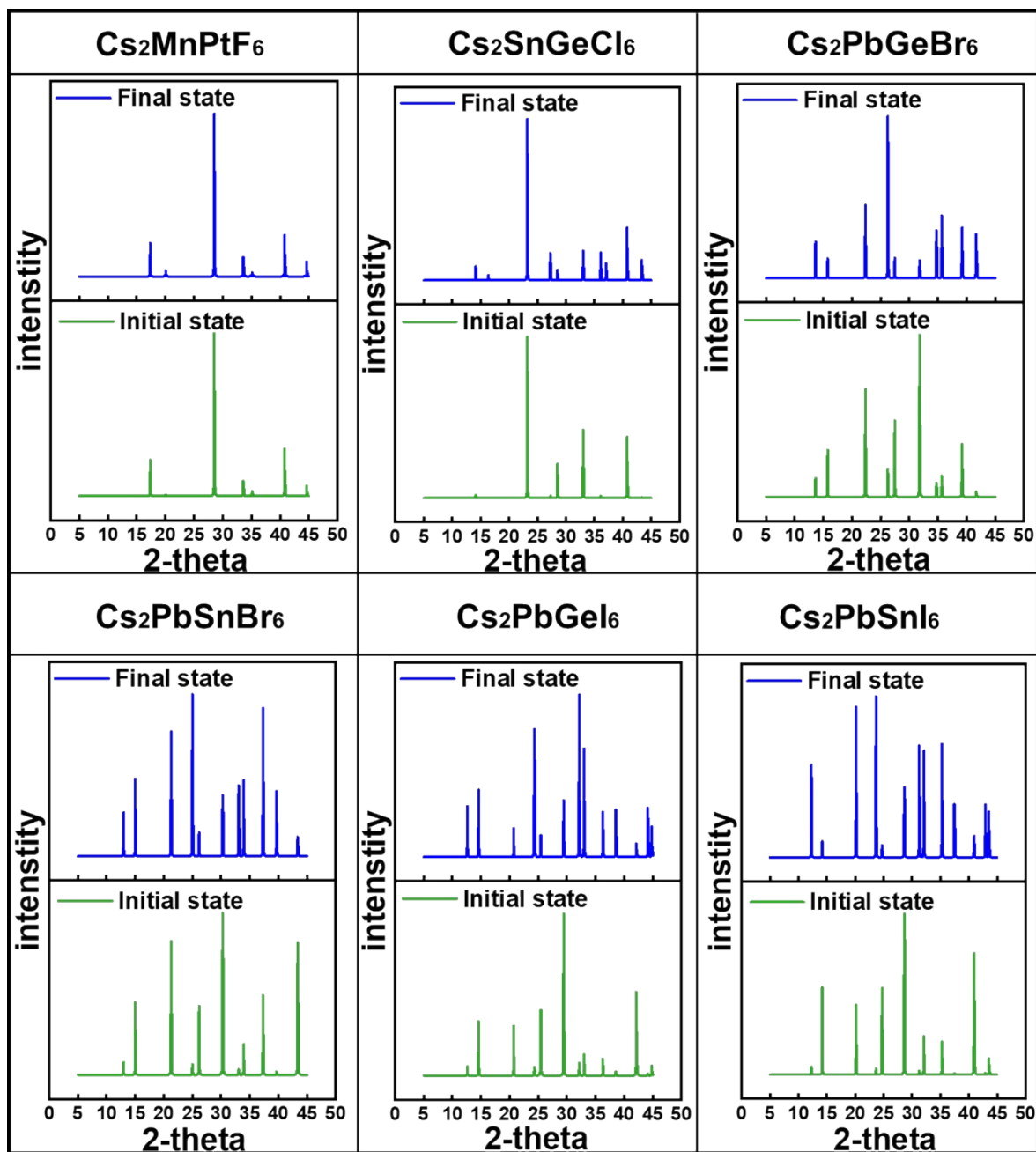


Figure S5. The X-ray diffraction evolution of cubic structure with the temperature of 800 K for $\text{Cs}_2\text{PbSnI}_6$, $\text{Cs}_2\text{PbGeI}_6$, $\text{Cs}_2\text{PbSnBr}_6$, $\text{Cs}_2\text{PbGeBr}_6$, $\text{Cs}_2\text{SnGeCl}_6$, $\text{Cs}_2\text{MnPtF}_6$.

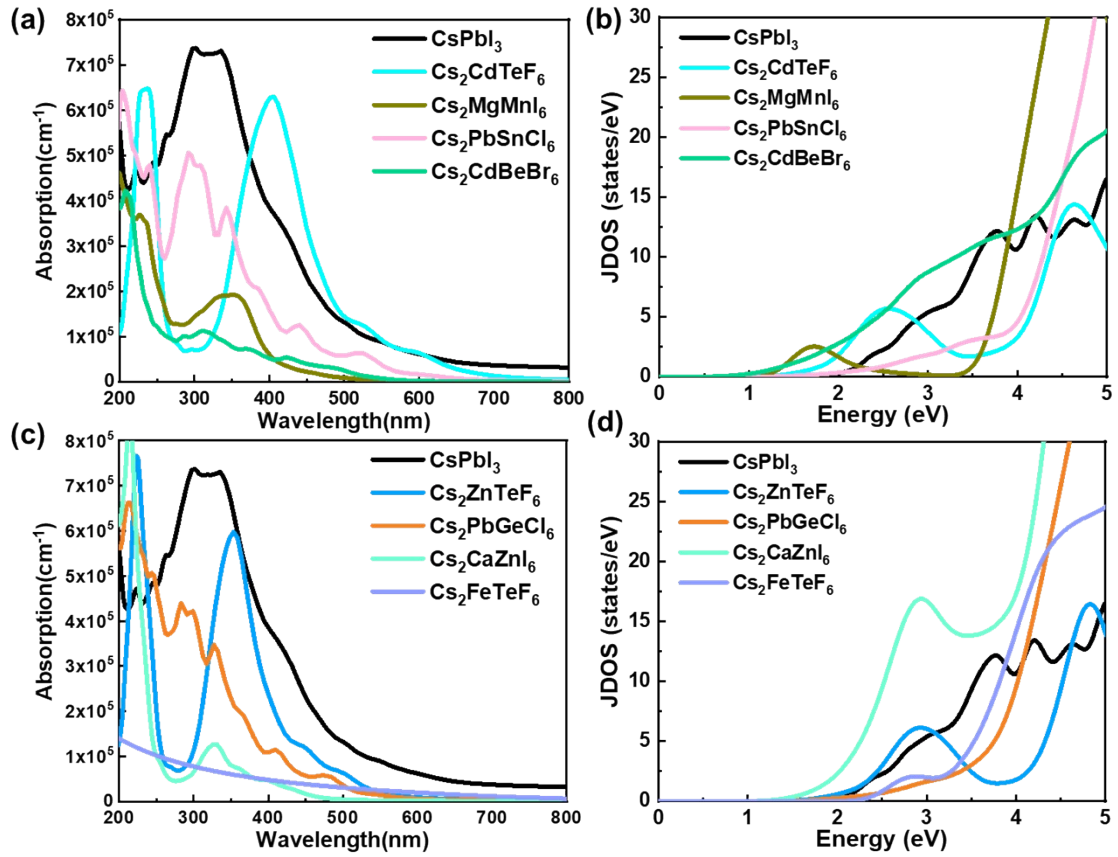


Figure S6. Calculated optical properties for Cs₂CdTeF₆, Cs₂MgMnI₆, Cs₂PbSnCl₆, Cs₂CdBeBr₆, Cs₂ZnTeF₆, Cs₂PbGeCl₆, Cs₂CaZnI₆, Cs₂FeTeF₆. Absorption coefficient: (a) and (c). Joint density of states (JDOS): (b) and (d).