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Stability and electronic properties of new inorganic perovskites from high-throughput ab initio calculations

Supplementary Information

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An illustrative binary convex hull for Sn–Cl is shown in panel (a) of Fig. ESI-1, while the ternary phase diagram of Sn–Cl–Rb is displayed in panel (b) of Fig. ESI-1. If a compound is stable with respect to decomposition, it lies by definition on the convex hull; otherwise it lies above the hull. In the binary phase diagram we can observe that SnCl lies above the hull. It is therefore unstable, in this case with respect to decomposition into $SnCl_2$ and Sn. On the other hand, $RbSnCl_3$ (here in the ilmenite crystal structure) lies on the hull of the ternary phase diagram, hence it is stable.

To some extent it is possible to find a relation between the possible value for the band-gap and the minimal difference in electronegativity between A or B and X elements, $\Delta\ \chi = \min(\chi(X)-\chi(B),\chi(X)-\chi(A))$. As we can see in Fig. ESI-2, band-gaps usually increase with $\Delta\ \chi$, although values are still quite scattered. The upper limit of the band gap can approximately be described by the straight line $E_g \leq 10/3\Delta\ \chi$.

Figure ESI-3 shows the dependency of the effective hole mass on the band gap. One may identify a trend to larger effective masses with larger band gaps for the compounds with direct gaps, whereas for the indirect band gap materials, the scattering is large (we can identify the direct band gap materials in the graph as the cases where direct and indirect band gap fall on top of each other).

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In Tables ESI-1 to ESI-3 we list the energy above the convex hull, E_{hull}, in eV/atom for each compound, together with the magnetic moment μ in units of μ_B, the indirect and direct band gaps from PBE and HSE, the effective hole mass in units of the electron mass, the modulus of the electric polarization $|P|$ in $\mu C/cm^2$, and the formation energy E_f in eV/atom, for all perovskite compounds which are within 25 meV/per atom from the convex hull of thermodynamic stability.

As a side comment, the concept of the effective mass is only valid for semiconductors, and although we obtain vanishing effective hole masses for the metallic compounds, in reality of course the electric conductivity of these compounds will be finite. Similarly, the ferroelectric polarization can only be larger than zero for materials with a band gap.

Where available, data for the same composition (not necessarily in the perovskite crystal structure) from databases are also included in the tables. The Materials Project database is abbreviated as "MP", the Computational Materials Repository [1] as "CMR", and the Open Quantum Materials Database as "OQMD". The formation energies in the CMR and most of those in the OQMD are those of the ideal cubic perovskites (space group 221). Since here we allow for structural distortions which can lower the energy, our formation energies are often more negative (stronger cohesion) than those of the CMR and the OQMD, whereas they usually are very close to those in the MP database.

References

1 https://cmr.fysik.dtu.dk, 2015.

Table ESI-1 Calculated properties of ABX_3 compounds: distance from the convex hull E_{hull} in eV/atom, magnetic moment μ per five-atom unit cell in units of the Bohr magneton, indirect and direct band gaps from PBE and HSE06 functionals, effective hole mass m_h^* in units of the electron mass, modulus of the ferroelectric polarization $|P|$ in the LDA, and formation energies E_{f} in eV/atom from this work and the MP, CMR, and OQMD databases. New compounds are marked by a •

			PBE gap		HSE gap			$\lvert P\rvert$	E_{f}			
composition	E_{hull}	μ/μ_B	ind.	direct	ind.	direct	m_h^*	(LDA)	this work	MP	CMR	OQMD
$PbTiO_3$	0.000	0.0	1.85	2.91	3.15	3.95	0.69	66	-2.848	-2.748	-2.187	-2.554
$BaNbO_3$	0.000	0.0	0.00	0.00	0.09	0.31	0.00	1	-3.333	-3.188	-2.544	-3.062
$TlZnF_3$•	0.000	0.0	4.01	4.09	5.52	5.80	1.95	3	-2.137			
$CsSnCl_3$	0.000	0.0	1.00	1.00	1.57	1.57	0.14	1	-1.460	-1.807		-1.719
$BaTiO_3$	0.000	-0.0	2.14	2.64	3.58	4.12	10.57	31	-3.580	-3.506	-2.948	-3.327
$KTaO_3$	0.000	0.0	2.12	2.79	3.39	4.10	2.31	0	-3.151	-3.098	-2.409	-2.967
$CsGeI_3$	0.000	0.0	1.17	1.17	1.48	1.48	0.29	7	-0.854	-0.849		-0.964
$NaNbO_3$	0.000	0.0	2.20	3.15	3.50	4.55	10.97	44	-3.028	-2.85	-2.168	-2.72
$KMgF_3$	0.000	0.0	7.01	7.32	9.28	9.58	3.97	0	-3.291	-3.289		-3.599
$SrFeO_3$	0.000	3.4	0.03	0.08	0.04	1.20	0.00	1	-2.509	-2.333	-1.851	
$KCdF_3$	0.000	0.0	3.07	4.48	5.28	6.69	1.13	7	-2.429	-2.455		-2.719
$TlMgF_3$•	0.000	0.0	4.25	4.29	5.38	5.47	1.81	1	-2.856			
$RbZnF_3$	0.000	0.0	3.66	4.79	6.24	7.16	1.27	0	-2.531	-2.534		-2.756
$RbCaF_3$	0.000	0.0	6.38	6.52	9.01	9.11	5.56	0	-3.463	-3.46		-3.772
$RbCdF_3$	0.000	0.0	3.14	4.39	5.36	6.61	1.16	4	-2.446	-2.447		-2.743
$RbCaCl_3$•	0.000	0.0	4.96	5.22	7.04	7.31	2.61	3	-2.245			
$RbMnF_3$	0.000	0.0	1.61	3.57	4.34	6.49	1.34	0	-2.560	-2.758		-2.878
$CsNaF_3$•	0.000	1.0	-0.01	0.02	-0.01	0.26	0.00	1	-2.176			
$CsInBr_3$•	0.000	0.0	0.03	0.03	0.49	0.49	0.00	1	-1.236			
$TlCdF_3$•	0.000	0.0	3.83	4.22	5.76	5.91	1.17	0	-2.039			
$RbNiF_3$	0.000	0.0	0.52	0.76	5.30	5.56	5.55	0	-2.120	-2.233		-2.353
$CsTlF_3$•	0.000	0.0	0.06	0.06	0.35	0.35	0.00	5	-2.231			
$CsCaF_3$	0.000	0.0	6.89	6.94	9.97	9.97	6.85	0	-3.472	-3.469		-3.781
$SrVO_3$	0.000	-0.0	0.02	0.02	0.04	0.04	0.00	1	-3.250	-2.895	-2.416	-2.864
$CsPbF_3$	0.000	0.0	3.07	3.07	4.79	4.79	0.41	12	-2.563	-2.533		-2.828
$CsSnBr_3$	0.000	0.0	0.64	0.64	1.11	1.11	0.11	1	-1.246	-1.249		-1.48
$CsCdF_3$	0.000	0.0	3.26	4.17	5.49	6.37	1.19	0	-2.455	-2.455		-2.753
$KZnF_3$	0.000	0.0	3.67	5.15	6.08	7.51	1.25	0	-2.556	-2.555		-2.852
$KTcO_3$	0.000	0.0	0.01	0.06	0.03	0.13	0.00	2	-2.131	-2.008		-1.878
$RbVF_3$	0.000	0.0	0.63	0.96	3.60	4.36	3.27	1	-2.613	-2.767		-2.908
$TlIO_3$	0.000	0.0	2.63	2.63	4.26	4.26	2.00	47	-1.054	-0.983		-0.883
$CsCaCl_3$•	0.000	0.0	5.34	5.55	7.08	7.30	2.70	0	-2.290			
$CsGeBr_3$	0.000	0.0	1.48	1.48	1.97	1.97	0.24	4	-1.146	-1.14		-1.356
$RbMgF_3$	0.000	0.0	7.03	7.16	9.45	9.55	4.47	0	-3.243	-3.252		-3.562
$CsIO_3$	0.000	0.0	3.12	3.12	4.18	4.18	1.42	35	-1.456	-1.397		-1.291
$BaHfO_3$	0.000	0.0	3.56	3.78	5.16	5.32	2.06	3	-3.852		-3.217	-3.671
$CaFeO_3$	0.000	3.3	0.00	0.09	-0.00	1.41	0.00	2	-2.486	-2.342	-1.821	-2.227
$BaZrO_3$	0.000	0.0	3.12	3.38	4.71	4.92	2.12	8	-3.778	-3.654	-3.133	-3.523
$CsInF_3$•	0.000	0.0	0.08	0.08	0.36	0.36	0.00	1	-2.438			
$CsGeCl_3$	0.000	0.0	2.17	2.17	2.84	2.84	0.32	6	-1.363	-1.708		-1.605
$CsCdCl_3$	0.000	0.0	1.72	2.13	3.06	3.55	1.11	0	-1.478	-1.839		-1.717
$CsAgCl_3$	0.000	0.0	0.06	0.06	0.37	0.37	0.00	1	-1.088	-1.445		-1.343
$BaSnO_3$	0.000	0.0	0.34	0.86	1.97	2.34	1.99	0	-2.679	-2.602	-2.008	-2.49
$KCuCl_3$	0.000	0.0	0.03	0.03	0.04	0.04	0.00	1	-1.087	-1.445		-1.298
$KNbO_3$	0.000	0.0	2.18	3.04	3.52	4.44	2.24	28	-3.047	-2.872	-2.187	-2.741
$TlAgCl_3$•	0.000	0.0	0.09	0.09	0.39	0.39	0.00	3	-0.657			
$LaAlO_3$	0.000	0.0	3.49	3.62	4.84	5.02	1.63	0	-3.794	-3.74	-3.053	-3.607
$TlPdF_3$•	0.000	0.0	0.06	0.48	0.14	1.04	0.00	4	-1.460			
$TlAgF_3$•	0.000	0.0	0.00	0.00	0.00	0.00	0.00	6	-1.474			
$CsTlBr_3$•	0.000	0.0	0.06	0.06	0.37	0.37	0.00	2	-1.126			
$RbPdCl_3$•	0.000	0.0	0.03	0.52	0.32	1.17	0.00	1	-1.085			
$CsAgBr_3$•	0.000	0.0	0.00	0.00	0.34	0.34	0.00	1	-0.932			
$SrTiO_3$	0.000	0.0	1.96	2.47	3.42	3.97	3.78	0	-3.647	-3.569	-3.008	-3.393
$TlHgF_3$•	0.000	0.0	2.06	3.06	3.86	4.57	11.37	70	-1.571			
$RbAgBr_3$•	0.000	0.0	0.00	0.00	0.38	0.38	0.00	0	-0.896			
$CsPbBr_3$	0.000	0.0	2.07	2.07	2.42	2.42	0.26	2	-1.323	-1.333		-1.531
$CsCaBr_3$	0.000	0.0	4.40	4.63	6.09	6.35	2.07	1	-1.999	-2.001		-2.219
$CsPbCl_3$	0.000	0.0	2.48	2.48	2.95	2.95	0.28	2	-1.538	-1.885		-1.775
KWO_3	0.001	0.0	0.01	0.01	0.08	0.08	0.00	1	-2.607		-1.83	
$RbHgF_3$	0.001	0.0	0.63	2.66	2.59	4.77	0.82	7	-1.963	-1.972		-2.238

Table ESI-2 Continuation of Table ESI-1

			PBE gap		HSE gap			$\|P\|$		E_f		
composition	E_{hull}	μ/μ_B	ind.	direct	ind.	direct	m_h^*	(LDA)	this work	MP	CMR	OQMD
$KAgBr_3$●	0.001	0.0	0.00	0.00	0.40	0.40	0.00	0	-0.866			
$KAgCl_3$●	0.001	0.0	0.00	0.00	0.01	0.01	0.00	0	-1.037			
$CsHgF_3$	0.001	0.0	0.70	2.41	2.65	4.51	0.80	4	-1.988	-1.997		-2.271
$RbTlF_3$●	0.001	0.0	0.05	0.05	0.01	0.01	0.00	0	-2.199			
$RbIO_3$	0.001	0.0	2.79	2.79	3.88	3.88	1.48	40	-1.446	-1.389		-1.286
$NaMoO_3$	0.001	0.0	0.00	0.00	0.02	0.02	0.00	0	-2.547		-1.714	-2.29
$LaReN_3$	0.001	0.0	-0.01	-0.01	0.04	0.04	0.00	4	-0.726		-0.442	
$RbAgCl_3$●	0.001	0.0	0.08	0.08	0.39	0.39	0.00	1	-1.063			
$KAgF_3$	0.001	0.0	0.03	0.03	0.32	0.54	0.00	2	-1.870	-2.138		
$KCuF_3$	0.001	0.0	0.03	0.26	1.76	2.28	0.00	0	-2.099	-2.381		-2.389
$TlCuF_3$	0.002	0.0	0.00	0.15	1.82	2.25	0.00	0	-1.670	-1.911		-1.926
$RbCuF_3$	0.002	0.0	0.04	0.27	1.79	2.20	0.00	1	-2.067	-2.076		-2.358
$CsSrCl_3$●	0.002	0.0	4.98	5.15	6.29	6.48	3.14	4	-2.300			
$BaBiO_3$	0.002	0.0	0.03	0.03	0.25	0.25	0.00	7	-2.284	-2.249	-1.654	-2.117
$RbAgF_3$	0.002	0.0	0.03	0.03	0.02	0.02	0.00	0	-1.882	-2.151		-2.173
$CsPdBr_3$●	0.002	0.0	0.02	0.49	0.00	0.01	0.00	1	-0.934			
$RbOsO_3$	0.002	0.0	0.01	0.01	0.00	0.00	0.00	1	-1.584			-1.405
$SrNbO_3$	0.003	0.0	0.00	0.00	0.08	0.08	0.00	2	-3.346	-3.195	-2.524	-3.061
$KMnF_3$	0.003	0.0	1.31	3.32	4.04	6.23	1.35	3	-2.566	-2.764		-2.882
$CsSnF_3$●	0.003	0.0	2.67	2.67	4.10	4.10	0.60	3	-2.515			
$InGeCl_3$●	0.004	0.0	2.41	2.41	3.03	3.03	0.53	26	-0.829			
$NaTcO_3$	0.004	0.0	0.00	0.08	0.01	0.13	0.00	1	-2.140	-2.0		-1.882
$CsSrF_3$	0.004	0.0	6.19	6.21	8.24	8.24	5.74	6	-3.423	-3.419		-3.715
$RbGeBr_3$	0.004	0.0	1.48	1.48	1.65	1.65	0.25	4	-1.095	-1.105		-1.318
$RbInCl_3$●	0.004	0.0	0.13	0.13	0.57	0.57	0.00	2	-1.390			
$RbCrCl_3$	0.004	4.0	0.01	0.35	0.16	0.83	0.00	0	-1.380	-1.726		-1.619
$PbHfO_3$	0.004	0.0	2.97	3.10	4.50	4.61	1.08	0	-3.078	-3.011	-2.408	-2.847
$RbPdBr_3$●	0.005	0.0	0.00	0.51	0.01	0.03	0.00	1	-0.912			
$RbSnBr_3$●	0.005	0.0	1.09	1.09	1.10	1.10	0.19	3	-1.197			
$TlMnF_3$●	0.005	0.0	1.37	2.42	3.92	4.78	1.32	0	-2.164			
$CsScBr_3$●	0.005	0.0	0.02	0.02	0.02	0.02	0.00	1	-1.613			
$NaWO_3$	0.006	0.0	0.00	0.00	0.01	0.01	0.00	0	-2.603	-2.114	-1.824	-2.419
$RbPbF_3$	0.007	0.0	3.20	3.20	4.80	4.91	0.39	15	-2.525	-2.522		-2.785
KIO_3	0.007	0.0	2.48	2.48	3.52	3.52	0.97	47	-1.439	-1.387		-1.277
$BaPbO_3$	0.007	0.0	0.00	0.06	0.64	1.35	0.00	0	-2.166	-2.127	-1.519	-1.989
$TlGeF_3$●	0.007	-0.0	2.80	3.07	3.99	4.33	1.73	11	-2.014			
$CsMnF_3$	0.008	0.0	2.11	3.94	4.67	6.98	1.40	0	-2.528	-2.74		-2.786
$TlFeF_3$●	0.008	0.0	0.00	0.02	2.51	2.85	0.00	0	-1.891			
$KCaF_3$	0.008	0.0	6.13	6.29	8.59	8.71	5.35	8	-3.445	-3.744		-3.748
$CsAgF_3$	0.009	0.0	0.02	0.02	0.02	0.02	0.00	1	-1.881	-2.154		-2.177
$CsSnI_3$	0.009	0.0	0.59	0.59	0.85	0.85	0.12	4	-0.960	-0.964		-1.097
$TlCuCl_3$●	0.009	0.0	0.04	0.04	0.05	0.05	0.00	0	-0.707			
$CsCaI_3$●	0.010	0.0	3.71	3.99	4.88	5.17	1.54	2	-1.607			
$KMnCl_3$	0.010	5.0	1.68	3.58	3.62	5.73	0.67	2	-1.416	-1.809		
$InSnBr_3$	0.011	0.0	1.13	1.13	1.58	1.58	0.25	0	-0.741	-0.727		
$InMnF_3$●	0.011	0.0	1.25	2.28	3.81	4.65	1.38	33	-2.065			
$RbInBr_3$●	0.013	0.0	0.03	0.03	0.50	0.50	0.00	2	-1.183			
$CsSrBr_3$●	0.013	0.0	4.18	4.38	5.35	5.58	2.47	4	-2.023			
$SrCrO_3$	0.013	0.0	-0.00	0.01	0.14	0.61	0.00	2	-2.880	-2.595	-2.164	-2.565
$KGeCl_3$●	0.014	0.0	1.48	1.48	2.16	2.16	0.19	5	-1.276			
$RbCuBr_3$●	0.014	0.0	0.00	0.00	0.24	0.24	0.00	1	-0.887			
$CsTlCl_3$●	0.014	0.0	0.00	0.00	0.45	0.45	0.00	1	-1.301			
$KNiF_3$	0.016	0.0	0.54	0.78	5.35	5.59	3.46	0	-2.153	-2.256		-2.449
$KHgF_3$	0.016	0.0	0.59	2.79	2.55	4.91	0.85	24	-1.937	-1.944		
$TlGeCl_3$●	0.016	0.0	1.37	1.37	2.02	2.02	0.17	0	-0.893			
$RbCuCl_3$	0.016	0.0	0.00	0.00	0.02	0.02	0.00	1	-1.094	-1.45		-1.311
$AgCuF_3$	0.017	0.0	0.00	0.00	0.12	0.12	0.00	4	-1.276			-1.532
$InSnCl_3$●	0.018	0.0	2.09	2.10	2.71	2.71	0.51	23	-0.937			
$LiSnCl_3$●	0.018	0.0	3.87	3.94	4.87	4.94	5.29	20	-1.322			
$KMgCl_3$	0.018	0.0	4.33	4.71	6.05	6.44	1.84	1	-1.889	-2.255		-2.15

Table ESI-3 Continuation of Table ESI-2

			PBE gap		HSE gap			$\|P\|$		E_f		
composition	E_{hull}	μ/μ_B	ind.	direct	ind.	direct	m_h^*	(LDA)	this work	MP	CMR	OQMD
$PbZrO_3$	0.019	-0.0	3.05	3.16	4.54	4.65	1.18	0	-3.008	-2.87	-2.316	-2.724
$RbMgCl_3$	0.019	0.0	4.20	4.54	5.76	6.11	1.97	0	-1.908	-2.278		-2.174
$NaTaO_3$	0.019	0.0	2.24	3.00	4.13	4.78	2.06	0	-3.136	-3.088	-2.404	-2.966
$InPbCl_3$●	0.019	0.0	2.87	2.89	3.69	3.71	0.86	0	-1.023			
$RbGeI_3$	0.020	0.0	1.21	1.21	1.35	1.35	0.31	8	-0.799	-0.809		-0.924
$RbGeCl_3$	0.020	0.0	1.73	1.73	2.45	2.45	0.24	5	-1.315	-1.682		-1.576
$BaHfS_3$●	0.020	0.0	0.71	1.13	1.45	1.93	1.01	7	-1.838			
$KCaCl_3$●	0.020	0.0	4.75	5.04	6.28	6.57	2.55	0	-2.207			
$RbTlBr_3$●	0.021	0.0	0.06	0.06	0.37	0.37	0.00	4	-1.069			
$RbMnCl_3$	0.021	0.0	1.67	3.52	3.58	5.56	0.67	1	-1.438	-1.815		-1.703
$NaReO_3$	0.021	0.0	0.00	0.10	0.25	0.46	0.00	1	-2.158	-2.098	-1.606	-1.971
$CsInI_3$●	0.022	0.0	0.05	0.05	0.35	0.35	0.00	1	-0.944			
$BaLiF_3$	0.022	0.0	6.58	6.58	8.64	8.64	3.65	1	-3.489	-3.478		-3.78
$CsSeBr_3$●	0.022	0.0	0.00	0.07	0.02	0.15	0.00	4	-0.790			
$RbSnCl_3$●	0.022	0.0	1.43	1.43	1.61	1.61	0.22	3	-1.408			
$KMoO_3$	0.023	0.0	0.00	0.00	0.07	0.07	0.00	1	-2.545		-1.723	-2.293
$CsSrI_3$●	0.023	0.0	3.61	3.84	4.74	4.84	1.85	4	-1.646			
$AgMgF_3$●	0.023	0.0	2.03	2.65	4.16	4.83	6.85	3	-2.485			
$LaWN_3$	0.023	0.0	0.46	1.37	0.97	2.09	0.93	73	-0.984		-0.564	
$RbCaBr_3$●	0.024	0.0	4.09	4.36	5.76	6.06	2.03	2	-1.947			
$TlCoF_3$●	0.024	0.0	-0.04	-0.01	4.27	4.70	0.00	0	-1.746			
$KHfO_3$	0.024	1.0	0.00	0.06	0.05	0.05	0.00	0	-3.018		-2.402	-2.83
$RbCdCl_3$	0.025	0.0	1.77	2.31	3.12	3.74	0.98	2	-1.443	-1.82		-1.693
$BaMoO_3$	0.025	0.2	0.00	0.01	0.00	0.18	0.00	1	-2.864	-2.595	-2.121	-2.632
$KCrCl_3$●	0.026	4.0	0.01	0.37	0.15	0.87	0.00	0	-1.364			
$KGeBr_3$●	0.026	0.0	1.37	1.38	1.47	1.47	0.22	7	-1.056			
$LaNiO_3$	0.026	0.3	0.02	0.29	0.03	0.03	0.00	1	-2.627	-2.378	-1.946	
$TlAgBr_3$●	0.027	0.0	0.03	0.03	0.43	0.43	0.00	9	-0.500			
$InCaBr_3$	0.028	0.0	3.49	3.64	4.32	4.47	3.42	22	-1.484	-1.519		-1.737
$LaCuO_3$	0.028	0.0	-0.00	0.42	0.14	1.18	0.00	0	-2.466	-2.44		
$TlCaF_3$●	0.029	0.0	4.47	4.48	6.21	6.25	1.56	27	-3.054			
$SrSnO_3$	0.030	-0.0	0.95	1.77	2.78	3.60	1.99	7	-2.684	-2.655	-2.0	
$SrHfO_3$	0.030	0.0	3.75	4.07	5.26	5.67	2.01	0	-3.847	-3.831	-3.2	-3.693
$LaFeO_3$	0.030	2.9	-0.02	0.02	0.02	0.02	0.00	1	-2.876	-2.94	-2.152	
$CsPbI_3$	0.033	0.0	1.51	1.51	2.04	2.04	0.23	3	-1.021	-1.053		
$BaZrS_3$	0.034	0.0	0.56	1.01	1.29	1.81	1.08	0	-1.822	-1.81		-2.008
$SrRuO_3$	0.034	1.9	0.00	0.04	0.00	0.34	0.00	4	-2.270	-2.206	-1.513	
$LaCoO_3$	0.034	1.4	0.00	0.02	0.11	0.43	0.00	108	-2.698	-2.64	-1.994	
$NaOsO_3$	0.034	0.0	-0.00	-0.00	0.04	0.04	0.00	1	-1.693			-1.518
$AgZnF_3$	0.035	0.0	1.56	2.27	3.86	4.45	1.17	9	-1.729	-1.736		
$RbSnI_3$	0.036	0.0	0.47	0.47	0.82	0.82	0.11	3	-0.899	-0.931		-1.061
$RbPbBr_3$●	0.036	0.0	2.06	2.06	2.40	2.40	0.26	0	-1.263			
$RbPbCl_3$●	0.037	0.0	2.46	2.46	2.92	2.92	0.28	0	-1.480			
$KCdCl_3$	0.038	-0.0	1.81	2.39	3.31	3.82	0.92	0	-1.410	-1.813		-1.688
$TlNiF_3$●	0.038	0.0	0.40	0.69	4.19	4.41	3.29	1	-1.726			
$RbSrCl_3$●	0.038	0.0	4.63	4.83	5.91	6.13	3.08	0	-2.242			
$AgTaO_3$	0.039	0.0	1.73	2.23	3.38	3.61	2.07	19	-2.461	-2.427	-1.774	
$BiNiO_3$	0.039	0.3	0.00	0.15	0.02	0.83	0.00	54	-1.410	-1.234		
$TlSnF_3$	0.040	0.0	2.33	2.70	3.45	3.96	1.25	21	-2.090	-2.363		
$TlGeBr_3$●	0.040	0.0	1.28	1.28	1.28	1.28	0.21	0	-0.683			
$RbSeBr_3$●	0.041	0.0	0.01	0.10	0.01	0.08	0.00	5	-0.747			
$TlCaCl_3$●	0.042	0.0	3.93	4.30	5.12	5.46	2.46	0	-1.824			
$SrTcO_3$	0.044	0.0	0.02	0.07	1.82	2.52	0.00	1	-2.578	-2.474		-2.335
$RbCaI_3$●	0.046	0.0	3.44	3.73	4.40	4.71	1.48	3	-1.548			
$SrZrO_3$	0.047	0.0	3.33	3.63	4.86	5.27	2.08	0	-3.757	-3.68	-3.105	-3.535
$AgNiF_3$●	0.047	2.0	0.56	0.82	3.33	4.36	2.05	2	-1.332			
$TlCdCl_3$	0.050	-0.0	1.86	2.57	3.38	3.99	0.87	0	-1.029	-1.433		-1.308
$RbSnF_3$●	0.052	-0.0	1.95	1.95	3.57	3.58	0.32	3	-2.460			
$LaCrO_3$	0.054	3.0	0.25	0.78	2.95	3.71	0.00	8	-3.207	-3.193	-2.494	
$LaMnO_3$	0.054	3.5	0.01	0.02	0.32	2.26	0.00	6	-3.089	-3.025	-2.428	

Table ESI-4 Continuation of Table ESI-3

composition	E_{hull}	μ/μ_B	PBE gap ind.	PBE gap direct	HSE gap ind.	HSE gap direct	m_h^*	$\lvert P\rvert$ (LDA)	E_f this work	E_f MP	E_f CMR	E_f OQMD
$KCaBr_3$•	0.054	0.0	3.92	4.20	5.11	5.36	1.98	0	-1.906			
$CaTiO_3$	0.055	0.0	1.97	2.48	3.44	4.03	2.19	0	-3.589	-3.573	-2.976	-3.396
$LaVO_3$	0.058	1.3	-0.04	0.07	0.26	2.29	0.00	3	-3.363	-3.286	-2.522	
$RbAuI_3$	0.059	-0.0	0.00	0.00	0.01	0.01	0.00	1	-0.630	-0.687		
$CsAuI_3$	0.059	0.0	0.00	0.00	0.01	0.01	0.00	1	-0.675	-0.73		
$TlInCl_3$•	0.059	0.0	0.13	0.13	0.32	0.32	0.00	19	-0.966			
$RbPbI_3$	0.060	0.0	1.58	1.58	2.01	2.01	0.23	3	-0.958	-1.017		
$LaTiO_3$	0.061	-0.0	0.00	0.00	0.03	0.10	0.00	10	-3.684	-3.657	-2.973	-3.494
$CsAuBr_3$	0.061	0.0	0.03	0.03	0.28	0.28	0.00	1	-0.856	-0.912		
$CsAuCl_3$	0.063	0.0	0.00	0.00	0.25	0.25	0.00	1	-0.986	-1.408		-1.304
$BaZrSe_3$•	0.072	-0.0	0.25	0.77	1.01	1.44	0.82	0	-1.586			
$CaTcO_3$	0.078	0.1	0.00	0.00	2.09	2.71	0.00	0	-2.496			-2.356
$LaGaO_3$	0.080	0.0	3.30	3.58	4.77	5.08	1.98	9	-3.131	-3.116	-2.408	
$KCoF_3$	0.099	3.0	0.00	0.01	4.02	4.71	0.00	1	-2.166	-2.503		
$RbCoF_3$	0.119	3.0	-0.00	0.00	4.03	4.60	0.00	2	-2.137	-2.382		
$YNiO_3$	0.137	0.2	0.01	0.41	0.02	0.02	0.00	31	-2.497	-2.382		-2.392
$TlNiO_3$	0.149	0.0	0.00	0.00	-0.00	-0.00	0.00	1	-0.975	-0.87		
$YReN_3$	0.149	0.0	0.00	0.00	0.12	0.12	0.00	0	-0.554		-0.354	
$SrCoO_3$	0.149	2.5	0.00	0.02	0.28	0.88	0.00	2	-2.202	-1.979	-1.565	

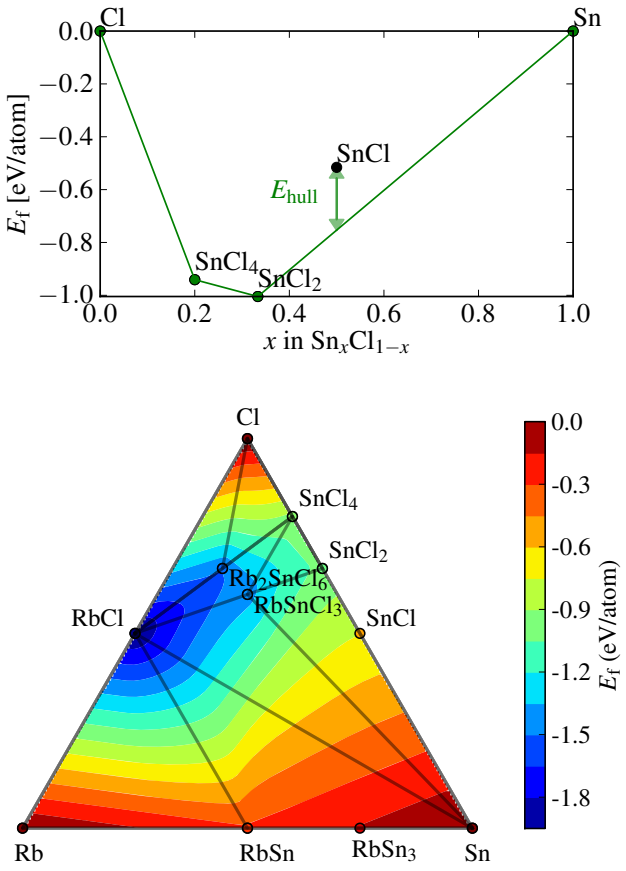

Fig. ESI-1 (Color online) Panel (a): Formation energy (in units of eV/atom) as a function of composition for the system Sn–Cl. Panel (b): Projected formation energy (in units of eV/atom) as a function of composition for the system Rb–Sn–Cl. The color map represents the formation energy E_f. Stable compounds (those on the convex hull) are connected by lines. For the sake of readability, most unstable or metastable phases are omitted.

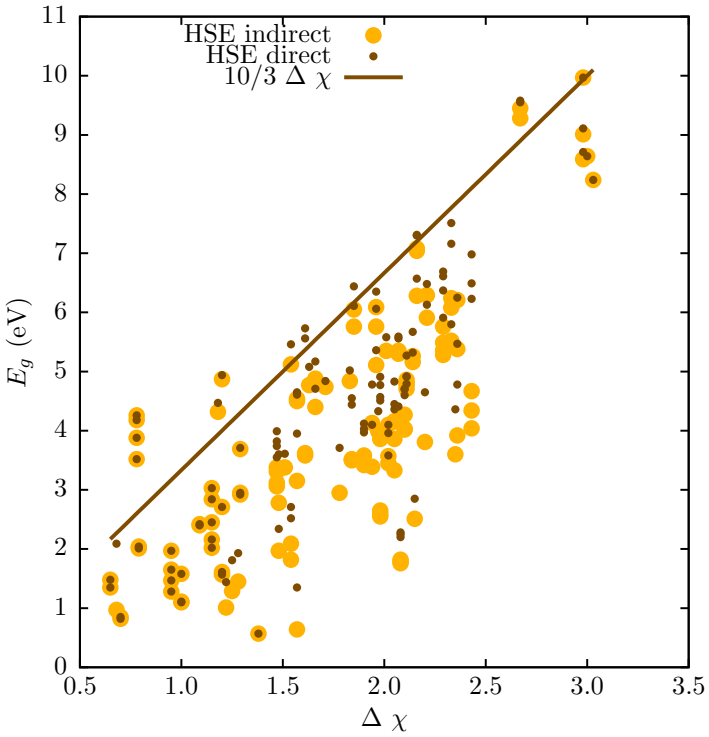

Fig. ESI-2 (Color online) band gaps of the stable perovskites *vs* electronegativity difference between cations and X anion (see text).

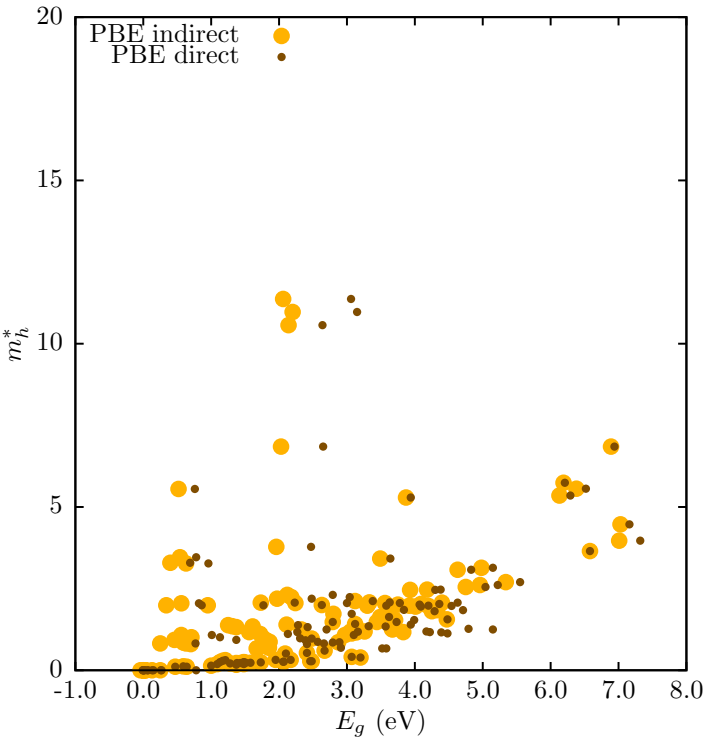

Fig. ESI-3 (Color online) Effective hole mass m_h^* *vs.* band gap for the stable perovskites.