SUPPLEMENTARY INFORMATION

Investigation of thermal control in phase-changing ABO_3 perovskites via first-principles predictions: General mechanism of solar absorbance

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

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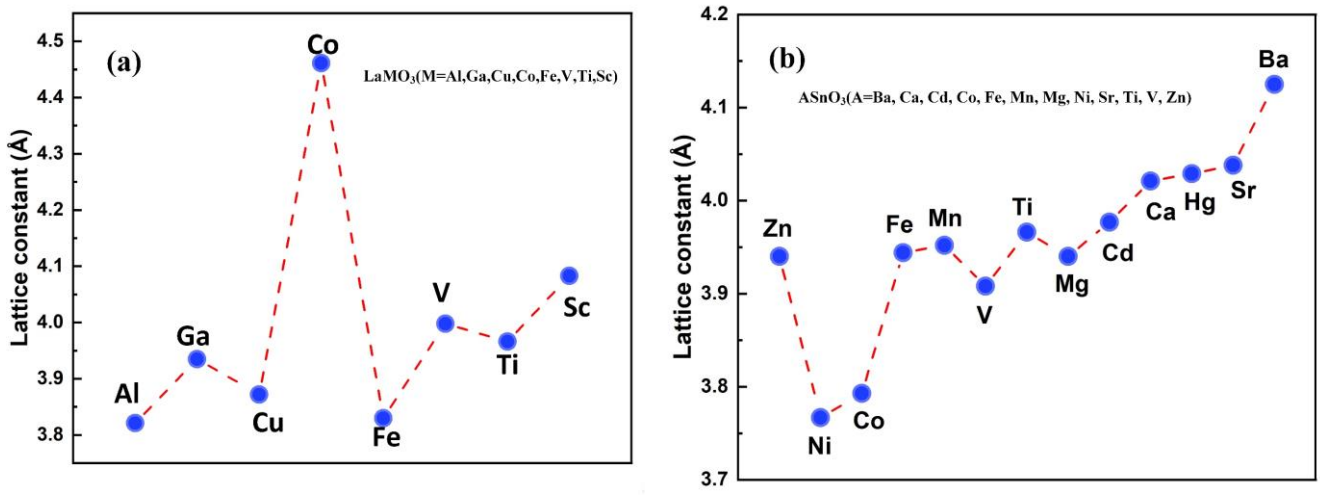

FIG. S1. Variation of lattice constant of cubic $LaMO_3$ (M=Al, Ga, Sc, Fe, Co, Cr, Ti, V) and $ASnO_3$ (A=Ba, Ca, Cd, Co, Fe, Mn, Mg, Ni, Sr, Ti, V, Zn).

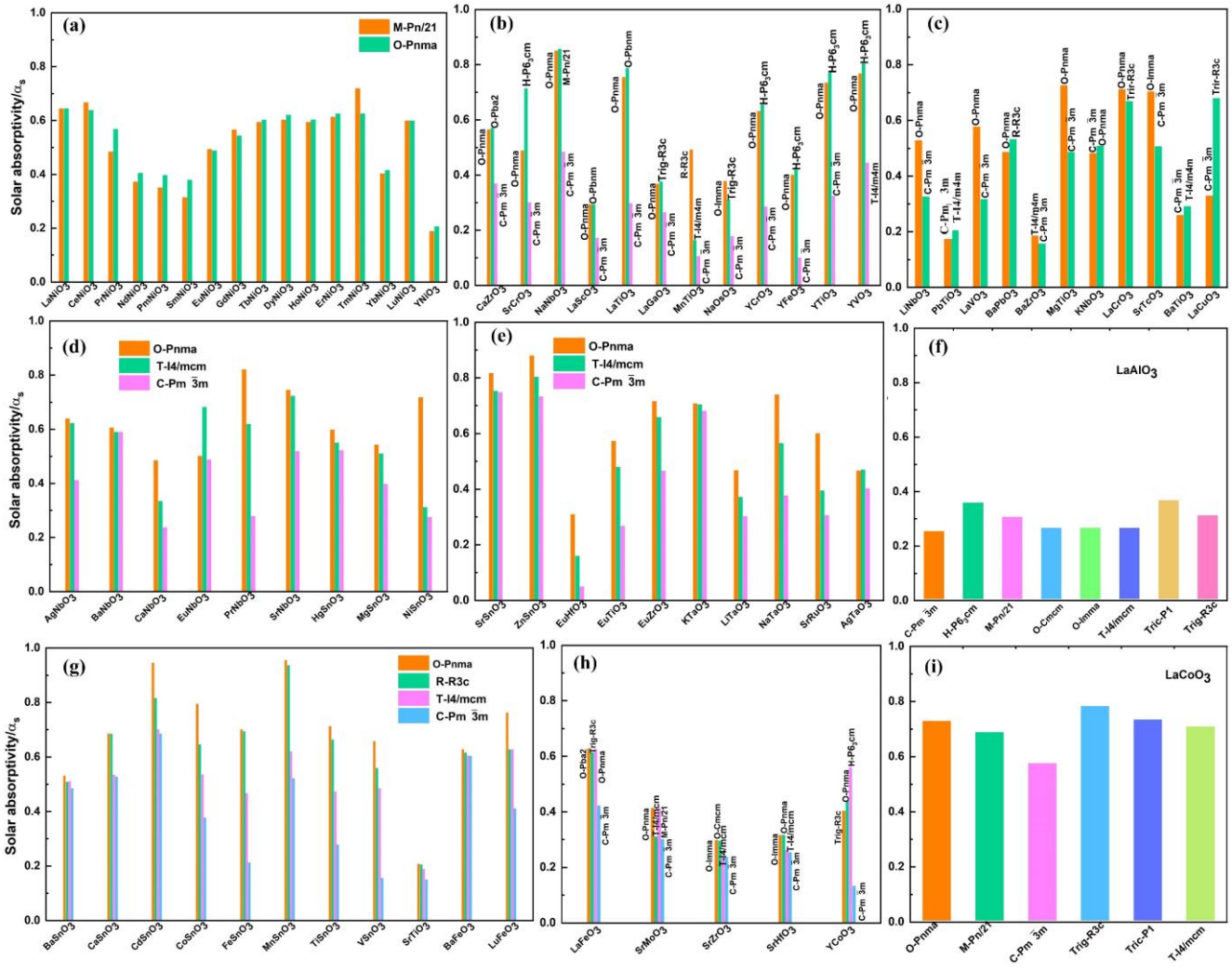

FIG. S2. Average solar absorptivity (250–2500 *n*m) of 76 ABO_3 perovskites.

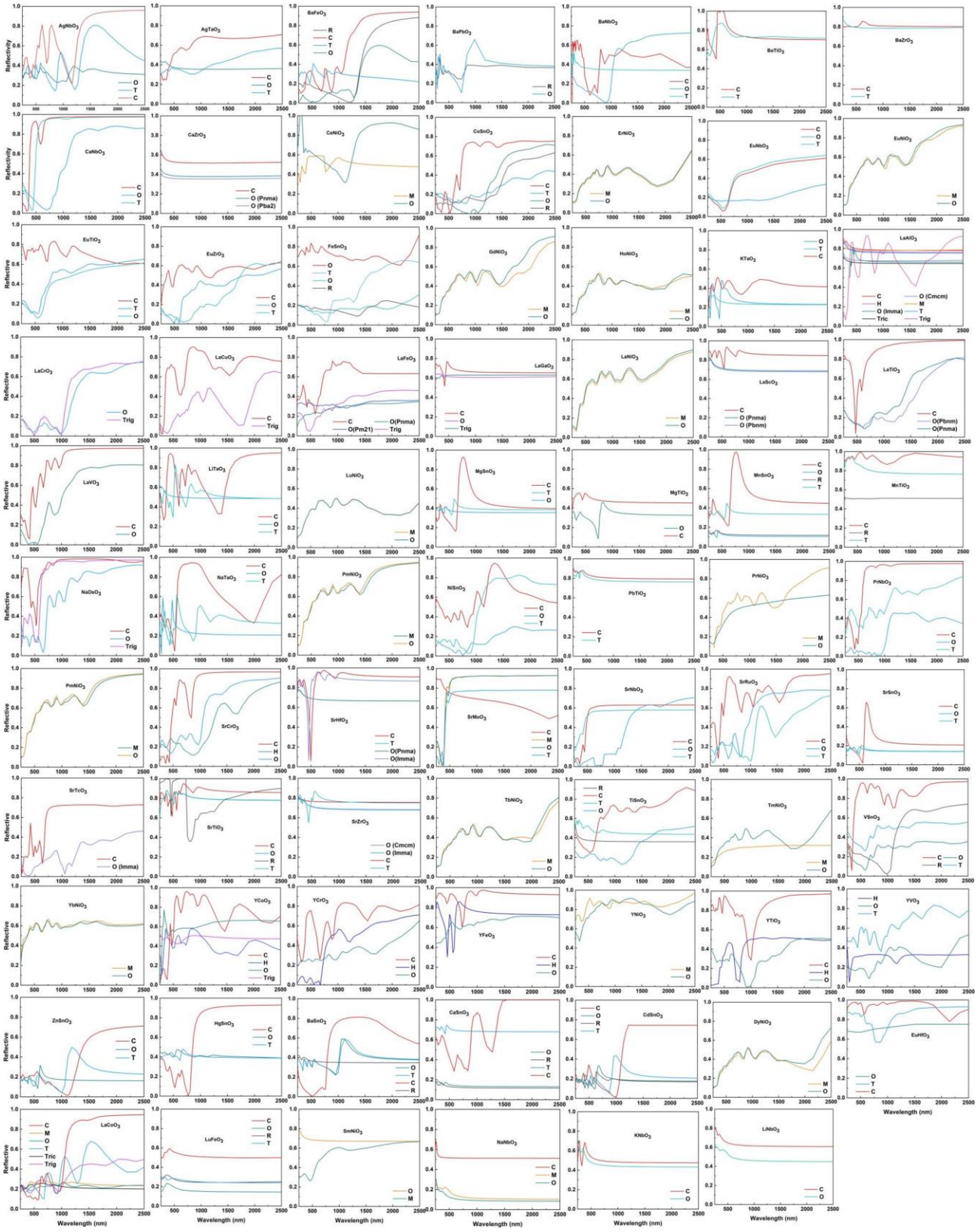

FIG. S3. Reflectivity (250–2500 *n*m) of 76 ABO_3 perovskites.

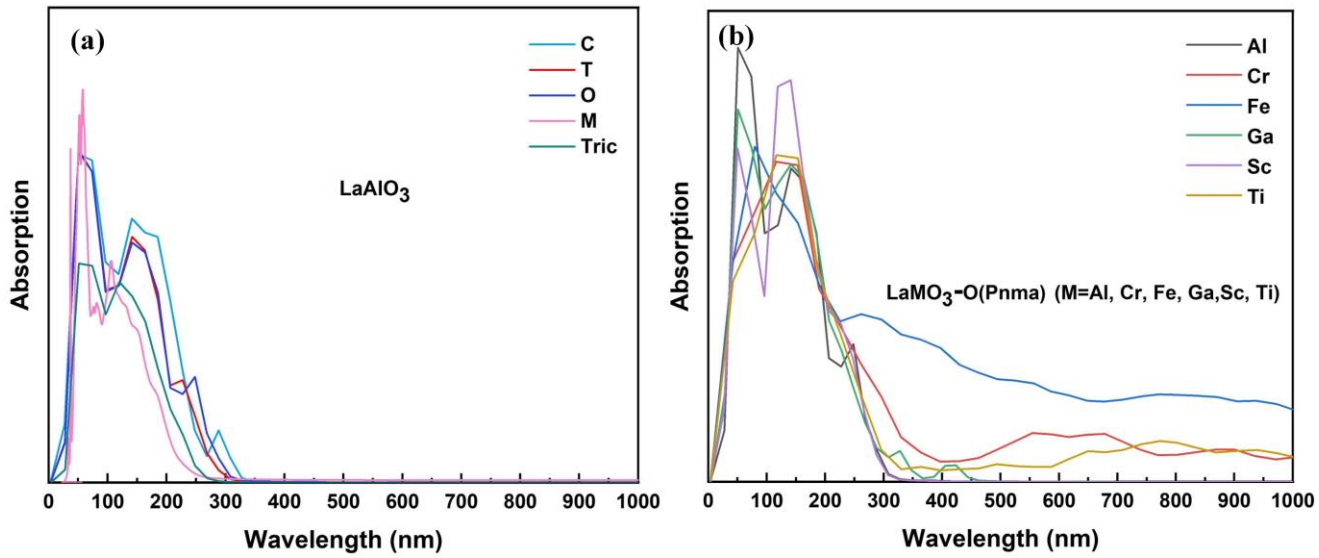

FIG. S4. Absorption spectra (0–1000*n*m) of $LaAlO_3$-C, $LaAlO_3$-T, $LaAlO_3$-Tric, $LaAlO_3$-M, $LaAlO_3$-O, $LaCrO_3$-O, $LaFeO_3$-O, $LaGaO_3$-O, $LaScO_3$-O, and $LaTiO_3$-O.

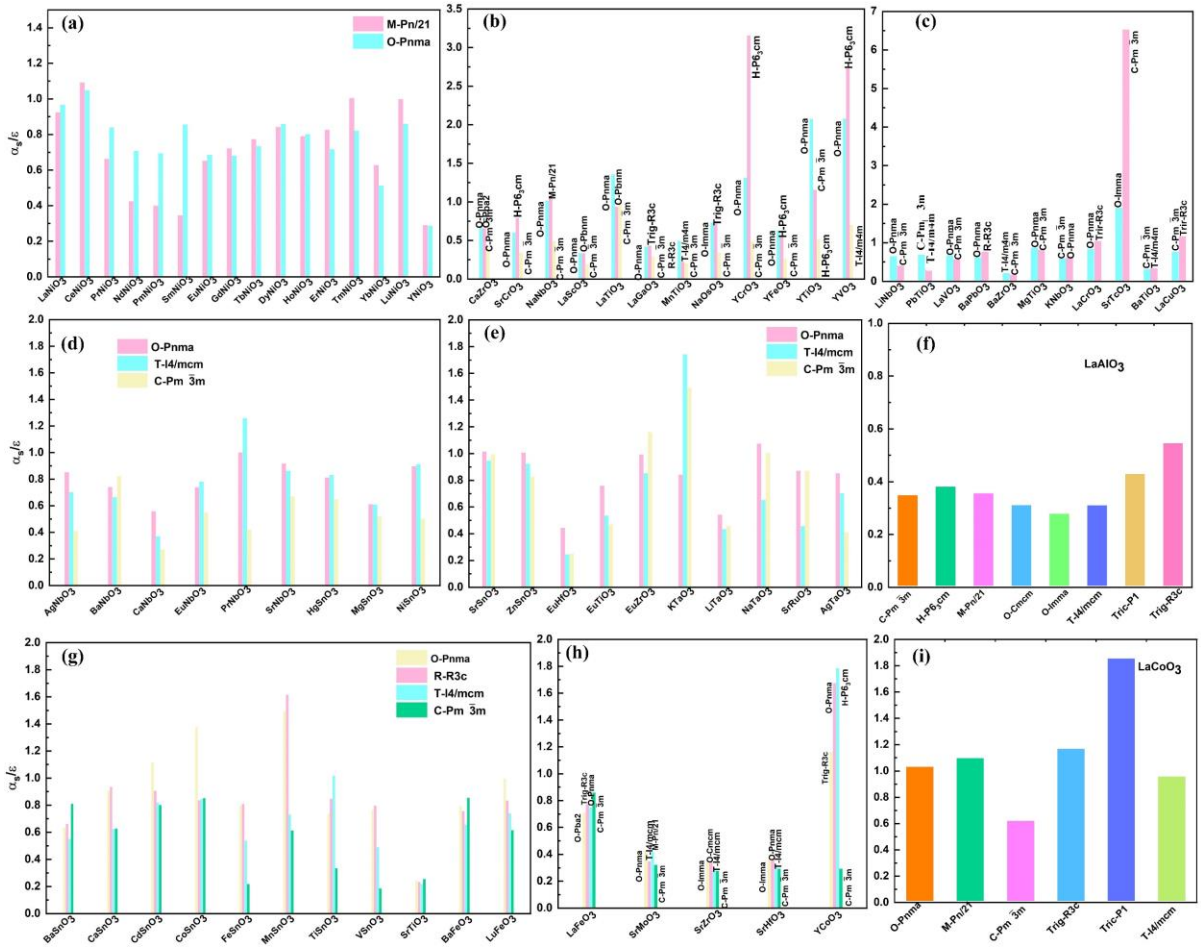

FIG. S5. The ratio of solar absorption (250-2500 nm) to IR emittance (2.5-25 μm) (α_S/ε) of 76 ABO_3 perovskites.

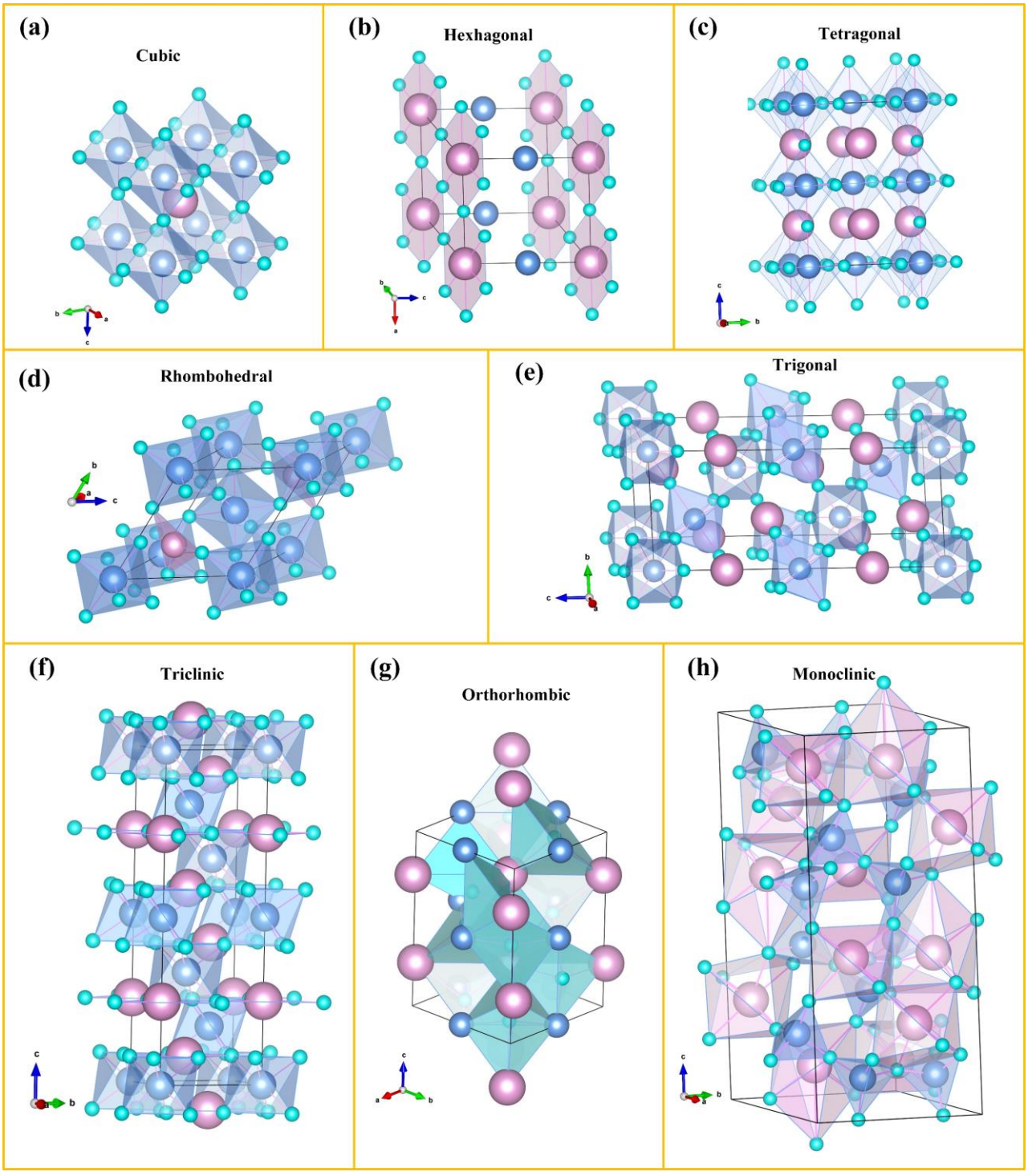

FIG. S6. The atomic models of Cubic (a), Hexhagonal (b), Tetragonal (c), Rhombohedral (d), Trigonal (e), Triclinic (f), Orthorhombic (g), and Monoclinic (h) for ABO_3 perovskites. The small turquoise balls are oxygen atoms, big darkslateblue balls are B-site atoms, and grey-pink balls are A-site atoms.

Table S1 Lattice constants and formation energies of 76 kinds of ABO_3 perovskites.

	Lattice constants (Å)	Formation energy (eV/atom)		Lattice constants (Å)	Formation energy (eV/atom)
$AgNbO_3$-O(Pmc21)	a=5.645,b=5.748,c=15.743	-3.19	$MgTiO_3$-C	a=b=c=3.832	-2.83978
$AgNbO_3$-C	a=b=c=4.024	-3.159	$MgTiO_3$-O	a=5.103,b=5.308,c=7.469	-2.93196
$AgNbO_3$-O(Cmcm)	a=7.92,b=7.965,c=8.017	-3.279	$MnSnO_3$-C	a=b=c=3.952	-2.67861
$AgNbO_3$-O(Pbcm)	a=5.671,b=5.748,c=15.763	-3.181	$MnSnO_3$-O	a=5.340,b=5.499,c=7.788	-2.76962
$AgNbO_3$-Te	a=5.63,b=5.63,c=4.021	-2.6418	$MnSnO_3$-R	a=5.355,b=4.638,c=14.674	-2.77837
$AgTaO_3$-C	a=b=c=3.9993	-3.409	$MnSnO_3$-T	a=5.492,b=5.492,c=7.809	-2.73215
$AgTaO_3$-O	a=5.544,b=6.002,c=9.103	-3.98989	MnTiO3-T	a=5.492,b=5.492,c=7.809	-2.96744
MnTiO3-C	a=b=c=3.820	-2.88798	MnTiO3-R	a=5.511,b=4.669,c=4.348	-3.03535
$BaNbO_3$-O	a=5.819,b=5.820,c=8.308	-3.06098	$NaOsO_3$-C	a=b=c=3.877	-2.673
BaSnO3-C	a=b=c=4.125	-2.62801	$NaOsO_3$-O	a=5.391,b=5.431,c=7.653	-2.666
$BaSnO_3$-O	a=5.826,b=5.827,c=8.238	-2.62741	$NaOsO_3$-Trig	a=5.429,b=4.701,c=13.187	-2.647
$BaSnO_3$-R	a=5.690,b=4.928,c=17.336	-2.6052	$NaTaO_3$-C	a=b=c=4.008	-3.07331
$BaSnO_3$-T	a=5.841,b=5.841,c=8.224	-2.62765	$NaTaO_3$-T	a=5.566,b=5.620,c=7.921	-3.08139
$BaTiO_3$-C	a=b=c=4.482	-2.10246	$NiSnO_3$-C	a=b=c=3.767	-2.41431
$BaTiO_3$-T	a=4.003,b=4.003,c=4.199	-3.00279	$NiSnO_3$-O	a=5.367,b=5.229,c=7.660	-2.54846
$CaNbO_3$-C	a=b=c=4.021	-3.03918	$NiSnO_3$-T	a=5.495,b=5.495,c=7.565	-2.4698
$CaNbO_3$-O	a=5.520,b=5.676,c=7.932	-3.06056	$PbTiO_3$-C	a=b=c=3.960	-2.89245
$CaSnO_3$-C	a=b=c= 3.977	-2.2287	$CaSnO_3$-R	a= 5.453,b= 5.453,c= 15.187	-2.65349
$CaSnO_3$-O	a= 5.463,b=5.600,c=7.884	-2.65375	$CaSnO_3$-T	a= 5.547,b=5.547,c=7.911	-2.64205
$CaNbO_3$-T	a=5.578,b=5.578,c=4.042	-3.05462	$PbTiO_3$-T	a=3.849,b=3.849,c=4.629	-2.9025
$CdSnO_3$-C	a=b=c=3.977	-2.29175	$PrNbO_3$-C	a=b=c=4.056	-3.14219
$CdSnO_3$-O	a=5.463,b=5.600,c=7.884	-2.35864	$PrNbO_3$-O	a=5.833,b=5.734,c=7.988	-3.15619
$CdSnO_3$-R	a=5.453,b=4.723,c=15.187	-2.36544	$PrNbO_3$-T	a=5.581,b=5.581,c=4.211	-3.15809
$CdSnO_3$-T	a=5.547,b=5.547,c=7.911	-2.33707	$SrCrO_3$-C	a=b=c=3.821	-2.8868
$CeNiO_3$-O	a=5.243,b=6.493,c=6.990	-2.89911	$SrCrO_3$-H	a=5.465,b=4.733,c=13.333	-3.83352
$CoSnO_3$-C	a=b=c= 3.793	-2.34985	$SrHfO_3$-C	a=b=c=4.141	-3.30398
$CoSnO_3$-O	a=5.343,b=5.341,c=7.676	-2.57128	$SrHfO_3$-O(Cmcm)	a=8.182,b=8.270,c=8.229	-3.3081
$CoSnO_3$-R	a=5.280,b=4.572,c=14.198	-2.58095	$SrHfO_3$-O(Imma)	a=5.827,b=5.837,c=8.187	-3.31168
$CoSnO_3$-T	a=5.440,b=4.440,c=7.800	-2.50386	$SrHfO_3$-O(Pnma)	a=5.800,b=5.833,c=8.213	-3.31239
$EuHfO_3$-C	a=b=c= 4.106	-3.34513	$SrHfO_3$-T	a=4.138,b=4.138,c=4.147	-3.30397
$EuHfO_3$-O	a=5.559,b=6.118,c=7.704	-3.40063	SrMoO3-C	a=b=c=4.001	-2.97663
$EuHfO_3$-T	a=5.612,b=5.612,c=8.426	-3.38028	$SrMoO_3$-M	a=5.727,b=7.934,c=5.670	-2.97392
$EuNbO_3$-O(Imma)	a=5.992,b=5.517,c=7.887	-3.15449	$SrMoO_3$-O(Imma)	a=5.662,b=5.678,c=7.937	-2.97641
$EuNbO_3$-T	a=5.509,b=5.509,c=4.165	-3.14735	$SrMoO_3$-T	a=5.677,b=5.677,c=7.939	-2.97661
$EuZrO_3$-C	a=b=c=4.137	-3.11453	$SrNbO_3$-C	a=b=c=4.062	-3.04892
EuZrO3-O	a=5.605,b=6.108,c=7.785	-3.18827	$SrNbO_3$-O	a=5.709,b=5.712,c=8.148	-3.05182
$EuZrO_3$-T	a=5.648,b=5.648,c=8.464	-3.15694	$SrNbO_3$-T	a=5.712,b=5.712,c=4.087	-3.05092
$FeSnO_3$-C	a=b=c=3.944	-2.54068	$SrRuO_3$-C	a=b=c=3.956	-2.72338
$FeSnO_3$-O	a=5.365,b=5.405,c=7.711	-2.66128	$SrRuO_3$-O	a=5.580,b=5.618,c=7.889	-2.73147
$FeSnO_3$-R	a=5.337,b=4.576,c=14.489	-2.66816	$SrRuO_3$-T	a=5.593,b=5.593,c=7.887	-2.73058
$FeSnO_3$-T	a=5.472,b=5.472,c=7.713	-2.61383	$SrSnO_3$-C	a=b=c=4.038	-2.62636
$HgSnO_3$-C	a=b=c=4.029	-2.20568	$SrSnO_3$-O	a=5.710,b=5.701,c=8.061	-2.63118
$HgSnO_3$-O	a=5.577,b=5.626,c=7.997	-2.25823	$SrSnO_3$-T	a=5.666,b=5.666,c=8.181	-2.63035
$HgSnO_3$-T	a=5.638,b=5.638,c=7.931	-2.24854	$SrTcO_3$-C	a=b=c=3.961	-2.463

$KTaO_3$-C	a=b=c=4.031	-3.05692	$SrTcO_3$-O(Imma)	a=5.583,b=5.604,c=7.941	-3.462
$KTaO_3$-O	a=5.707,b=5.695,c=8.066	-3.05677	$SrTiO_3$-C	a=b=c=3.942	-3.00751
$LaAlO_3$-C	a=b=c=3.821	-2.99468	SrTiO3-O	a=5.573,b=5.575,c=7.881	-3.00689
$LaAlO_3$-H	a=4.755,b=4.119,c=6.537	-2.26354	$SrTiO_3$-R	a=5.573,b=5.573,c=5.573	-3.00702
$LaAlO_3$-O(Imma)	a=5.428,b=5.430,c=7.631	-2.95439	$SrTiO_3$-T	a=5.568,b=5.568,c=7.907	-3.00766
$LaAlO_3$-O(Cmcm)	a=7.158,b=12.434,c=10.289	-2.98019	$SrZrO_3$-C	a=b=c=4.175	-3.07009
$LaAlO_3$-T	a=5.384,b=5.384,c=7.784	-2.95762	$SrZrO_3$-O(Imma)	a=5.867,b=5.869,c= 8.231	-3.07993
$LaAlO_3$-Tric	a=7.281,b=7.682,c=8.442	-2.98166	$SrZrO_3$-O(Pnma)	a=5.819,b=5.885,c= 8.259	-2.97273
$LaAlO_3$-Trig	a=5.430,b=4.692,c=13.261	-2.97003	$SrZrO_3$-T	a=4.156,b=4.156,c=4.252	-3.07039
$LaCoO_3$-O	a=5.467,b=5.550,c=7.810	-2.75185	$TiSnO_3$-C	a=b=c=3.966	-2.76035
$LaCoO_3$-C	a=b=c=4.461	-2.12355	$TiSnO_3$-O	a=5.511,b=5.533,c=7.676	-2.72487
$LaCoO_3$-M	a=6.551,b=5.092,c=4.711	-2.69256	$TiSnO_3$-R	a=5.161,b=5.161,c=21.244	-2.80835
$LaCoO_3$-T	a=5.391,b=5.391,c=7.682	-2.73486	$TiSnO_3$-T	a=5.797,b=5.548,c=7.947	-2.7643
$LaCrO_3$-O	a=5.483,b=5.466,c=7.763	-3.09579	$VSnO_3$-C	a=b=c=3.908	-2.66184
LaCrO3-Trig	a=5.496,b=4.760,c=13.292	-3.0959	$VSnO_3$-O	a=5.347,b=5.557,c=7.710	-2.73003
$LaCuO_3$-Trig	a=5.565,b=4.819,c=13.199	-3.297	$VSnO_3$-R	a=5.106,b=5.091,c= 20.244	-2.71488
$LaCuO_3$-C	a=b=c=3.872	-3.268	$LaFeO_3$-C	a=b=c=3.830	-2.77208
$LaGaO_3$-C	a=b=c=3.935	-2.78937	$VSnO_3$-T	a=5.336,b=5.553,c=7.700	-2.71761
$LaGaO_3$-O(Imma)	a=5.564,b=5.622,c=7.884	-2.80447	YCoO3-C	a=b=c=3.735	-3.431
$LaScO_3$-C	a=b=c=4.083	-3.13486	$YCoO_3$-H	a=3.498,b=3.498,c=11.493	-3.556
$LaScO_3$-O(Pbnm)	a=5.720,b=5.849,c=8.182	-3.18157	$YCoO_3$-O	a=5.154,b=5.524,c=7.389	-3.661
$LaScO_3$-O(Pnma)	a=5.719,b=5.853,c=8.161	-3.18167	$YCoO_3$-Trig	a=5.146,b=5.528,c=7.391	-3.65
$LaTiO_3$-C	a=b=c=3.959	-3.17187	$YCrO_3$-C	a=b=c=3.774	-2.908
$LaTiO_3$-O(Pbnm)	a=5.631,b=5.621,c=7.954	-3.17977	$YCrO_3$-H	a=3.498,b=3.498,c=11.493	-3.032
$LaTiO_3$-O(Pnma)	a=5.584,b=5.679,c=7.950	-3.18063	$YCrO_3$-O(Pnma)	a=5.180,b=5.577,c=7.476	-3.212
$LaVO_3$-C	a=b=c=3.998	-3.14085	$YFeO_3$-C	a=b=c=3.736	-2.603
$LaVO_3$-O(Pbnm)	a=5.548,b=7.795,c=5.532	-3.14304	$YFeO_3$-H	a=3.498,b=3.498,c=11.493	-2.935
$LiTaO_3$-C	a=b=c=3.966	-3.07331	$YFeO_3$-O	a=5.148,b=5.520,c=7.407	-2.932
$LiTaO_3$-O	a=4.752,b=5.120,c=8.836	-3.08139	$YTiO_3$-C	a=b=c=3.893	-3.576
$LiTaO_3$-T	a=5.430,b=5.430,c=3.944	-3.08729	$YTiO_3$-H	a=6.073,b=6.073,c=11.997	-3.624
$MgSnO_3$-C	a=b=c=3.940	-2.45401	$YTiO_3$-O	a=5.328,b=5.688,c=7.690	-3.166
$MgSnO_3$-O	a=5.255,b=5.398,c=7.701	-2.57542	YVO_3-O	a=5.235,b=5.629,c=7.559	-3.28
$MgSnO_3$-T	a=5.465,b=5.465,c=7.733	-2.51587	YVO_3-T	a=3.819,b=3.819,c=3.819	-2.927
$ZnSnO_3$-C	a=b=c=3.940	-2.26759	$ZnSnO_3$-T	a=5.510,b=5.510,c=7.592	-1.34911
$ZnSnO_3$-O	a=5.265,b=5.314,c=7.767	-2.41496	YVO_3-H	a=3.449,b=3.449,c=12.143	-3.126

Table S2. Bandgap (indirect gap or direct gap) E_g and the average solar absorptivity (α_S) of 76 kinds of ABO_3 perovskites.

	Bandgap (E_g)	Type of Bandgap	Solar absorption		Bandgap (E_g)	Type of Bandgap	Solar absorption
$AgNbO_3$-O(Pmc21)	2.902	Indirect gap	0.63122	$MgTiO_3$-C	2.901	Direct gap	0.48575
$AgNbO_3$-C	2.801	Indirect gap	0.41192	$MgTiO_3$-O	3.701	Direct gap	0.209
$AgNbO_3$-O(Cmcm)	2.001	Indirect gap	0.68974	$MnSnO_3$-C	1.9	Indirect gap	0.62177
$AgNbO_3$-O(Pbcm)	3.002	Indirect gap	0.63589	$MnSnO_3$-O	2.403	Direct gap	0.42518
$AgNbO_3$-Te	2.401	Direct gap	0.62326	$MnSnO_3$-R	2.99	Direct gap	0.43699
$AgTaO_3$-C	3.601	Indirect gap	0.40332	$MnSnO_3$-T	1.903	Direct gap	0.68203
$AgTaO_3$-O	3.467	Indirect gap	0.46679	MnTiO3-T	2.087	Direct gap	0.16445
MnTiO3-C	2.3694	Indirect gap	0.12480	MnTiO3-R	2.4825	Direct gap	0.49614
$BaNbO_3$-O	2.901	Indirect gap	0.41103	$NaOsO_3$-C	0.8	Indirect gap	0.77864
BaSnO3-C	1.501	Indirect gap	0.58523	$NaOsO_3$-O	0.12	Indirect gap	0.77804
$BaSnO_3$-O	2.1	Direct gap	0.61152	$NaOsO_3$-Trig	0.04	Indirect gap	0.11142
$BaSnO_3$-R	2.001	Direct gap	0.60561	$NaTaO_3$-C	3.4712	Indirect gap	0.37696
$BaSnO_3$-T	2.601	Direct gap	0.66139	$NaTaO_3$-T	3.491	Indirect gap	0.36525
$BaTiO_3$-C	3.201	Direct gap	0.19601	$NiSnO_3$-C	3.703	Indirect gap	0.27575
$BaTiO_3$-T	3.402	Direct gap	0.29145	$NiSnO_3$-O	3.903	Direct gap	0.20186
$CaNbO_3$-C	4.13	Indirect gap	0.13759	$NiSnO_3$-T	3.603	Indirect gap	0.21212
$CaNbO_3$-O	4.302	Direct gap	0.18585	$PbTiO_3$-C	3.403	Indirect gap	0.27806
$CaNbO_3$-T	4.201	Indirect gap	0.23505	$PbTiO_3$-T	3.301	Indirect gap	0.30568
$CaSnO_3$-C	2.16	Indirect gap	0.64320	$CaSnO_3$-R	3.03	Direct gap	0.95321
$CaSnO_3$-O	2.83	Direct gap	0.93763	$CaSnO_3$-T	2.33	Direct gap	0.63689
$CdSnO_3$-C	2.802	Indirect gap	0.68513	$PrNbO_3$-C	3.602	Direct gap	0.27958
$CdSnO_3$-O	3.02	Direct gap	0.30635	$PrNbO_3$-O	3.902	Direct gap	0.27161
$CdSnO_3$-R	2.957	Indirect gap	0.31586	$PrNbO_3$-T	3.401	Direct gap	0.31951
$CdSnO_3$-T	2.901	Direct gap	0.3017	$SrCrO_3$-C	2.3288	Direct gap	0.50093
$CeNiO_3$-O	1.703	Indirect gap	0.39177	$SrCrO_3$-H	2.3239	Direct gap	0.51435
$CoSnO_3$-C	2.93	Direct gap	0.73781	$SrHfO_3$-C	5.903	Indirect gap	0.16496
$CoSnO_3$-O	2.876	Direct gap	0.31561	$SrHfO_3$-O(Cmcm)	6.103	Indirect gap	0.13332
$CoSnO_3$-R	2.702	Direct gap	0.31564	$SrHfO_3$-O(Imma)	6.101	Indirect gap	0.13317
$CoSnO_3$-T	2.801	Direct gap	0.28874	$SrHfO_3$-O(Pnma)	6.101	Indirect gap	0.13164
$EuHfO_3$-C	2.5619	Direct gap	0.20503	$SrHfO_3$-T	6.003	Indirect gap	0.16281
$EuHfO_3$-O	4.5469	Direct gap	0.10976	SrMoO3-C	1.909	Indirect gap	0.46023
$EuHfO_3$-T	4.0426	Direct gap	0.16003	$SrMoO_3$-M	1.906	Indirect gap	0.4625
$EuNbO_3$-O(Imma)	0.801	Direct gap	0.85015	$SrMoO_3$-O(Imma)	2.001	Indirect gap	0.46431
$EuNbO_3$-T	0.603	Indirect gap	0.76682	$SrMoO_3$-T	2.003	Indirect gap	0.46201
$EuZrO_3$-C	2.513	Direct gap	0.41664	$SrNbO_3$-C	4.202	Indirect gap	0.16777
EuZrO3-O	2.402	Direct gap	0.42632	$SrNbO_3$-O	4.102	Direct gap	0.14598
$EuZrO_3$-T	2.957	Direct gap	0.35886	$SrNbO_3$-T	4.152	Indirect gap	0.12392
$FeSnO_3$-C	0.1	Indirect gap	0.31318	$SrRuO_3$-C	0.4	Indirect gap	0.70673
$FeSnO_3$-O	1.903	Indirect gap	0.79484	$SrRuO_3$-O	0.6	Direct gap	0.70114
$FeSnO_3$-R	2.09	Indirect gap	0.74697	$SrRuO_3$-T	0.52	Direct gap	0.6952

$FeSnO_3$-T	1.67	Indirect gap	0.83603	$SrSnO_3$-C	4.102	Indirect gap	0.34863
$HgSnO_3$-C	1.49	Indirect gap	0.85225	$SrSnO_3$-O	4.002	Direct gap	0.34729
$HgSnO_3$-O	1.622	Direct gap	0.78759	$SrSnO_3$-T	3.902	Direct gap	0.34538
$HgSnO_3$-T	1.506	Direct gap	0.79504	$SrTcO_3$-C	0.7	Indirect gap	0.74134
$KTaO_3$-C	3.2632	Indirect gap	0.42122	$SrTcO_3$-O(Imma)	1.7	Indirect gap	0.70477
$KTaO_3$-O	3.2565	Direct gap	0.42084	$SrTiO_3$-C	3.439	Indirect gap	0.37509
$LaAlO_3$-C	4.702	Indirect gap	0.26144	SrTiO3-O	3.202	Direct gap	0.3688
$LaAlO_3$-H	1.701	Indirect gap	0.66519	$SrTiO_3$-R	3.242	Direct gap	0.3664
$LaAlO_3$-O(Imma)	6.003	Direct gap	0.13001	$SrTiO_3$-T	3.152	Direct gap	0.36895
$LaAlO_3$-O(Cmcm)	5.602	Direct gap	0.12928	$SrZrO_3$-C	5.403	Indirect gap	0.23758
$LaAlO_3$-T	4.502	Direct gap	0.33014	$SrZrO_3$-O(Imma)	5.603	Direct gap	0.29905
$LaAlO_3$-Tric	5.703	Indirect gap	0.14191	$SrZrO_3$-O(Pnma)	5.603	Direct gap	0.29616
$LaAlO_3$-Trig	4.702	Indirect gap	0.29115	$SrZrO_3$-T	5.503	Indirect gap	0.20103
$LaCoO_3$-O	0.53	Direct gap	0.73586	$TiSnO_3$-C	2.451	Indirect gap	0.67858
$LaCoO_3$-C	1.2	Indirect gap	0.64196	$TiSnO_3$-O	1.801	Direct gap	0.68789
$LaCoO_3$-M	0.403	Indirect gap	0.69477	$TiSnO_3$-R	1.701	Indirect gap	0.66412
$LaCoO_3$-T	0.5	Indirect gap	0.71563	$TiSnO_3$-T	2.601	Indirect gap	0.67363
$LaCrO_3$-O	3.325	Direct gap	0.71188	$VSnO_3$-C	0.8	Indirect gap	0.85615
LaCrO3-Trig	3.3041	Direct gap	0.66982	$VSnO_3$-O	0.6	Direct gap	0.78433
$LaCuO_3$-Trig	0.3	Direct gap	0.68003	$VSnO_3$-R	1	Indirect gap	0.86672
$LaGaO_3$-C	4.602	Indirect gap	0.22485	$VSnO_3$-T	0.5	Direct gap	0.88506
$LaGaO_3$-O(Imma)	4.703	Indirect gap	0.2778	YCoO3-C	2.301	Indirect gap	0.43828
$LaScO_3$-C	5.403	Direct gap	0.13726	$YCoO_3$-H	2.601	Indirect gap	0.46133
$LaScO_3$-O(Pbnm)	5.803	Direct gap	0.29375	$YCoO_3$-O	2.701	Direct gap	0.52939
$LaScO_3$-O(Pnma)	5.703	Direct gap	0.29389	$YCoO_3$-Trig	2.751	Direct gap	0.50459
$LaTiO_3$-C	0.001	Direct gap	0.01298	$YCrO_3$-C	2.001	Indirect gap	0.58541
$LaTiO_3$-O(Pbnm)	0.7	Direct gap	0.75572	$YCrO_3$-H	1.1	Indirect gap	0.74647
$LaTiO_3$-O(Pnma)	1.2	Direct gap	0.888	$YCrO_3$-O(Pnma)	1.7	Direct gap	0.71199
$LaVO_3$-C	0.6576	Indirect gap	0.82134	$YFeO_3$-C	1.3	Indirect gap	0.71008
$LaVO_3$-O(Pbnm)	1.0997	Direct gap	0.76444	$YFeO_3$-H	0.3	Indirect gap	0.81992
$LiTaO_3$-C	3.1804	Indirect gap	0.30298	$YFeO_3$-O	1.2	Indirect gap	0.71369
$LiTaO_3$-O	3.0795	Indirect gap	0.31805	$YTiO_3$-C	4.102	Indirect gap	0.20153
$LiTaO_3$-T	3.6154	Indirect gap	0.27185	$YTiO_3$-H	4.203	Indirect gap	0.27712
$MgSnO_3$-C	3.007	Indirect gap	0.4982	$YTiO_3$-O	3.102	Indirect gap	0.33455
$MgSnO_3$-O	4.03	Indirect gap	0.36323	YVO_3-O	2.601	Indirect gap	0.46821
$MgSnO_3$-T	3.795	Indirect gap	0.35108	YVO_3-T	2.49875	Indirect gap	0.54444
$ZnSnO_3$-C	3.901	Direct gap	0.42336	$ZnSnO_3$-T	4.101	Direct gap	0.22804
$ZnSnO_3$-O	4.201	Direct gap	0.22054	YVO_3-H	2.702	Indirect gap	0.4283