

## Unraveling the relationships between chemical bonding and thermoelectric properties: n-type $ABO_3$ perovskites

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**Table S1.** The lattice parameter, band gaps ( $E_g$ ), density of states (DOS) at conduction band minima (CBM) +0.1 eV, deformation potential  $E_{\text{def}}$  (eV), and the coefficient of determination  $R^2$  of the 46 compounds.

	Composition	Lattice Parameter (Å)	$E_g$ (eV)	DOS (a.u.)	$E_{\text{def}}$ (eV)	$R^2$
1	SrHfO <sub>3</sub>	4.14	5.22	0.27	1.55	1.00
2	EuHfO <sub>3</sub>	4.09	5.33	0.24	2.96	1.00
3	CaZrO <sub>3</sub>	4.14	4.28	0.33	4.36	1.00
4	SrZrO <sub>3</sub>	4.18	4.29	0.38	43.83	0.23
5	EuZrO <sub>3</sub>	4.13	4.40	0.34	4.30	1.00
6	KTaO <sub>3</sub>	4.04	3.69	0.52	2.29	1.00
7	NaTaO <sub>3</sub>	3.99	4.00	0.55	2.06	0.94
8	RbTaO <sub>3</sub>	4.08	3.48	0.52	2.61	0.95

9	TiTaO <sub>3</sub>	4.09	1.50	0.68	0.85	0.25
10	AgNbO <sub>3</sub>	4.00	2.50	0.58	6.14	0.7
11	NaNbO <sub>3</sub>	3.98	2.73	0.56	2.30	0.99
12	KNbO <sub>3</sub>	4.03	2.50	0.56	-0.11	0
13	TiNbO <sub>3</sub>	4.09	0.42	0.67	62.49	0.32
14	SrTiO <sub>3</sub>	3.97	3.13	0.82	9.08	0.62
15	SnTiO <sub>3</sub>	3.97	1.82	1.04	1.99	1.00
16	PbTiO <sub>3</sub>	4.00	2.64	1.17	1.74	0.99
17	CaTiO <sub>3</sub>	3.92	3.26	0.73	2.50	1.00
18	EuTiO <sub>3</sub>	3.91	3.31	0.69	2.67	0.04
19	YbTiO <sub>3</sub>	3.88	3.43	0.72	2.65	1.00
20	PbHfO <sub>3</sub>	4.15	3.58	0.1	2.01	1.00
21	PbZrO <sub>3</sub>	4.19	3.54	0.1	3.29	0.93
22	BiAlO <sub>3</sub>	3.79	2.63	0.05	-1.07	0.93
23	BiGaO <sub>3</sub>	3.85	2.46	0.05	-0.92	0.92
24	BiInO <sub>3</sub>	4.15	1.05	0.08	-0.73	0.57
25	BiScO <sub>3</sub>	4.11	1.43	0.06	3.37	1.00
26	EuGeO <sub>3</sub>	3.77	2.90	0.02	-10.66	1.00
27	PbGeO <sub>3</sub>	3.90	0.84	0.02	-9.28	1.00
28	SrGeO <sub>3</sub>	3.86	1.92	0.02	-9.84	1.00
29	YbGeO <sub>3</sub>	3.74	3.39	0.02	-11.15	1.00
30	CaSiO <sub>3</sub>	3.61	4.74	0.02	-12.29	1.00
31	SnSiO <sub>3</sub>	3.70	1.09	0.02	-11.71	1.00
32	SrSiO <sub>3</sub>	3.69	3.68	0.02	-11.36	1.00

33	EuSiO <sub>3</sub>	3.61	4.69	0.02	-22.49	1.00
34	PbSiO <sub>3</sub>	3.75	1.83	0.02	-20.38	1.00
35	CaSnO <sub>3</sub>	3.99	4.32	0.03	-8.27	0.88
36	EuSnO <sub>3</sub>	3.98	4.57	0.02	-13.97	1.00
37	PbSnO <sub>3</sub>	4.06	3.64	0.03	-12.69	1.00
38	SrSnO <sub>3</sub>	4.04	3.80	0.02	-10.62	1.00
39	BaSnO <sub>3</sub>	4.13	0.94	0.01	-9.33	1.00
40	NdGaO <sub>3</sub>	3.83	4.06	0.09	3.32	1.00
41	PrGaO <sub>3</sub>	3.84	4.03	0.09	3.29	1.00
42	SmGaO <sub>3</sub>	3.80	4.20	0.09	3.34	1.00
43	DyAlO <sub>3</sub>	3.71	4.61	0.09	0.011	0.01
44	NdAlO <sub>3</sub>	3.77	4.13	0.08	3.31	1.00
45	PrAlO <sub>3</sub>	3.80	4.09	0.08	3.23	1.00
46	LaAlO <sub>3</sub>	3.83	3.12	0.07	2.91	1.00

**Table S2.** The Young's modulus ( $G$ ), lattice thermal conductivity ( $\kappa_L$ ),  $ZT_{max}$ , carrier concentrations  $n$ , electrical conductivity ( $\sigma$ ), and Seebeck coefficients ( $S$ ) of the 46 compounds at 700 K.

Composition	Young's modulus $G$ (GPa)	$\kappa_L$ (W/mK)	$ZT_{max}$	$n$ ( $10^{20}$ cm <sup>-3</sup> )	$\sigma$ (S/m)	$S$ ( $\mu$ V/K)
SrHfO <sub>3</sub>	250.59	13.28	0.37	2.45	233428.91	-191.72
EuHfO <sub>3</sub>	256.83	13.43	0.36	2.30	233753.64	-191.84
CaZrO <sub>3</sub>	213.69	11.53	0.32	3.26	184653.90	-187.40
SrZrO <sub>3</sub>	226.04	13.34	0.38	3.39	249419.19	-191.77

EuZrO <sub>3</sub>	230.62	11.07	0.46	2.81	232863.31	-199.79
KTaO <sub>3</sub>	302.16	21.31	0.52	4.30	474028.37	-205.73
NaTaO <sub>3</sub>	281.84	15.21	0.72	3.89	416043.56	-222.03
RbTaO <sub>3</sub>	297.99	26.44	0.42	4.66	504262.48	-196.76
TlTaO <sub>3</sub>	267.20	11.03	0.78	3.87	306974.73	-227.34
AgNbO <sub>3</sub>	215.81	6.66	0.96	3.29	220389.72	-237.10
NaNbO <sub>3</sub>	262.49	16.53	0.70	3.89	432490.82	-222.24
KNbO <sub>3</sub>	281.84	23.04	0.52	4.35	487882.69	-209.40
TiNbO <sub>3</sub>	244.68	10.43	0.83	3.65	304976.31	-230.39
SrTiO <sub>3</sub>	270.33	18.58	0.40	7.54	334971.79	-196.83
SnTiO <sub>3</sub>	222.31	9.02	0.65	6.75	217452.55	-219.94
PbTiO <sub>3</sub>	233.33	9.34	0.69	6.93	232877.94	-221.82
CaTiO <sub>3</sub>	259.84	19.39	0.32	7.87	297336.90	-187.73
EuTiO <sub>3</sub>	289.89	20.86	0.39	7.12	381912.11	-194.07
YbTiO <sub>3</sub>	278.52	16.28	0.50	6.65	350063.88	-204.59
PbHfO <sub>3</sub>	223.87	7.92	0.51	0.77	176521.06	-205.83
PbZrO <sub>3</sub>	200.75	7.13	0.48	0.83	152049.09	-203.03
BiAlO <sub>3</sub>	290.30	14.44	0.36	0.59	253503.67	-190.72
BiGaO <sub>3</sub>	227.24	8.02	0.46	0.54	165844.00	-200.81
BiInO <sub>3</sub>	143.96	2.92	0.66	0.49	78634.59	-219.06
BiScO <sub>3</sub>	367.50	8.57	0.53	0.45	195848.10	-207.84
EuGeO <sub>3</sub>	322.84	23.86	0.01	0.47	17926.02	-134.08
PbGeO <sub>3</sub>	245.07	11.14	0.01	0.38	9730.26	-133.14
SrGeO <sub>3</sub>	277.07	23.50	0.01	0.39	12724.63	-133.26

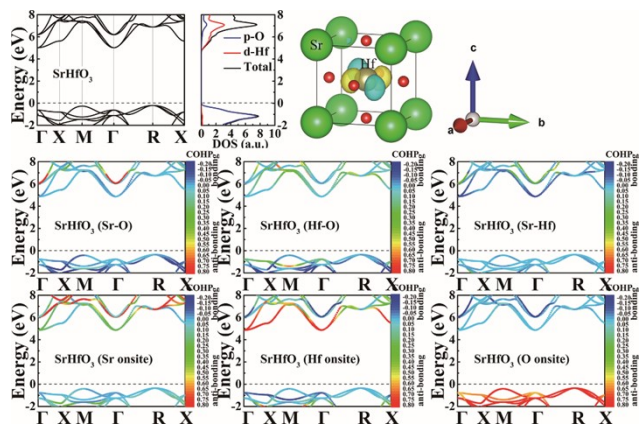
YbGeO <sub>3</sub>	318.29	19.64	0.01	0.50	19689.00	-135.79
CaSiO <sub>3</sub>	365.32	35.55	0.01	0.67	16186.06	-136.68
SnSiO <sub>3</sub>	294.23	15.32	0.01	0.61	15562.07	-134.86
SrSiO <sub>3</sub>	346.23	30.90	0.01	0.58	20534.92	-136.00
EuSiO <sub>3</sub>	421.75	37.25	0.01	0.65	27906.13	-137.73
PbSiO <sub>3</sub>	291.81	13.26	0.01	0.57	15410.93	-134.50
CaSnO <sub>3</sub>	210.88	10.95	0.01	0.56	8603.92	-136.41
EuSnO <sub>3</sub>	234.69	11.16	0.01	0.54	11894.26	-138.11
PbSnO <sub>3</sub>	202.97	7.95	0.02	0.69	10608.51	-133.38
SrSnO <sub>3</sub>	217.99	12.82	0.01	0.50	10821.88	-137.12
BaSnO <sub>3</sub>	219.68	14.06	0.01	0.23	7528.25	-135.98
NdGaO <sub>3</sub>	263.43	12.89	0.17	1.41	126406.88	-167.56
PrGaO <sub>3</sub>	263.35	13.25	0.17	1.38	128851.64	-167.13
SmGaO <sub>3</sub>	261.75	12.33	0.17	1.46	122732.81	-168.79
DyAlO <sub>3</sub>	344.74	24.10	0.13	1.65	192951.90	-162.45
NdAlO <sub>3</sub>	337.76	25.89	0.12	1.49	186751.64	-159.42
PrAlO <sub>3</sub>	333.63	25.40	0.12	1.45	186283.27	-159.75
LaAlO <sub>3</sub>	317.62	23.30	0.13	1.21	184365.77	-160.28

Table S3. The band gaps in this work calculated with mBJ+U ( $E_{g\text{-mBJ+U}}$ ), PBE+U ( $E_{g\text{-PBE+U}}$ ), and experimental band gaps of cubic ABO<sub>3</sub> ( $E_{g\text{-exp.}}$ ).

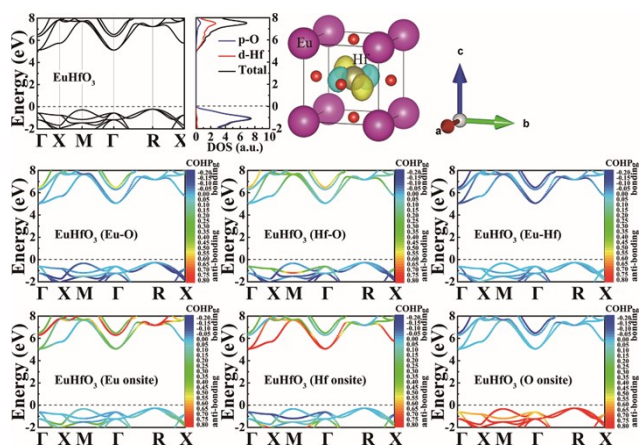
Compound	$E_{g\text{-mBJ+U}}$ (eV)	$E_{g\text{-PBE+U}}$ (eV)	$E_{g\text{-exp.}}$ (eV)
KTaO <sub>3</sub>	3.69	2.33	3.64 <sup>1</sup>
NaTaO <sub>3</sub>	4.00	2.51	~4.00 <sup>2</sup>
AgNbO <sub>3</sub>	2.50	1.82	2.78 <sup>3</sup>
SrTiO <sub>3</sub>	3.13	2.32	3.22 <sup>4</sup>
PrAlO <sub>3</sub>	4.09	2.89	3.19 <sup>5</sup>

**Fig. S1.** The electronic structures, DOS, wave functions, and band-resolved COHPs for 46 compounds.

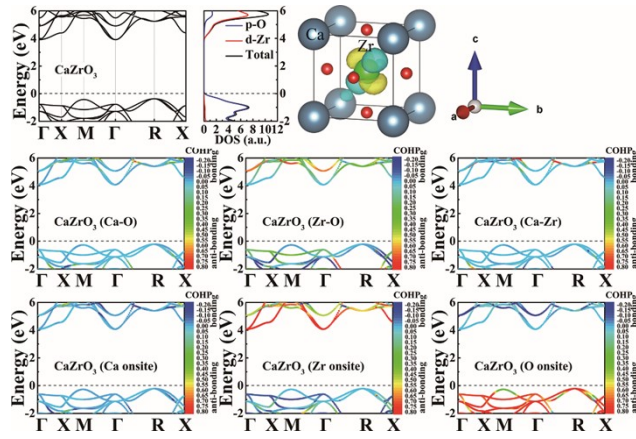
1. SrHfO<sub>3</sub>



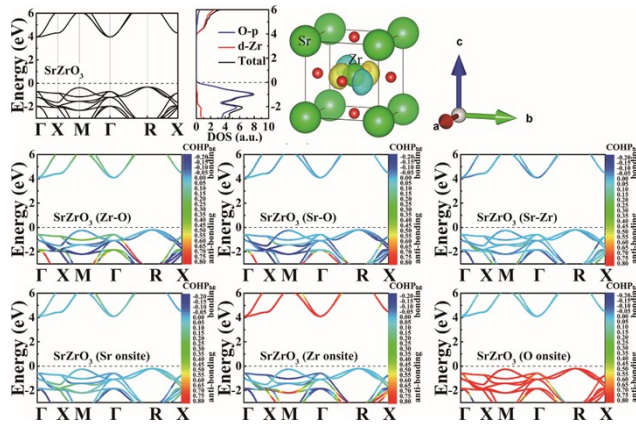
2. EuHfO<sub>3</sub>



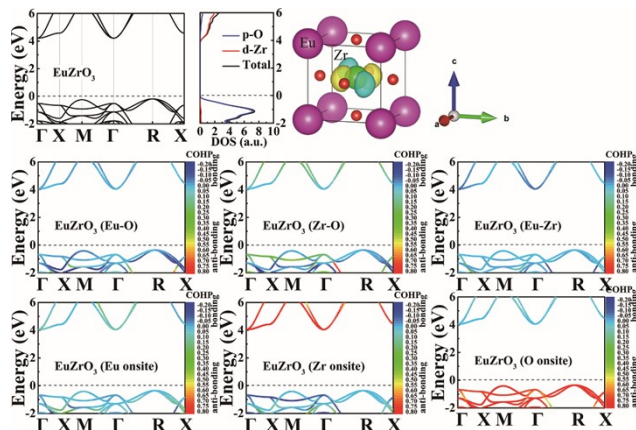
### 3. CaZrO<sub>3</sub>



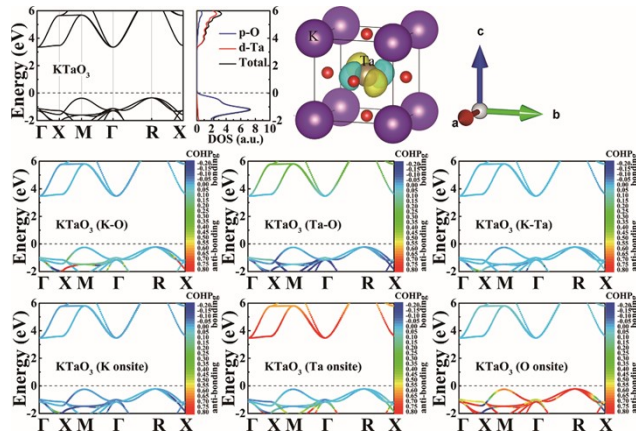
### 4. SrZrO<sub>3</sub>



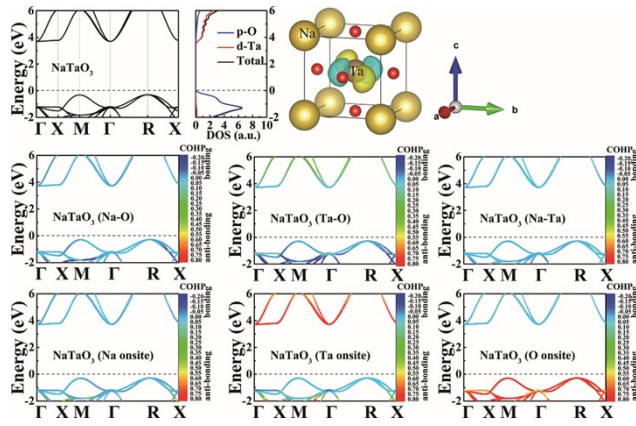
### 5. EuZrO<sub>3</sub>



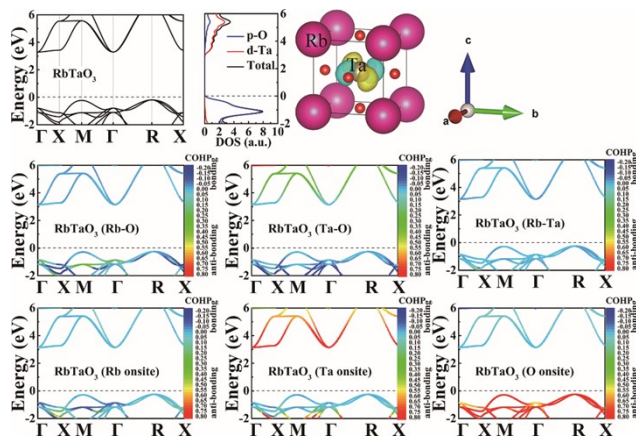
## 6. $\text{KTaO}_3$



## 7. $\text{NaTaO}_3$

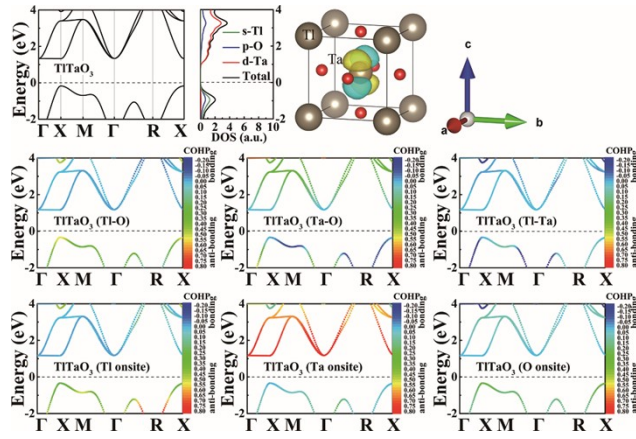


## 8. $\text{RbTaO}_3$

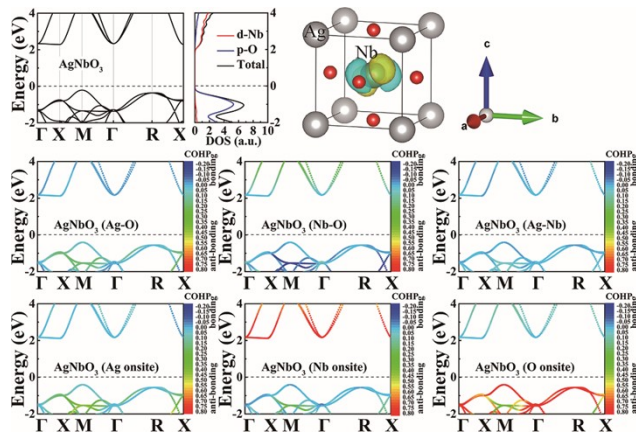




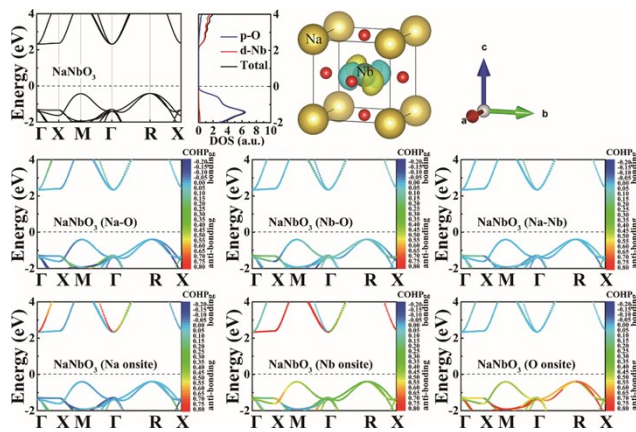
## 9. $\text{TiTaO}_3$



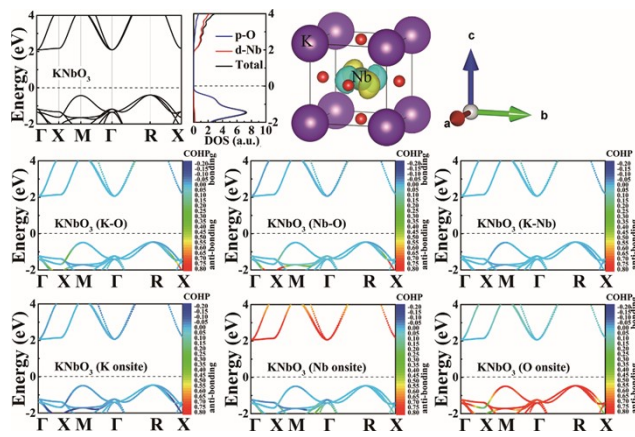
## 10. $\text{AgNbO}_3$



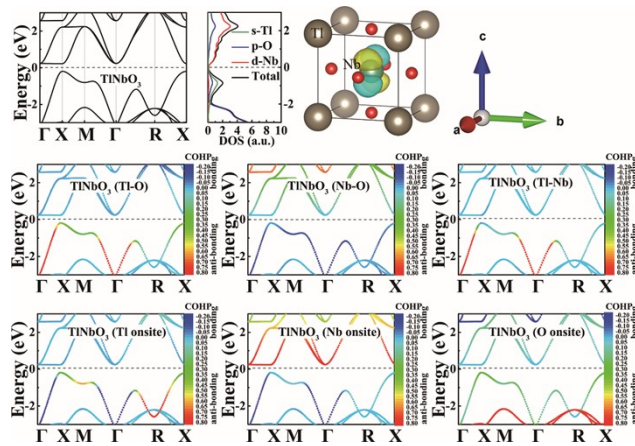
## 11. $\text{NaNbO}_3$



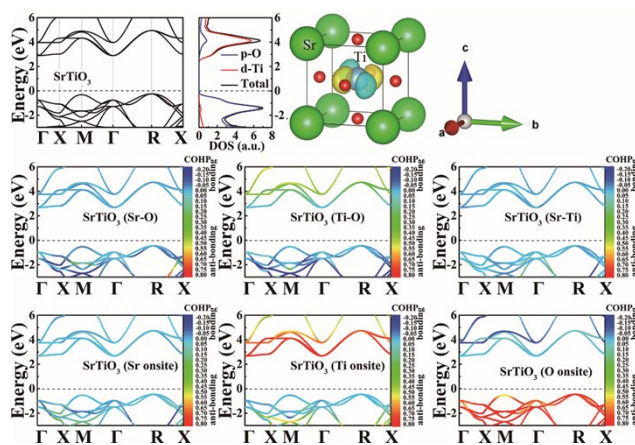
## 12. KNbO<sub>3</sub>



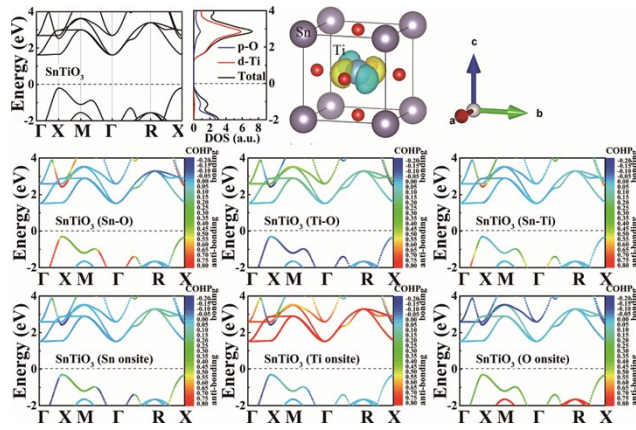
## 13. TiNbO<sub>3</sub>



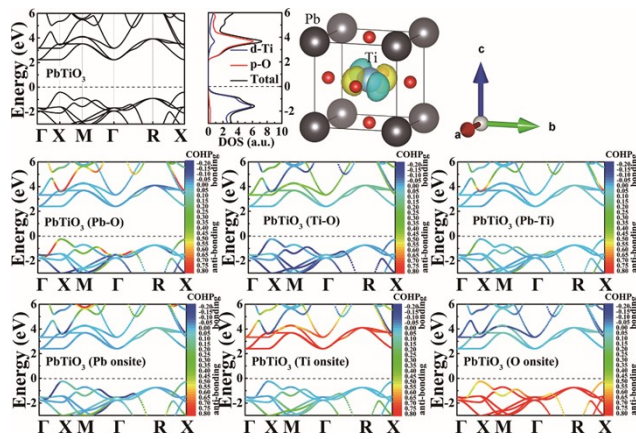
## 14. SrTiO<sub>3</sub>



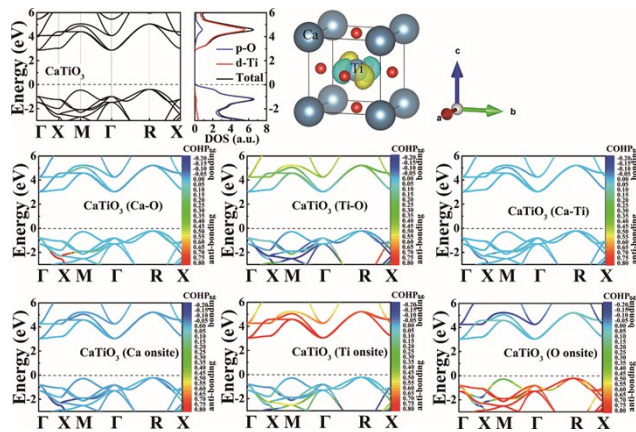
### 15. SnTiO<sub>3</sub>



### 16. PbTiO<sub>3</sub>

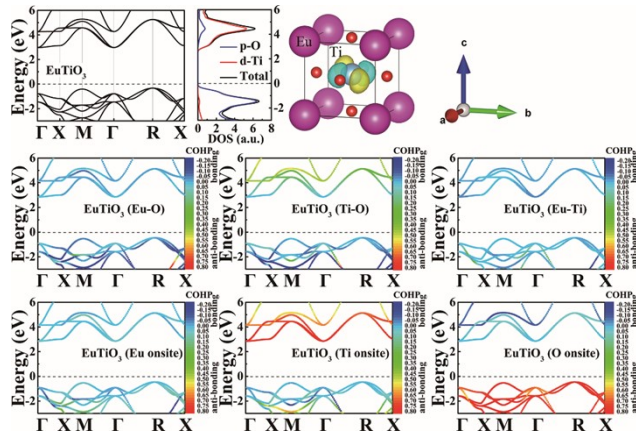


### 17. CaTiO<sub>3</sub>

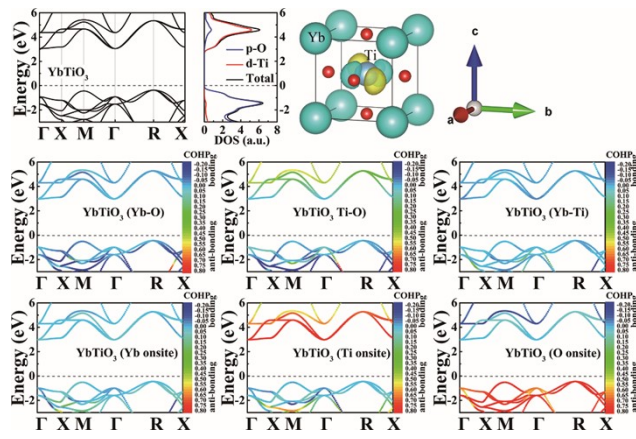




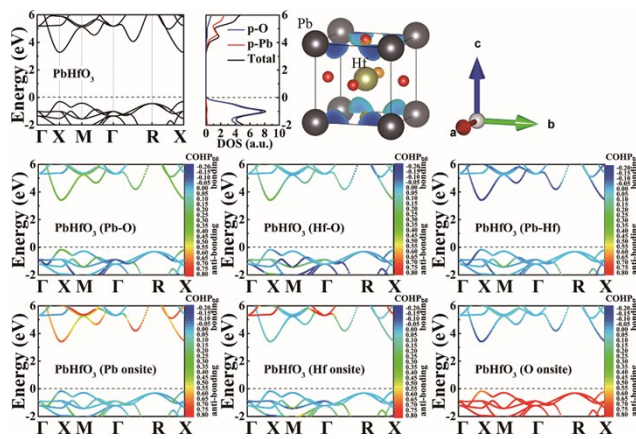
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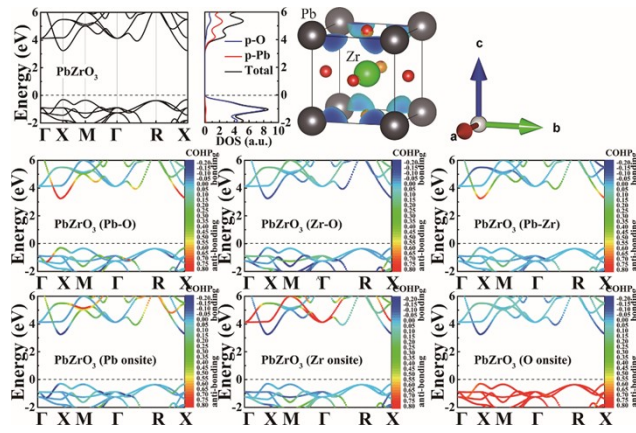
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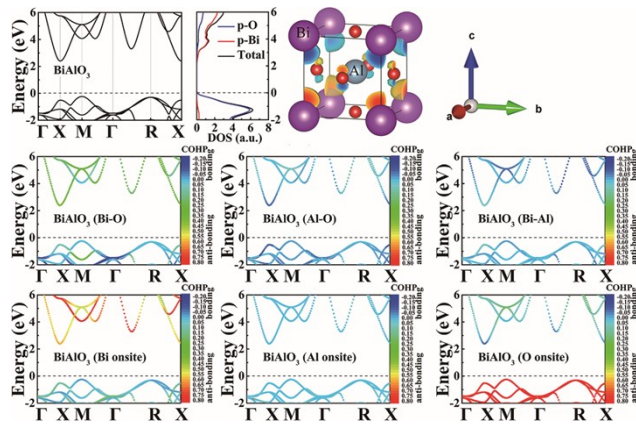
### 20. $\text{PbHfO}_3$



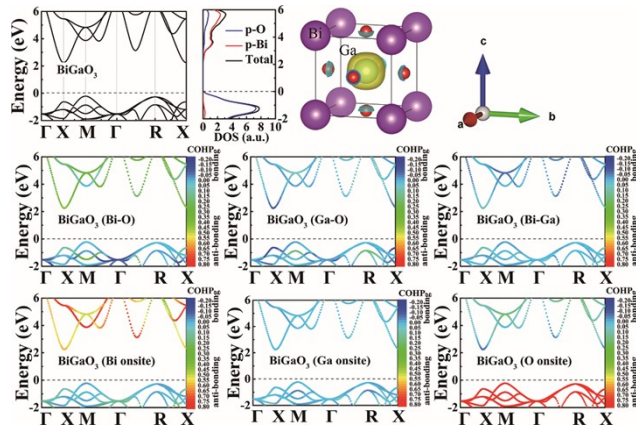
## 21. PbZrO<sub>3</sub>



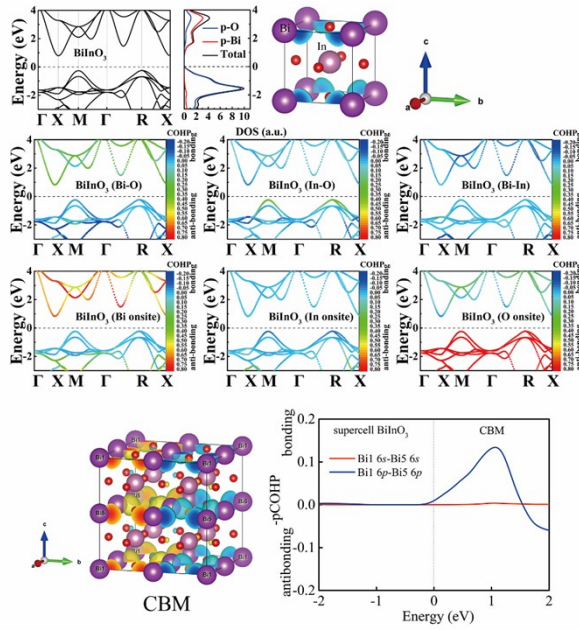
## 22. BiAlO<sub>3</sub>



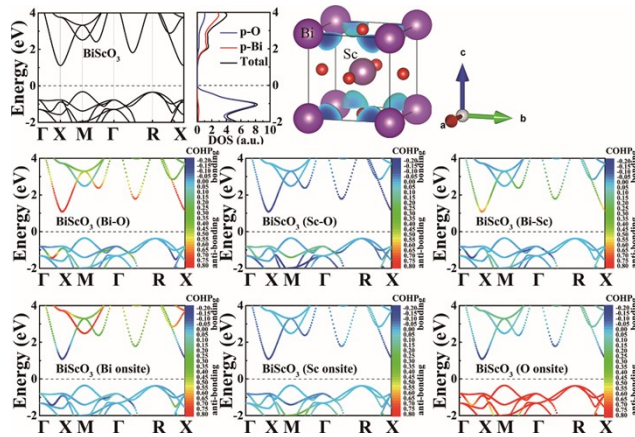
## 23. BiGaO<sub>3</sub>



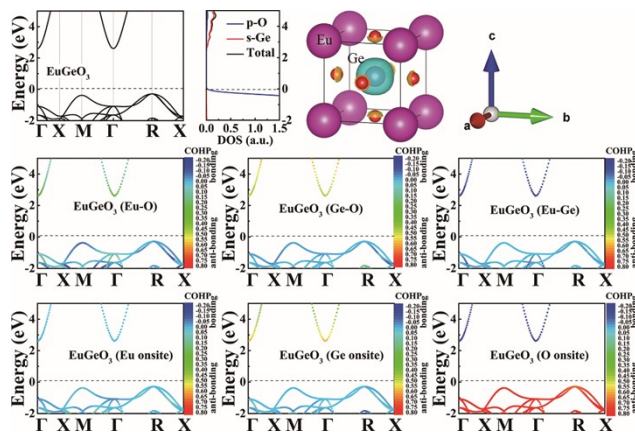
## 24. BiInO<sub>3</sub>



## 25. BiScO<sub>3</sub>

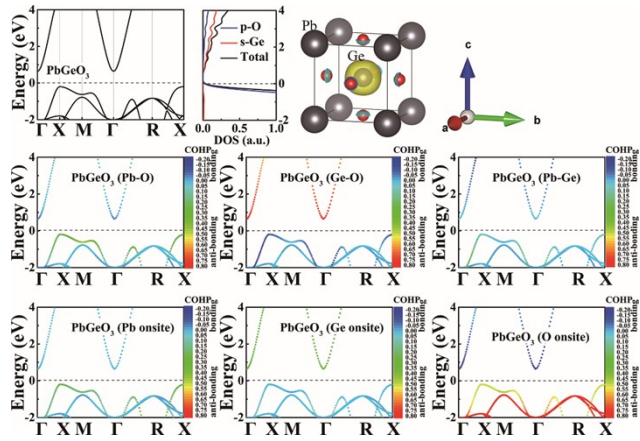


## 26. EuGeO<sub>3</sub>

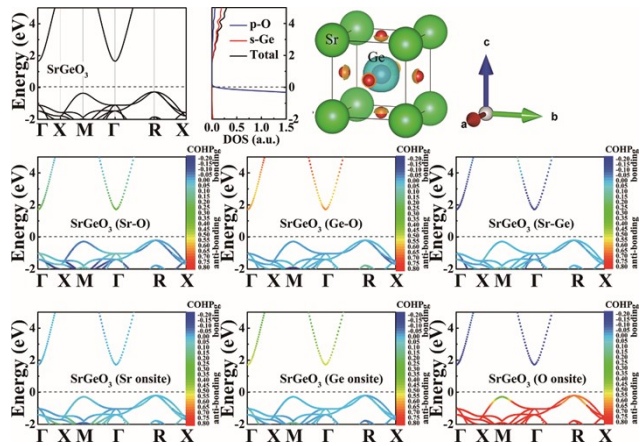




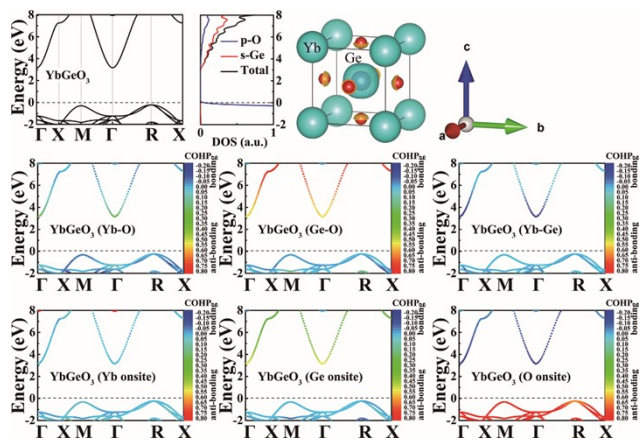
### 27. $\text{PbGeO}_3$



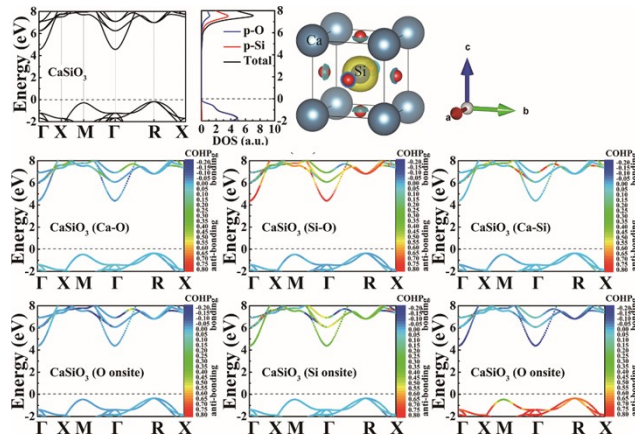
### 28. $\text{SrGeO}_3$



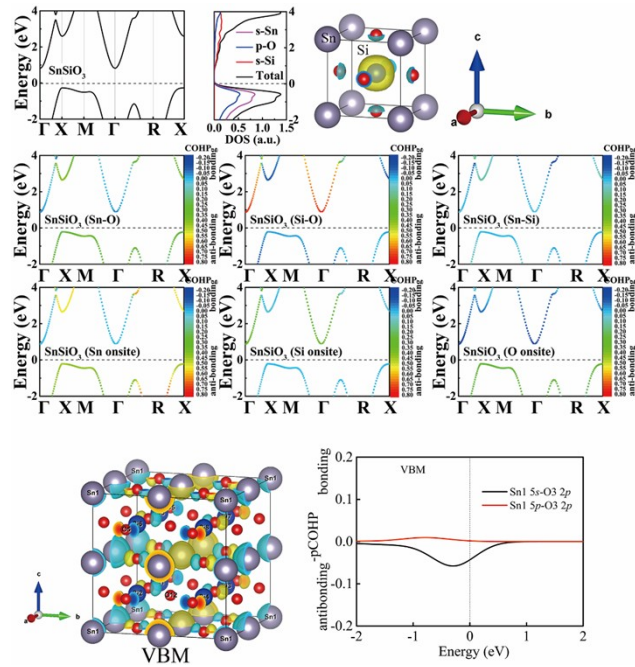
### 29. $\text{YbGeO}_3$



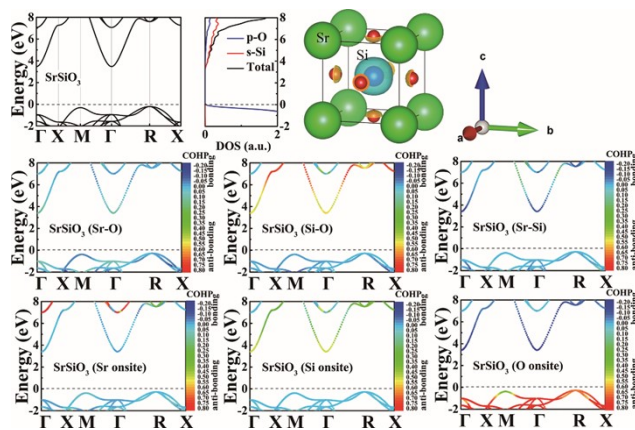
### 30. CaSiO<sub>3</sub>



### 31. SnSiO<sub>3</sub>

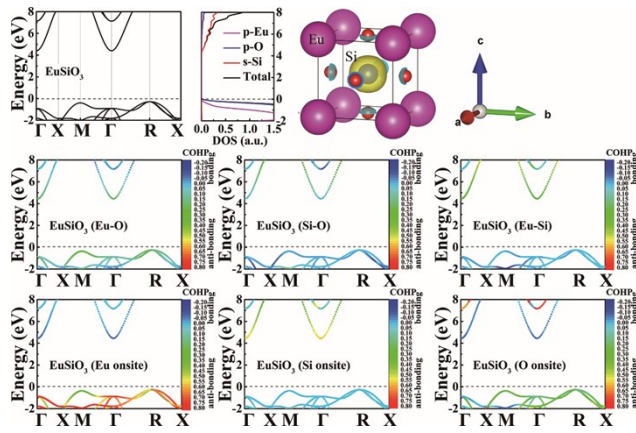


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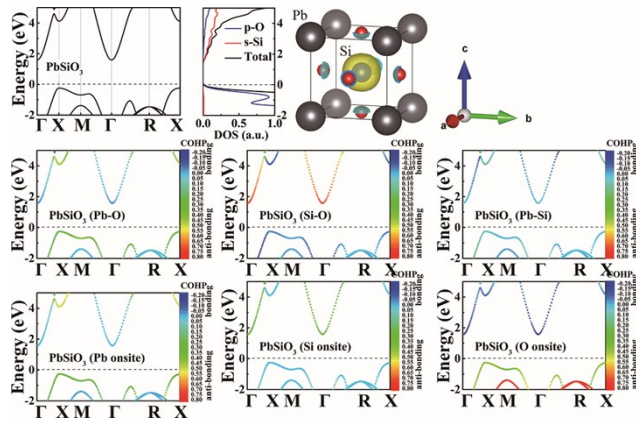




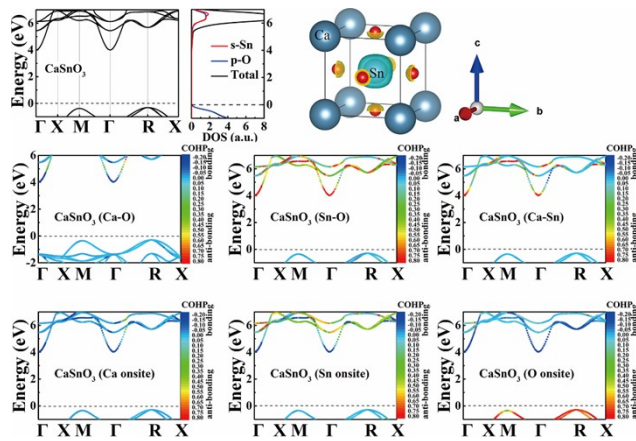
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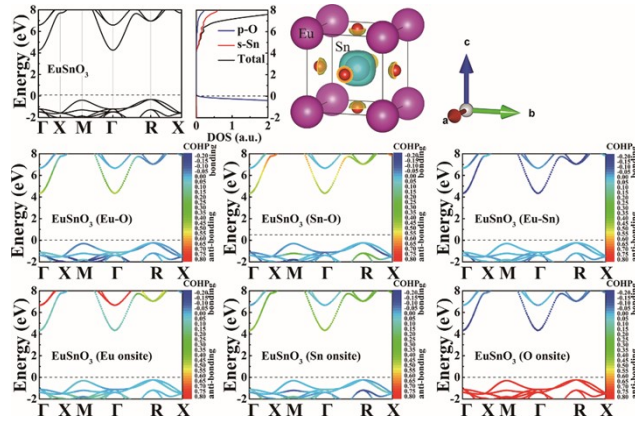
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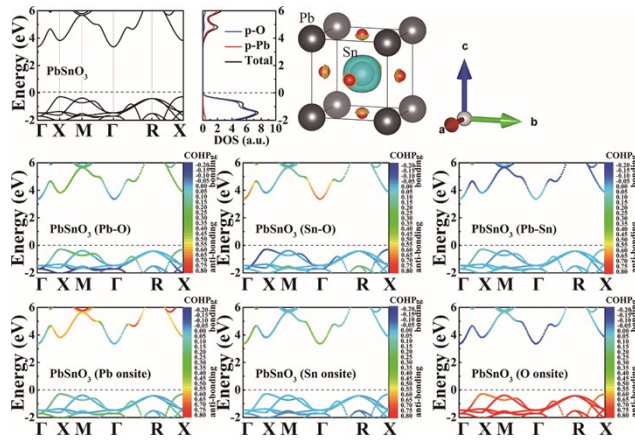
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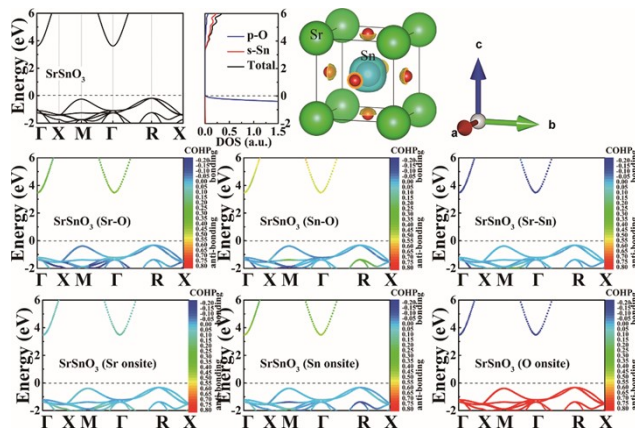
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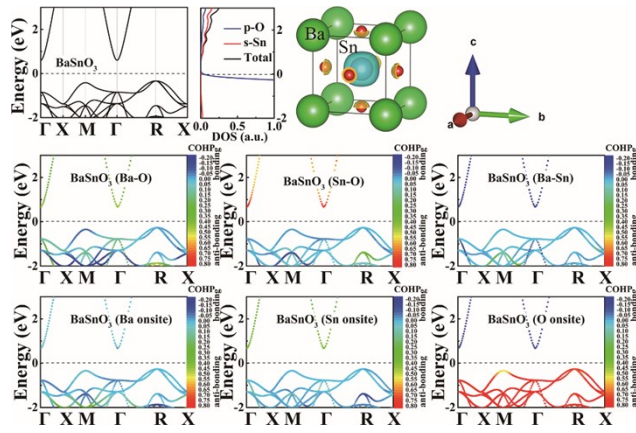
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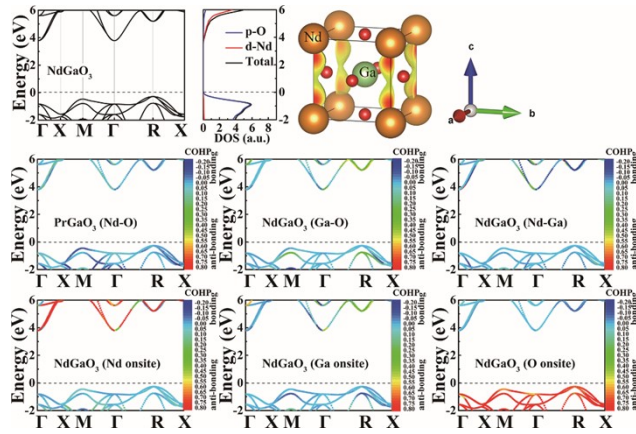
### 38. $\text{SrSnO}_3$



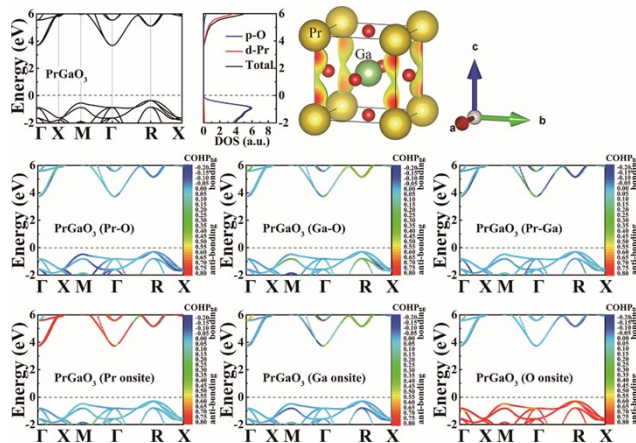
### 39. BaSnO<sub>3</sub>



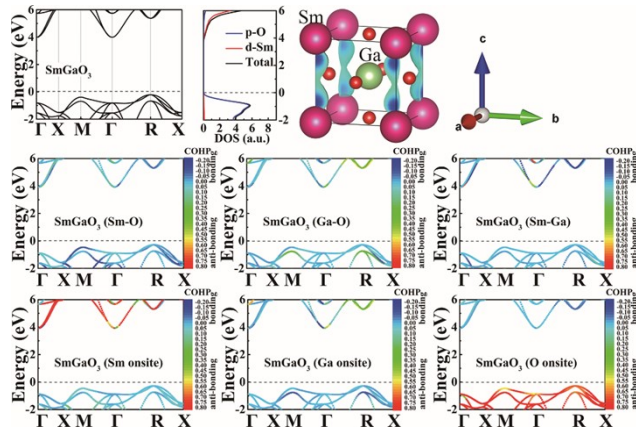
### 40. NdGaO<sub>3</sub>



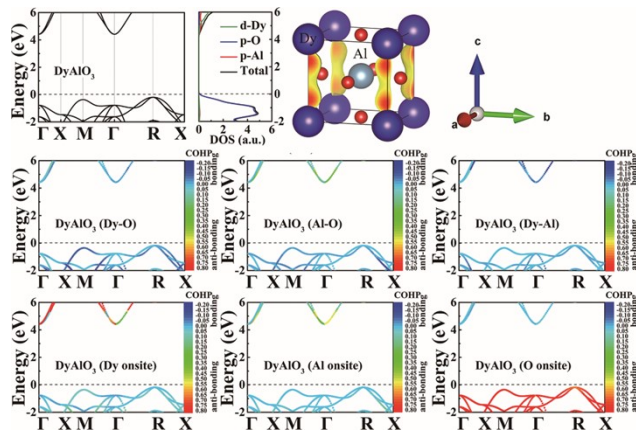
### 41. PrGaO<sub>3</sub>



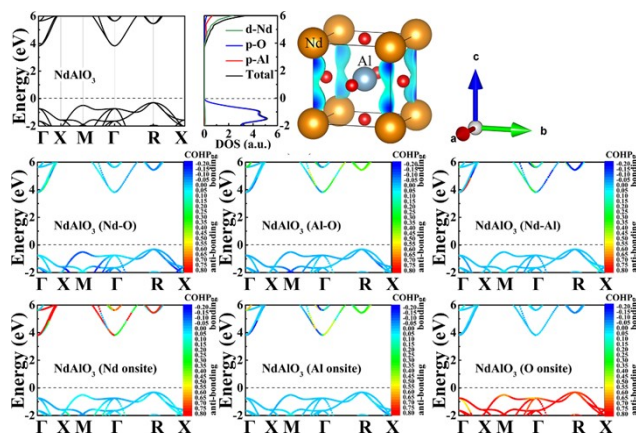
## 42. SmGaO<sub>3</sub>



## 43. DyAlO<sub>3</sub>

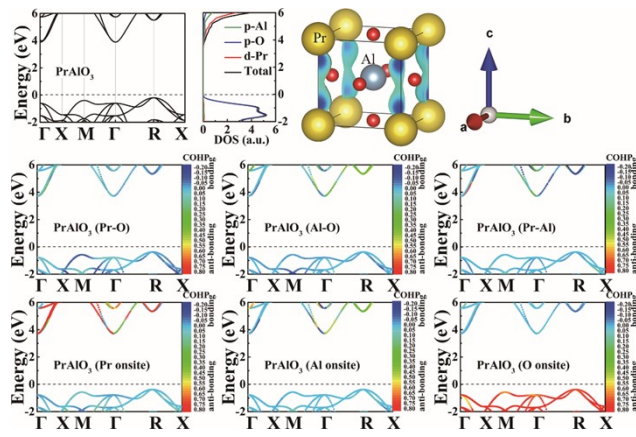


## 44. NdAlO<sub>3</sub>

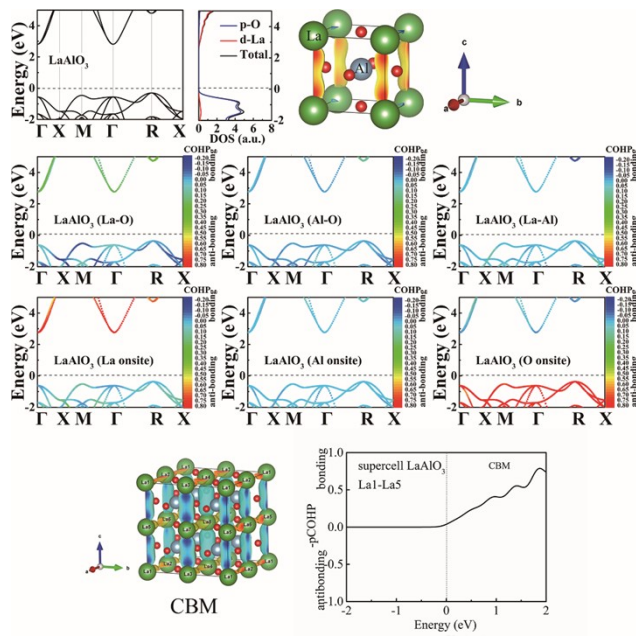


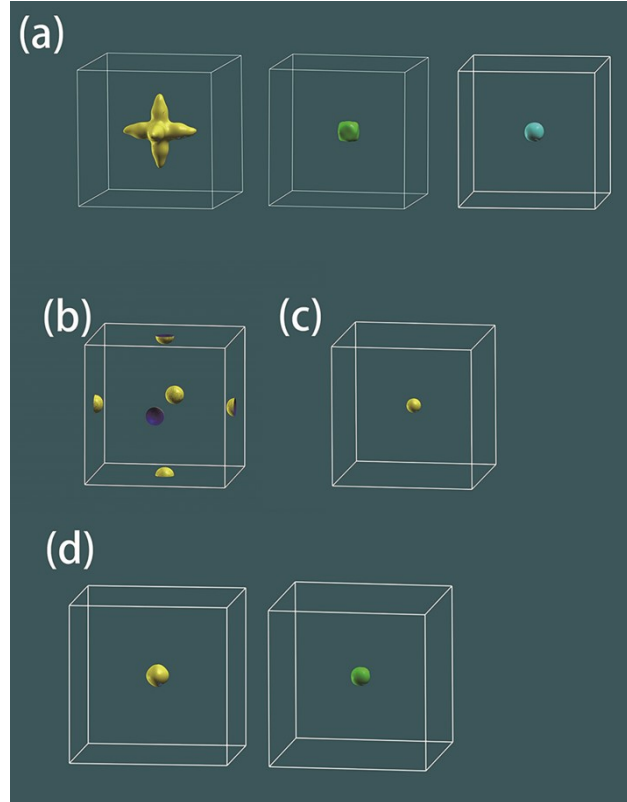


### 45. PrAlO<sub>3</sub>

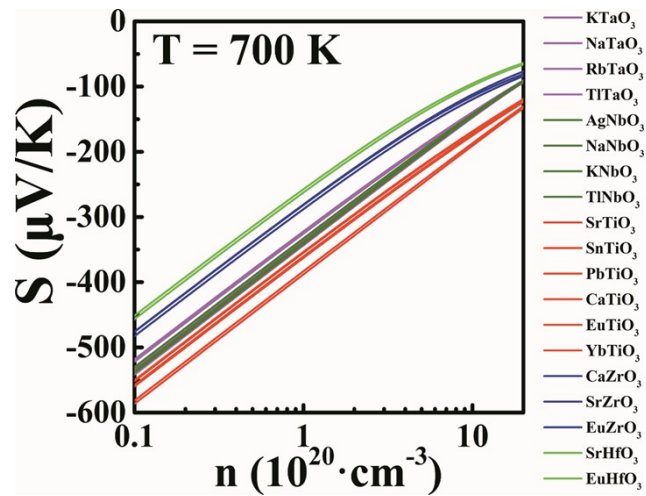


### 46. LaAlO<sub>3</sub>





**Fig. S2** The Fermi surfaces of (a) SrTiO<sub>3</sub>, (b) BiInO<sub>3</sub>, (c) CaSnO<sub>3</sub> (d) LaAlO<sub>3</sub>.



**Fig. S3** The correlations between Seebeck coefficient ( $S$ ) and carrier concentration ( $n$ ) of type I compounds.

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