

Material	Electronegativity (eV)	Band gap (eV)	Conduction band bottom(eV)	Valence band top (eV)
Ag <sub>2</sub> O	5.29	1.20	-4.69	-5.89
BaTiO <sub>3</sub>	5.12	3.30	-4.58	-7.88
Bi <sub>2</sub> O <sub>3</sub>	6.23	2.80	-4.83	-7.63
CdO	5.71	2.20	-4.61	-6.81
CdFe <sub>2</sub> O <sub>4</sub>	5.83	2.30	-4.68	-6.98
Ce <sub>2</sub> O <sub>3</sub>	5.20	2.40	-4.00	-6.40
CoO	5.69	2.60	-4.39	-6.99
CoTiO <sub>3</sub>	5.76	2.25	-4.64	-6.89
Cr <sub>2</sub> O <sub>3</sub>	5.68	3.50	-3.93	-7.43
CuO	5.81	1.70	-4.96	-6.66
Cu <sub>2</sub> O	5.32	2.20	-4.22	-6.42
CuTiO <sub>3</sub>	5.81	2.99	-4.32	-7.31
FeO	5.53	2.40	-4.33	-6.73
Fe <sub>2</sub> O <sub>3</sub>	5.88	2.20	-4.78	-6.98
Fe <sub>3</sub> O <sub>4</sub>	5.78	0.10	-5.73	-5.83
FeTiO <sub>3</sub>	5.69	2.80	-4.29	-7.09
Ga <sub>2</sub> O <sub>3</sub>	5.35	4.80	-2.96	-7.76
HgO	6.08	1.90	-5.13	-7.03
In <sub>2</sub> O <sub>3</sub>	5.28	2.80	-3.88	-6.68
KNbO <sub>3</sub>	5.29	3.30	-3.64	-6.94
KTaO <sub>3</sub>	5.32	3.50	-3.57	-7.07
La <sub>2</sub> O <sub>3</sub>	5.28	5.50	-2.53	-8.03
LiNbO <sub>3</sub>	5.52	3.50	-3.77	-7.27
LiTaO <sub>3</sub>	5.55	4.00	-3.55	-7.55
MgTiO <sub>3</sub>	5.60	3.70	-3.75	-7.45
MnO'	5.29	3.60	-3.49	-7.09
MnO <sub>2</sub>	5.95	0.25	-5.83	-6.08
MnTiO <sub>3</sub>	5.59	3.10	-4.04	-7.14
Nb <sub>2</sub> O <sub>5</sub>	6.29	3.40	-4.59	-7.99
NiO	5.75	3.50	-4.00	-7.50
NiTiO <sub>3</sub>	5.79	2.18	-4.70	-6.88
PbO	5.42	2.80	-4.02	-6.82
PdO	5.79	1.00	-5.29	-6.29
Sb <sub>2</sub> O <sub>3</sub>	6.32	3.00	-4.82	-7.82
SnO	5.69	4.20	-3.59	-7.79
SnO <sub>2</sub>	6.25	3.50	-4.50	-8.00
SrTiO <sub>3</sub>	4.94	3.40	-3.24	-6.64
Ta <sub>2</sub> O <sub>3</sub>	6.33	4.00	-4.33	-8.33
TiO <sub>2</sub>	5.81	3.20	-4.21	-7.41
V <sub>2</sub> O <sub>5</sub>	6.10	2.80	-4.70	-7.50
WO <sub>3</sub>	6.59	2.70	-5.24	-7.94
ZnO	5.79	3.20	-4.19	-7.39
ZnTiO <sub>3</sub>	5.80	3.06	-4.27	-7.34
ZrO <sub>2</sub>	5.91	5.00	-3.41	-8.41

Material	Electronegativity (eV)	Band gap (eV)	Conduction band bottom (eV)	Valence band top (eV)
Ag <sub>2</sub> S	4.96	0.92	-4.50	-5.42
As <sub>2</sub> S <sub>3</sub>	5.83	2.50	-4.58	-7.08
CdS	5.18	2.40	-3.98	-6.38
CoS	5.17	0.00	-5.17	-5.17
CoS <sub>2</sub>	5.49	0.00	-5.49	-5.49
CuS	5.27	0.00	-5.27	-5.27
CuS <sub>2</sub>	4.99	0.00	-5.57	-5.57
CuFeS <sub>2</sub>	5.15	0.35	-4.97	-5.32
FeS	5.02	0.10	-4.97	-5.07
FeS <sub>2</sub>	5.39	0.95	-4.92	-5.87
In <sub>2</sub> S <sub>3</sub>	4.70	2.00	-3.70	-5.70
MnS	4.81	3.00	-3.31	-6.31
MnS <sub>2</sub>	5.24	0.50	-4.99	-5.49
MoS <sub>2</sub>	5.32	1.17	-4.73	-5.90
NiS	5.23	0.40	-5.03	-5.43
NiS <sub>2</sub>	5.54	0.30	-5.39	-5.69
PbS	4.92	0.37	-4.74	-5.11
PbCuSbS <sub>3</sub>	5.22	1.23	-4.61	-5.84
PtS <sub>2</sub>	6.00	0.95	-5.53	-6.48
Rh <sub>2</sub> S <sub>3</sub>	5.36	1.50	-4.61	-6.11
RuS <sub>2</sub>	5.58	1.38	-4.89	-6.27
Sb <sub>2</sub> S <sub>3</sub>	5.63	1.72	-4.72	-6.44
SnS	5.17	1.01	-4.66	-5.67
SnS <sub>2</sub>	5.49	2.10	-4.44	-6.54
TiS <sub>2</sub>	5.11	0.70	-4.76	-5.46
WS <sub>2</sub>	5.54	1.35	-4.86	-6.21
ZnS	5.26	3.60	-3.46	-7.06
ZnS <sub>2</sub>	5.56	2.70	-4.21	-6.91
Zn <sub>3</sub> In <sub>2</sub> S <sub>6</sub>	5.00	2.81	-3.59	-6.40
ZrS <sub>2</sub>	5.20	1.82	-4.29	-6.11

The values are calculated using the following two equations

$$E_c = -A = -\chi + 0.5 E_g$$

$E_v = -I = -\chi - 0.5 E_g$  where  $\chi$  is electronegativity,  $E_g$  is the band gap,  $A$  is electron affinity and  $I$  is the ionization potential.