Appendix

B Band Edge Data

Table B.1 ***Data of Band edges and band gap of common sulphide semiconductors***

Material	*Electronegativity*	*Band Gap*	*Conduction Band*	*Valence Band*
Ag_2S	4.96	0.92	-4.50	-5.42
As_2S_3	5.83	2.50	-4.58	-7.08
CdS	5.18	2.40	-3.98	-6.38
$CuFeS_2$	5.15	0.35	-4.97	5.32
FeS	5.02	0.10	-4.97	-5.07
FeS_2	5.39	0.95	-4.92	5.87
In_2S_3	4.70	2.00	-3.70	-5.70
MnS	4.81	3.00	-3.31	-6.31
MnS_2	5.24	0.50	-4.99	-5.49
MoS_2	5.32	1.17	-4.73	-5.90
NiS	5.23	0.40	-5.03	-5.43
NiS_2	5.54	0.30	-5.39	-5.69
PbS	4.92	0.37	-4.74	-5.11
$PbCuSbS_3$	5.22	1.23	-4.61	-6.11
PtS_2	6.00	0.95	-5.53	-6.48
Rh_2S_3	5.36	1.50	-4.61	-6.11
RuS_2	5.58	1.38	-4.89	-6.27
Sb_2S_3	5.63	1.72	-4.72	-6.44
SnS	5.17	1.01	-4.66	-5.67
SnS_2	5.49	2.10	-4.44	-6.54
TiS_2	5.11	0.70	-4.76	-5.46
WS_2	5.54	1.35	-4.86	-6.21
ZnS	5.26	3.60	-3.46	–7.06
ZnS_2	5.56	2.70	-4.21	-6.91
$Zn_3In_2S_6$	5.00	2.81	-3.59	-6.40
ZrS_2	5.20	1.82	-4.29	-6.11

The values are calculated using the following two equations $E_c = -A = -\chi + 0.5E_g$ $E_v = -I = -\chi - 0.5E_g$ where χ is electronegativity, E_g is the value of band gap and A is electron affinity and I is the ionization potential

Table B.2 ***Data of Band edges and band gap of common oxide semiconductors***

Material	*Electronegativity*	*Band Gap*	*Conduction Band*	*Valence Band*
	eV	(eV)	Bottom (eV)	top (eV)
Ag_2O	5.29	1.20	-4.69	-5.89
$BaTiO_3$	5.12	3.30	-4.58	-7.88
Bi_2O_3	6.23	2.80	-4.83	-7.63
CdO	5.71	2.20	-4.61	-6.81
$CdFe_2O_4$	5.83	2.30	-4.68	-6.98
Ce_2O_3	5.20	2.40	-4.00	-6.40
CoO	5.69	2.60	-4.39	-6.40
$CoTiO_3$	5.76	2.25	-4.64	-6.89
Cr_2O_3	5.68	3.50	-3.93	-7.43
CuO	5.81	1.70	-4.96	-6.66
Cu_2O	5.32	2.20	-4.22	-6.42
$CuTiO_3$	5.76	2.99	-4.32	-7.31
FeO	5.53	2.40	-4.33	-6.73
Fe_2O_3	5.88	2.20	-4.78	-6.98
Fe_3O_4	5.78	0.10	-5.73	-5.83
$FeTiO_3$	5.69	2.80	-4.29	-7.09
Ga_2O_3	5.35	4.80	-2.96	-7.76
HgO	6.08	1.90	-5.13	-7.03
In_2O_3	5.28	2.80	-3.88	-6.68
$KNbO_3$	5.29	3.30	-3.64	-6.94
$KTaO_3$	5.32	3.50	3.57	-7.07
La_2O_3	5.28	5.50	-2.53	-8.03
$LiNbO_3$	5.52	3.50	-3.77	-7.27
$LiTaO_3$	5.55	4.00	-3.55	-7.55
$MgTiO_3$	5.60	3.70	-3.75	7.45
MnO	5.29	3.60	-3.49	-7.09
MnO_2	5.95	0.25	-5.83	-6.08
$MnTiO_3$	5.59	3.10	-4.04	-7.14
Nb_2O_5	6.29	3.40	-4.59	-7.99

Table B.2 ***(Continued)***

Material	*Electronegativity*	*Band Gap*	*Conduction Band*	*Valence Band*
NiO	5.75	3.50	-4.00	-7.50
$NiTiO_3$	5.79	2.18	-4.70	-6.88
PbO	5.42	2.80	-4.02	-6.82
Nb_2O_5	6.29	3.40	-4.59	-7.99
NiO	5.75	3.50	-4.00	-7.50
$NiTiO_3$	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_2O_3	6.32	3.00	-4.82	-7.82
SnO	5.69	4.20	-3.59	-7.79
SnO_2	6.25	3.50	-4.50	-8.00
$SrTiO_3$	4.94	3.40	-3.24	6.64
Ta_2O_3	6.33	4.00	-4.33	-8.33
TiO_2	5.81	3.20	-4.21	-8.33
V_2O_5	6.10	2.80	-4.70	-7.50
WO_3	6.59	2.70	-5.24	-7.94
ZnO	5.79	3.20	-4.19	-7.39
$ZnTiO_3$	5.80	3.06	-4.27	-7.34
ZrO_2	5.91	5.00	-3.41	-8.41

The values are calculated using the following two equations $E_c = -A = -\chi + 0.5E_g$ $E_v = -I = -\chi - 0.5E_g$ where χ is electrongativity, E_g is the value of band gap and A is electron affinity and I is the ionization potential.